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### 0.1 What's this course about?

The goal of this course is to introduce you to a variety of concepts and methods that are useful when dealing with data. You can think of data as any information that could potentially be studied to learn more about something.

Some simple examples:

1. Sales records for a company
2. Won/Lost records for a sports team
3. Web log listings
4. Email messages
5. Demographic Information found on the web

What may be surprising is that some of the data (for example web log listings or email) consists of text, not numbers. It's increasingly important to be able to deal with text in order to look at the wide variety of information that is available.

In most statistics courses, a lot of time is spent working on the preliminaries (formulas, algorithms, statistical concepts) in order to prepare the student for the interesting part of statistics, which is studying data for a problem that matters to you. Unfortunately, by the time these preliminaries are covered, many students are bored or frustrated, and they leave the course with a distorted view of statistics. In this class, we're going to do things differently. We will concentrate on:

1. Computer Languages - which will let us read in and manipulate data.
2. Graphical Techniques - which will allow us to display data in a way that makes it easier to understand and easier to make decisions based on the data.
3. Technologies - so that we can present these techniques to someone who's not as knowledgeable as us without too much misery.

The main computer language that we will be using in the course is a statistical programming environment known as R (http://r-project.org). R is freely downloadable and copyable, and you are strongly encouraged to install R on your own computer for use in this course and beyond. We will use this language for both data acquisition, data manipulation and producing graphical output. R is not the ideal language for all of the tasks we're going to do, but in the interest of efficiency, we'll try to use it for most things, and point you in the direction of other languages that you might want to explore sometime in the future.

Another tool that we'll use are UNIX shell commands, which allow you to store, copy and otherwise manipulate files which contain data, documents or programs. The computer accounts for this course will allow you to access computers running a version of the UNIX operating system

More and more commonly, data is stored on database servers, not in ordinary files. Most database servers use some version of a language known as the Structured Query Language (SQL). We'll use the open-source MySQL database as an example of an SQL database.

While you shouldn't have any problems understanding any of the statistical techniques we study in this class, a certain level of complexity arises when various techniques are combined together and presented as a start-to-finish solution. To learn how we can make techniques we've developed to others, we'll look at graphical user interfaces (GUIs) as well as using web servers to get information from users and display results.

### 0.2 Some Basic Concepts in Computing with Data

Most real-life projects that involve data can be broken down into several steps:

1. Data Acquisition - we need to find (or collect) the data, and get some representation of it into the computer
2. Data Cleaning - Inevitably, there will be errors in the data, either because they were entered incorrectly, we misunderstood the nature of the data, records were duplicated or omitted. Many times data is presented for viewing, and extracting the data in some other form becomes a challenge.
3. Data Organization - Depending on what you want to do, you may need to reorganize your data. This is especially true when you need to produce graphical representations of the data. Naturally, we need the appropriate tools to do these tasks.
4. Data Modeling and Presentation - We may fit a statistical model to our data, or we may just produce a graph that shows what we think is important. Often, a variety of models or graphs needs to be considered. It's important to know what techniques are available and whether they are accepted within a particular user community.

Further, techniques such as simulation and resampling have been developed to allow us to get information even in cases where we don't have exactly the data that we'd like to have.

### 0.3 A Short Note on Academic Integrity

One of the main ways you are going to learn in this course is by discussing the material in class and in lab sections, and I feel that this is one of the most important aspects of the course. However, the programs you write are like an essay or term paper, and you should not share them with others, or ask others to give their programs to you.

The University has a very detailed code of student conduct, available at http://students.berkeley.edu/ug vii.asp. Please refer to that document or talk to me if there are any questions.

## Chapter 1

## Operating Systems

### 1.1 Operating Systems

The operating system of a computer is the set of programs that control the basic operations of the computer (reading data, performing calculations) and that knows how to interface to the computer hardware (the screen, disk drives, tapes, CDs, etc.). The goal of the operating system is to provide a stable and usable environment from which we can run applications (like web browsers, R, databases, servers, etc.). Modern operating systems offer a desktop to their users, which is an graphical interface where things can be displayed and various controls can be manipulated.

Notice that while the operating system controls things such as the way files are created, named, and moved around, if all you're interested in is a particular application (like a web browser or a word processor) it doesn't make that big of a difference what operating system you use.

The most common operating systems used in computers today are Microsoft Windows, Mac OS X, Linux, and other variants of UNIX (Sun's Solaris, IBM's AIX, H-P HPUX, etc.) Traditionally, Linux/UNIX operating systems have not relied on graphical interfaces but have concentrated on the command line, where sometimes arcane and complex commands are typed into a window instead of being selected through drop-down menus, checkboxes, etc. The program that a user of such a computer uses to communicate with the operating system and launch other programs is known as a shell. There are a variety of different shells available on most Linux/UNIX computers. Microsoft Windows, on the other hand relies on graphical elements for most user input; many Windows users never use the DOS shell, which is the only command-line-oriented tool available under Windows. Modern Linux/UNIX systems have come a long way in providing graphically-oriented programs to replace or supplement the shell, but the command line still remains the most effective method of getting things done on Linux/UNIX systems.

Mac OS X is unusual in that it has a UNIX core, offering a variety of shells and most of the commands that other UNIX systems offer, but they also provide a very advanced graphical interface. Many Mac users are not aware of the UNIX underpinnings, but it should be mentioned that most UNIX/Linux knowledge can be transfered easily to the Mac, by opening the Terminal application.

### 1.2 File System

One of the most important functions of a computer is to manage the files that the computer has access to. Files are used to hold everything on a computer - pictures, programs, documents, music, web pages, and anything else that can be stored on a computer. Regardless of the operating system, files are organized pretty much the same way: groups of related files are stored together in a directory (sometimes called a folder); each of these directories can contain as many directories as necessary to organize the files they contain, and the same is true for the directories within the directories, and so on. This naturally describes a hierarchical arrangement of files, which can be found on any operating system. On UNIX-style
systems, the topmost branch of the hierarchy is known as the root of the file system, and is represented by a forward slash (/). On Windows, each drive represents a hierarchical arrangement starting at $\mathrm{X}: \backslash$, where X is the drive letter, for example " C " for the main disk on most Windows computers. Each directory, adds one more piece to the file's name; for example on the SCF UNIX system, there is a directory called class in the root of the file system, holding a directory called $u$ for undergraduate classes and $g$ for graduate classes. In these directories are separate directories for each class; in those directories is a separate directory for each student in the class where they can store their personal files. Thus, a particular student might use the directory /class/u/s133/s133xx to store their files. (On a corresponding Windows system, the path might be d:\class\u\s133\s133xx .) The area on the computer where each user stores their own files is known as the user's home directory.

Naturally, it would be tedious to have to type this entire name (refered to as the full pathname) everytime you wanted to access a file. (Notice on a graphically-oriented file system, this is not nearly so large of an issue, since you can navigate through the file system with a few clicks and visual cues (names and icons) are provided to help you find the file you want.) On command-line oriented systems there are a few features to make things more manageable. First, there is the concept of a working directory. When you have type commands into a UNIX-style computer, you can set a working directory, and filenames that you type will be resolved relative to the working directory. When you first log in, your working directory is set to your home directory. Suppose you are user s133xx, and your home directory is /class/u/s133/s133xx. If you refer to a filename as myfile, it will automatically treated as /class/u/s133/s133x/myfile. In other words, when you refer to a filename that doesn't begin with a slash (/), it is evaluated relative to your current directory.

In addition, most modern shells have a feature called tab completion. If you type part of the name of a file, and there is only one file in the current directory that starts with what you've typed, hitting the tab key will automatically complete the file name; if there's more than one file that starts with what you've typed, hitting the tab key a second time will briefly display the names of the matching files. As you're working with files in the shell, try using this feature - it's a real time (and keystroke) saver.

### 1.3 How information is stored on the Computer

Most of us have heard the cliche that everything on the computer is just a series of zeroes and ones. While this is true, it's sometimes helpful to understand how the zeroes and ones are actually arranged. The basic unit of information in a computer is called a bit, which is an abbreviation for "binary digit". A bit can either be on or off. Since this only offers two choices, it's fairly limited, so we usually refer to a collection of eight bits, which is known as a byte. For example, a single character, like an A, would be stored in the computer using one byte. Since there are eight bits in a byte, and each of the bits can be either 0 or 1 (independent of any of the other bits), there are $2^{8}$ or 256 possible bit patterns that can be stored in a single byte. However, there are only a limited number of printable characters
that the computer can display: 26 upper case letters, 26 lower case letters, 10 digits, and perhaps 40 or so punctuation symbols. That leaves well over 100 bit combinations that don't have a printable representation. These other non-printable characters are used in non-text or so-called binary files, and they will look very strange if you ask the computer to display them as if they were text. Of course, if we're thinking about something like a photograph (for example, a photo from a digital camera stored as a JPG file), there will be image viewers that understand how to use the binary information in the file to display a picture on the computer, so these bit combinations certainly do not go to waste. In fact, the same combinations of bits will behave very differently depending on whether they are in a text file, an image file or an MP3 file, so it's important to use the right application to deal with the different files on your computer.

Since the patterns of binary digits can naturally be interpreted as numbers, it's not surprising that one way of storing integers is to simply interpret the bits directly. In the diagram below, there's a binary representation of the number $154(128+16+8+2)$.

| 128 | 64 | 32 | 16 | 8 | 4 | 2 | 1 |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 0 | 0 | 1 | 1 | 0 | 1 | 0 |

This actually represents an unsigned integer - in practice, one of the bits is usually interpreted as a sign bit - i.e. if that bit is set to 1 , the number will be interpreted as negative. But using only 8 bits to store a number limits us to a range of 0 to 256 , or -128 to +128 , which isn't nearly enough for practical use. On real computers, groups of bytes (usually 4 or 8 ) are grouped together to store a single number. Consider an integer stored in 4 bytes. Assuming one bit is for the sign, that leaves 31 bits for holding the number, allowing a range of $-2^{31}$ to $2^{31}$, or -2147483648 to 2147483648 .

While that range seems really large, integers aren't suitable for storing all the information that we might encounter. One difficulty is that there is no provision for numbers after the decimal point; another is that in many cases we need to work with very small numbers simultaneously with very large numbers. To solve these problems, another way of storing numbers, known as floating point storage is used. Floating point numbers are usually stored in either four or eight bytes; one bit is used for sign, and the other bits are divided between the mantissa (which stores the important digits), and the exponent, which records the scale of the number. For example, to store the number 10325.25, one of the bits would be used for the sign, some of the bits would be used to store 1.032525, and other bits would be used to store an exponent of 4 , i.e. the number is stored as $1.032525 \times 10^{4}$ using binary digits.

The important part of this is not the specifics of how these things are stored, just the understanding that, to the computer the character string " 1 ", the integer 1 , and the floating point number 1.0 are all stored inside the computer in different ways.

### 1.4 Types of Files

As mentioned before, just about everything that's on a computer is a file. People often organize their files by putting similar files together in the same directory, but there is also information about a file that is available regardless of where the file is.

Most files have an extension that gives a clue to the type of file. For example, a file called xyz.jpg has an extension of "jpg", which is an image file (jpg stands for "Joint Photographic Experts Group, and sometimes the extension jpeg is used). Since early DOS computers could only handle extensions of three characters or less, you'll notice that many files have 3 character extensions, for example mp3, avi, pdf, and txt. However, this is no longer a limitation, and file extensions may be longer, for example mpeg or html. Windows and Mac OS X desktops give you the option of suppressing the display of these extensions, and they usually map each extension to a different icon to help remind you of what the file is. When files are displayed in a graphical interface, the operating system often uses the file extension to figure out what program should be called when you double-click on a file's icon.

It is important to realize that these extensions are simply part of the file's name, and, changing an extension of a file doesn't actually change the file itself - it just confuses all the programs that think they know how to handle that file! For example, suppose you've downloaded a music file using the open-source Ogg Vorbis format; such files usually have an extension of ogg, like song. ogg. If your portable music player can only play mp3 files, you can't just rename the file to song.mp3, and expect for it to play properly. You would need to locate a program that can convert an Ogg Vorbis file to an MP3 file.

In order to reduce dependence on extensions, developers of different file formats generally include a common string somewhere near the beginning of each file that definitively defines what type of file it is, eliminating the need to rely on the file extension. These strings are known as "magic numbers"; on UNIX systems, the file command can be used to identify a file by its magic number.

## Chapter 2

## R

### 2.1 The Basics

Most of the time you will use R, you'll use it in interactive mode. The program will print a greater-than sign $(>)$ to indicate it's ready for input, and will display the result of the commands that you type in as soon as they are calculated. On a UNIX system, start R by typing

R
at the UNIX prompt. Under windows, double click the "R" icon (if you let R put a icon on your desktop), or find $R$ in a folder in the Program Files folder with a name like R-2.1.0

When you use $R$ interactively, the value of an object is displayed when you type the objects name, and the values of calculations are displayed if they are not assigned to a variable. Thus, to use $R$ as a calculator, we can just enter the expression we wish to calculate:

```
> 10 + 12
```

[1] 22
> $59.95 * 1.0725$
[1] 64.29637
It may come as a surprise that typing a function's name also displays the value of the function. For example, to exit your R session, you need to invoke the q (for quit) function. But if you just type q into the R interpreter, here's what you'll see:

```
>q
function (save = "default", status = 0, runLast = TRUE)
.Internal(quit(save, status, runLast))
<environment: namespace:base>
```

To actually quit, you need to invoke q as a function with no arguments, i.e.
q()
When you do quit $R$, you'll be asked the following question:
Save workspace image? [y/n/c]:
If you answer yes, all of the variables you have created during your $R$ session will be saved in a file called .Rdata; if you start an R session later on in the same directory, your workspace (the collection of variables and other objects that you've created) will be restored to the way it was when you quit R. Sometimes it's more efficient to just save selected items; the save function allows you to do that. Once you've saved all or part of your workspace, you can transfer the file that R saves to another computer (even one running a different operating system) and use the load function to bring all of your objects into the workspace.
$R$ can also be used in a non-interactive way in several fashions:

1. Suppose you have a file called commands.r, and you'd like to see a full transcript (input, output and error messages) of the R session in output.txt. Type

R CMD BATCH command.r output.txt
at the UNIX prompt.
2. Suppose you want to run the commands in commands.r, but you wanted the results only (no echoing of input commands) to go to standard output. Type

```
R --slave < commands.r
```

at the UNIX prompt. You could also redirect the output to any file that you wanted.
3. Suppose you are running an interactive $R$ session, and you want to execute the commands commands.r as part of the current session. Type
source('commands.r')
at the R prompt.
When you execute commands this way, R shuts off it's automatic printing, so if you use the source function, you need to explicitly call the print function when you want something to be displayed.

### 2.2 Getting Help in R

$R$ provides a number of mechanisms for getting help. The help function can be called for information about any of the functions in R. You can abbreviate the help command by preceding the name of the function you're interested in with a question mark. So either of the following forms will display help for the print function:

```
help(print)
?print
```

When using R under Windows, the help files will open in a separate window, making it very easy to refer to them as you continue to work on your program. Under Unix, however, the help files are displayed in the same window as the interpreter, making it difficult or impossible to refer to the pages while you're working. If a browser is available, you can call help.start () once at the beginning of your $R$ session, and $R$ will display its help pages in the browser.

If you don't know the name of the function you're looking for, you can pass a keyword (as a quoted string) to help.search, and it will show you the name of the functions in $R$ that might be relevant. As a shortcut, you can type two question marks instead of the function name, for example, these two commands are the same:

```
help.search('random numbers')
```

??'random numbers'

There is a very active mailing list of R users where a wide variety of questions are raised, discussed and ultimately answered. The archives of this list provide an invaluable resource for solving problems and learning about R. The R function RSiteSearch will open a browser window displaying the results of a search of these archives. Suppose you were curious about how to make a plot with multiple colors. The R command:
> RSiteSearch('plot multiple colors')
would open a window on the results of searching the R newsgroup archives for those keywords.
Finally, if you like to learn by looking at working examples of programs, the example function accepts the name of most functions and runs a few simple examples using that function. (The same examples can be found on the help page for the function.)

### 2.3 Data in R

While R can handle many types of data, the three main varieties that we'll be using are numeric, character and logical. In R, you can identify what type of object you're dealing with by using the mode function. For example:

```
> name = 'phil'
> number = 495
> happy = TRUE
> mode(name)
[1] "character"
> mode(number)
[1] "numeric"
> mode(happy)
[1] "logical"
```

Note that when we enter character data, it needs to be surrounded by quotes (either double or single), but the symbols TRUE and FALSE (without quotes) are recognized as values of a logical variable.

Another important characteristic of an object in $R$ is its class, because many functions know how to treat objects of different classes in a special way. You can find the class of an object with the class function.

### 2.4 Vectors

Occasionally it may be useful to have a variable (like name or happy in the above example) to have only a single value (like 'phil' or TRUE), but usually we'll want to store more than
a single value (sometimes refered to as a scalar) in a variable. A vector is a collection of objects, all of the same mode, that can be stored in a single variable, and accessed through subscripts. For example, consider the minimum temperature in Berkeley for the first 10 days of January, 2006:
50.752 .848 .653 .049 .947 .954 .147 .643 .645 .5

We could create a variable called mintemp as follows:
> mintemp $=c(50.7,52.8,48.6,53.0,49.9,47.9,54.1,47.6,43.6,45.5)$
The c function is short for catenate or combine, and it's used to put individual values together into vectors. You can find the number of elements in a vector using the length function.

Once you've created a vector, you can refer to the elements of the vector using subscripts. Numerical subscripts in R start at 1, and continue up to the length of the vector. Subscripts of 0 are silently ignored. To refer to multiple elements in a vector, simply use the c function to create a vector of the indexes you're interested in. So to extract the first, third, and fifth values of the mintemp vector, we could use:

```
> mintemp[c(1,3,5)]
[1] 50.7 48.6 49.9
```

If all of the subscripts of an object are negative, $R$ will ignore those values, and use just the remaining elements. To extract all of the elements of mintemp except the first and last (tenth), use:

```
> mintemp[-c(1,10)]
[1] 52.8 48.6 53.0 49.9 47.9 54.1 47.6 43.6
```

In most programming languages, once you're dealing with vectors, you also have to start worrying about loops and other programming problems. Not so in R! For example, suppose we want to use the conversion formula

$$
C=5 / 9(F-32)
$$

to convert our Fahrenheit temperatures into Celsius. We can act as if mintemp is just a single number, and R will do the hard part:

```
> mintempC = 5/9 * (mintemp - 32)
> mintempC
    [1] 10.388889 11.555556 9.222222 11.666667 9.944444 8.833333 12.277778
    [8] 8.666667 6.444444 7.500000
```

In fact, most similar operations in R are vectorized; that is they operate on entire vectors at once, without the need for loops or other programming.

There are some shortcuts to generate vectors. The colon operator lets you generate sequences of integers from one value to another. For example,

```
> x = 1:10
> X
    [1] }
```

For more control, see the help page for the seq function.
You can repeat values using the rep function. This function is very flexible; if called with scalars, it does the obvious:

```
> rep (5,3)
    [1] 5 5 5
```

with a vector and a scalar, it creates a new vector by repeating the old one:

```
> rep(y,3)
    [1] 3 4 5 6 7 3 4 5 6 7 3 4 5 6 7
```

Finally, if you call rep with two equal length vectors, it repeats the elements of the first vector as many times as the corresponding element of the second vector:

```
> rep(1:4,c(2,3,3,4))
    [1] 1 1 2 2 2 3 3 3 4 4 4 4
```

One surprising thing about vectors in R is that many times it will carry out an operation with two vectors that aren't the same size by simply recycling the values in the shorter vector. For example, suppose we try to add a vector with four numbers to one with just two numbers:

```
> c(1,2,3,4) + c(1,2)
[1] 2446
```

Notice that, for the two last elements, it simply recycled the 1 and 2 from the second vector to perform the addition. R will be silent when things like this happen, but if the length of the larger vector isn't an even multiple of the length of the smaller vector, $R$ will print a warning:

```
> c(1,2,3,4) + c(1,2,3)
[1] 2465
Warning message:
longer object length is not a multiple of shorter object
length in: c(1, 2, 3, 4) + c(1, 2, 3)
```

It's possible to provide names for the elements of a vector. Suppose we were working with purchases in a number of states, and we needed to know the sales tax rate for a given state. We could create a named vector as follows:

```
> taxrate = c(AL=4,CA=7.25,IL=6.25,KS=5.3,NY=4.25,TN=7)
> taxrate
    AL CA IL KS NY TN
4.00 7.25 6.25 5.30 4.25 7.00
```

To add names to a vector after a fact, you can use the names function:

```
> taxrate = c(4,7.25,6.25,5.3,4.25,7)
> taxrate
[1] 4.00 7.25 6.25 5.30 4.25 7.00
> names(taxrate) = c('AL','CA','IL','KS','NY','TN')
> taxrate
    AL CA IL KS NY TN
4.00 7.25 6.25 5.30 4.25 7.00
```

If you have a named vector, you can access the elements with either numeric subscripts or by using the name of the element you want:

```
> taxrate[3]
    IL
6.25
> taxrate['KS']
    KS
```

5.3

One of the most powerful tools in R is the ability to use logical expressions to extract or modify elements in the way that numeric subscripts are traditionally used. While there are (of course) many cases where we're interested in accessing information based on the numeric or character subscript of an object, being able to use logical expressions gives us a much wider choice in the way we can study our data. For example, suppose we want to find all of observations in taxrate with a taxrate less than 6. First, let's look at the result of just asking whether taxrate is less than 6 :

```
> taxrate < 6
    AL CA IL KS NY TN
TRUE FALSE FALSE TRUE TRUE FALSE
```

The result is a logical vector of the same length as the vector we were asking about. If we use such a vector to extract values from the taxrate vector, it will give us all the ones that correspond to TRUE values, discarding the ones that correspond to FALSE.

```
> taxrate[taxrate > 6]
    CA IL TN
7.25 6.25 7.00
```

As another example, suppose we want to find which of the states we have information about has the highest sales tax. The max function will find the largest value in a vector. (Once again, note that we don't have to worry about the size of the vector or looping over individual elements.)

```
> max(taxrate)
[1] 7.25
```

We can find the state which has the highest tax rate as follows:

```
> taxrate[taxrate == max(taxrate)]
    CA
```

7.25

Notice that we use two equal signs when testing for equality, and one equal sign when we are assigning an object to a variable.

Another useful tool for these kinds of queries is the which function. It converts between logical subscripts and numeric ones. For example, if we wanted to know the index of the element in the taxrate vector that was the biggest, we could use:
> which (taxrate $==\max ($ taxrate $))$
CA
2
Once you start working with larger amounts of data, it becomes very tedious to enter data into the c function, especially considering the need to put quotes around character values and commas between values. To read data from a file or from the terminal without the need for quotes and commas, you can use the scan function. To read from a file (or a URL), pass it a quoted string with the name of the file or URL you wish to read; to read from the terminal, call scan() with no arguments, and enter a completely blank line when you're done entering your data. Additionally, on Windows or Mac OS X, you can substitute a call to the file.choose() function for the quoted string with the file name, and you'll be presented with the familiar file chooser used by most programs on those platforms.

### 2.5 Missing Values

No matter how carefully we collect our data, there will always be situations where we don't know the value of a particular variable. For example, we might conduct a survey where we ask people 10 questions, and occasionally we forget to ask one, or people don't know the proper answer. We don't want values like this to enter into calculations, but we can't just eliminate them because then observations that have missing values won't "fit in" with the rest of the data.

In $R$, missing values are represented by the string NA. For example, suppose we have a vector of 10 values, but the fourth one is missing. I can enter a missing value by passing NA to the c function just as if it was a number (no quotes needed):
$\mathrm{x}=\mathrm{c}(1,4,7, \mathrm{NA}, 12,19,15,21,20)$
$R$ will also recognize the unquoted string NA as a missing value when data is read from a file or URL.

Missing values are different from other values in R in two ways:

1. Any computation involving a missing value will return a missing value.
2. Unlike other quantities in $R$, we can't directly test to see if something is equal to a missing value with the equality operator (==). We must use the builtin is.na function, which will return TRUE if a value is missing and FALSE otherwise.
Here are some simple R statements that illustrate these points:
```
> x = c(1,4,7,NA,12,19,15,21,20)
mean(x)
[1] NA
> x == NA
[1] NA NA NA NA NA NA NA NA NA
```

Fortunately, these problems are fairly easy to solve. In the first case, many functions (like mean, min, max, sd, quantile, etc.) accept an na.rm=TRUE argument, that tells the function to remove any missing values before performing the computation:

```
> mean(x,na.rm=TRUE)
```

[1] 12.375

In the second case, we just need to remember to always use is.na whenever we are testing to see if a value is a missing value.

```
> is.na(x)
[1] FALSE FALSE FALSE TRUE FALSE FALSE FALSE FALSE FALSE
```

By combining a call to is.na to the logical "not" operator (!) we can filter out missing values in cases where no na.rm= argument is available:

```
> x[!is.na(x)]
```

[1] $\begin{array}{lllllllll}1 & 4 & 7 & 12 & 19 & 15 & 21 & 20\end{array}$

### 2.6 Matrices

A very common way of storing data is in a matrix, which is basically a two-way generalization of a vector. Instead of a single index, we can use two indexes, one representing a row and the second representing a column. The matrix function takes a vector and makes it into a matrix in a column-wise fashion. For example,

```
> mymat = matrix(1:12,4,3)
> mymat
\begin{tabular}{lrrr} 
& {\([, 1]\)} & {\([, 2]\)} & {\([, 3]\)} \\
{\([1]\),} & 1 & 5 & 9 \\
{\([2]\),} & 2 & 6 & 10 \\
{\([3]\),} & 3 & 7 & 11 \\
{\([4]\),} & 4 & 8 & 12
\end{tabular}
```

The last two arguments to matrix tell it the number of rows and columns the matrix should have. If you used a named argument, you can specify just one dimension, and $R$ will figure out the other:

```
> mymat = matrix(1:12,ncol=3)
> mymat
\begin{tabular}{lrrr} 
& {\([, 1]\)} & {\([, 2]\)} & {\([, 3]\)} \\
{\([1]\),} & 1 & 5 & 9 \\
{\([2]\),} & 2 & 6 & 10 \\
{\([3]\),} & 3 & 7 & 11 \\
{\([4]\),} & 4 & 8 & 12
\end{tabular}
```

To create a matrix by rows instead of by columns, the byrow=TRUE argument can be used:

```
> mymat = matrix(1:12,ncol=3,byrow=TRUE)
> mymat
```

|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| :--- | ---: | ---: | ---: |
| $[1]$, | 1 | 2 | 3 |
| $[2]$, | 4 | 5 | 6 |
| $[3]$, | 7 | 8 | 9 |
| $[4]$, | 10 | 11 | 12 |

When data is being read from a file, you can simply imbed a call to scan into a call to matrix. Suppose we have a file called matrix.dat with the following contents:

712194
187123
95842
We could create a $3 \times 4$ matrix, read in by rows, with the following command:

```
matrix(scan('matrix.dat'),nrow=3,byrow=TRUE)
```

To access a single element of a matrix, we need to specify both the row and the column we're interested in. Consider the following matrix, containing the numbers from 1 to 10 :

```
> m = matrix(1:10,5,2)
>m
    [,1] [,2]
[1,] 1 6
[2,] 2 7
[3,] 3 8
[4,] 4 9
[5,] 5 10
```

Now suppose we want the element in row 4 and column 1:

```
> m[4,1]
```

[1] 4

If we leave out either one of the subscripts, we'll get the entire row or column of the matrix, depending on which subscript we leave out:

```
> m[4,]
[1] 4 9
> m[,1]
[1] 1 2 3 4 5
```


### 2.7 Data Frames

One shortcoming of vectors and matrices is that they can only hold one mode of data; they don't allow us to mix, say, numbers and character strings. If we try to do so, it will change the mode of the other elements in the vector to conform. For example:
> c(12,9, "dog",7,5)
[1] "12" "9" "dog" "7" "5"
Notice that the numbers got changed to character values so that the vector could accomodate all the elements we passed to the c function. In R, a special object known as a data frame resolves this problem. A data frame is like a matrix in that it represents a rectangular array of data, but each column in a data frame can be of a different mode, allowing numbers, character strings and logical values to coincide in a single object in their original forms. Since most interesting data problems involve a mixture of character variables and numeric variables, data frames are usually the best way to store information in R. (It should be mentioned that if you're dealing with data of a single mode, a matrix may be more efficient than a data frame.) Data frames correspond to the traditional "observations and variables"
model that most statistical software uses, and they are also similar to database tables. Each row of a data frame represents an observation; the elements in a given row represent information about that observation. Each column, taken as a whole, has all the information about a particular variable for the data set.

For small datasets, you can enter each of the columns (variables) of your data frame using the data.frame function. For example, let's extend our temperature example by creating a data frame that has the day of the month, the minimum temperature and the maximum temperature:

```
> temps = data.frame(day=1:10,
+ min = c(50.7,52.8,48.6,53.0,49.9,47.9,54.1,47.6,43.6,45.5),
+ max = c(59.5,55.7,57.3,71.5,69.8,68.8,67.5,66.0,66.1,61.7))
> head(temps)
    day min max
1 1 50.7 59.5
2 2 52.8 55.7
3 3 48.6 57.3
4 53.0 71.5
5 5 49.9 69.8
6 647.9 68.8
```

Note that the names we used when we created the data frame are displayed with the data. (You can add names after the fact with the names function.) Also, instead of typing the name temps to see the data frame, we used a call the the head function instead. This will show me just the first six observations (by default) of the data frame, and is very handy to check to make sure a large data.frame really looks the way you think. (There's a function called tail that shows the last lines in an object as well.)

Suppose we want to concentrate on the maximum daily temperature (which we've called max in our data frame) among the days recorded. There are several ways we can refer to the columns of a data frame:

1. Probably the easiest way to refer to this column is to use a special notation that eliminates the need to put quotes around the variable names (unless they contain blanks or other special characters). Separate the data frame name from the variable name with a dollar sign (\$):
```
> temps$max
    [1] 59.5 55.7 57.3 71.5 69.8 68.8 67.5 66.0 66.1 61.7
```

2. We can treat the data frame like it was a matrix. Since the maximum temperature is in the third column, we could say
```
> temps[,3]
    [1] 59.5 55.7 57.3 71.5 69.8 68.8 67.5 66.0 66.1 61.7
```

3. Since we named the columns of temps we can use a character subscript:
```
> temps[,"max"]
    [1] 59.5 55.7 57.3 71.5 69.8 68.8 67.5 66.0 66.1 61.7
```

4. When you use a single subscript with a data frame, it refers to a data frame consisting of just that column. R also provides a special subscripting method (double brackets) to extract the actual data (in this case a vector) from the data frame:
```
> temps['max']
    max
1 59.5
2 55.7
3 57.3
41.5
569.8
6 68.8
767.5
86.0
966.1
1061.7
> temps[['max']]
> temps[['max']]
[1] 59.5 55.7 57.3 71.5 69.8 68.8 67.5 66.0 66.1 61.7
```

Notice that this second form is identical to temps\$max. We could also use the equivalent numerical subscript (in this case 3) with single or double brackets.
5. If you want to work with a data frame without having to constantly retype the data frame's name, you can use the with function. Suppose we want to convert our minimum and maximum temperatures to centigrade, and then calculate the difference between them. Using with, we can write:

```
> with(temps,5/9*(max-32) - 5/9*(min-32))
    [1] 4.888889 1.611111 4.833333 10.277778 11.055556 11.611111 
    [8] 10.222222 12.500000 9.000000
```

which may be more convenient than typing out the data frame name repeatedly:

```
> 5/9*(temps$max-32) - 5/9*(temps$min-32)
    [1] 4.888889 1.611111 4.833333 10.277778 11.055556 11.611111 
    [8] 10.222222 12.500000 9.000000
```

6. Finally, if the goal is to a add one or more new columns to a data frame, you can combine a few operations into one using the transform function. The first argument to transform is the name of the data frame that will be used to construct the new columns. The remaining arguments to transform are name/value pairs describing the new columns. For example, suppose we wanted to create a new variable in the temps data frame called range, representing the difference between the min and max values for each day. We could use transform as follows:
```
> temps = transform(temps,range = max - min)
> head(temps)
    day min max range
1 1 50.7 59.5 8.8
2 2 52.8 55.7 2.9
3 3 48.6 57.3 8.7
4 4 53.0 71.5 18.5
5 5 49.9 69.8 19.9
6 47.9 68.8 20.9
```

As can be seen, transform returns a new data frame like the original one, but with one or more new columns added.

### 2.8 Reading Data Frames from Files and URLs

It's actually pretty rare to enter a data frame the way we've done in these examples; usually you'll be reading data from a file or possibly a URL. In these cases, the read.table function (or one of its' closely related variations described below) can be used. read.table tries to be clever about figuring out what type of data you'll be using, and automatically determines how each column of the data frame should be stored. One problem with this scheme is has to do with a special type of variable known as a factor. A factor in R is a variable that is stored as an integer, but displayed as a character string. By default, read.table will automatically turn all the character variables that it reads into factors. You can recognize factors by using either the is.factor function or by examining the objects class, using the class function. Factors are very useful for storing large data sets compactly, as well as for statistical modeling and other tasks, but when you're first working with R they'll most likely just get in the way. To avoid read.table from doing any factor conversions, pass the stringsAsFactors=TRUE argument as shown in the examples below.

By default, R expects there to be at least one space or tab between each of the data values in your input file; if you're using a different character to separate your values, you can specify it with the sep= argument. Two special versions of read.table are provided to handle two common cases: read.csv for files where the data is separated by commas, and read.delim when a tab character is used to separate values. On the other hand, if the variables in your input data occupy the same columns for every line in the file, the read.fwf can be used to turn your data into a data frame.

If the first line of your input file contains the names of the variables in your data separated with the same separator used for the rest of the data, you can pass the header=TRUE argument to read.table and its variants, and the variables (columns) of your data frame will be named accordingly. Otherwise, names like V1, V2, etc. will be used.

As an example of how to read data into a data frame, the URL http://www.stat.berkeley.edu/classes/s13 contains information about literacy, gross domestic product, income and military expenditures for about 150 countries. Here are the first few lines of the file:
country,gdp,income,literacy,military
Albania, 4500,4937, 98.7,56500000
Algeria, 5900, 6799, 69.8,2.48e+09
Angola, 1900,2457,66.8,183580000
Argentina, 11200, 12468, 97.2,4.3e+09
Armenia, $3900,3806,99.4,1.35 \mathrm{e}+08$
Since the values are separated by commas, and the variable names can be found in the first line of the file, we can read the data into a data frame as follows:
world = read.csv('http://www.stat.berkeley.edu/classes/s133/data/world.txt', header=TRUE,
Now that we've created the data frame, we need to look at some ways to understand what our data is like. The class and mode of objects in $R$ is very important, but if we query them for our data frame, they're not very interesting:

```
> mode(world)
[1] "list"
> class(world)
[1] "data.frame"
```

Note that a data frame is also a list. We'll look at lists in more detail later. In order to see the modes and classes of the individual columns, we can use the sapply function. This function will apply a function to each element of a list; for a data frame these elements represent the columns (variables), so it will do exactly what we want:

```
> sapply(world,mode)
    country gdp income literacy military
"character" "numeric" "numeric" "numeric" "numeric"
> sapply(world,class)
    country gdp income literacy military
"character" "integer" "integer" "numeric" "numeric"
```

You might want to experiment with sapply using other functions to get familiar with some strategies for dealing with data frames.

You can always view the names of the variables in a data frame by using the names function, and the size (number of observations and number of variables) using the dim function:

```
> names(world)
[1] "country" "gdp" "income" "literacy" "military"
> dim(world)
[1] 154 5
```

Suppose we want to see the country for which military spending is the highest. We can still use logical subscripts just as we did with vectors, but extra care is needed to make sure we get the piece of the data frame we want. Since each country occupies one row in the data frame, we want all of the columns in that row, and we can leave the second index of the data frame blank:

```
>
> world[world$military == max(world$military,na.rm=TRUE),]
    country gdp income literacy military
142 USA 37800 39496 99.9 3.707e+11
```

The 142 at the beginning of the line is the row number of the observation. If you'd like to use a more informative label for the rows, look at the row.names= argument in read.table and data.frame, or use the assignment form of the row. names function if the data frame already exists.

These types of queries, where we want to find observations from a data frame that have certain properties, are so common that R provides a function called subset to make them
easier and more readable. The subset function requires two arguments: the first is a data frame, and the second is the condition that you want to use to create the subset. An optional third argument called select= allows you to specify which of the variables in the data frame you're interested in. The return value from subset is a data frame, so you can use it anywhere that you'd normally use a data frame. A very attractive feature of subset is that you can refer to the columns of a data frame directly in the second or third arguments; you don't need to keep retyping the data frame's name, or surround all the variable names with quotes. So the previous query could be rewritten as:

```
> subset(world,military==max(military,na.rm=TRUE))
    country gdp income literacy military
141 USA 37800 39496 99.9 3.707e+11
```

One other nice feature of the select= argument is that it converts variable names to numbers before extracting the requested variables, so you can use "ranges" of variable names to specify contiguous columns in a data frame. For example, here are the names for the world data frame:

```
> names(world)
[1] "country" "gdp" "income" "literacy" "military"
```

To create a data frame with just the last three variables, we could use

```
> subset(world,select=income:military)
```

If we were interested in a particular variable, it would be useful to reorder the rows of our data frame so that they were arranged in descending or ascending order of that variable. It's easy enough to sort a variable in R ; using literacy as an example, we simply call the sort routine:

```
> sort(world$literacy)
    [1] 12.8 14.4 19.0 25.5 29.6 33.6 39.3 39.6 41.0 41.1 41.5 46.5 47.0 48.6 48.6
[16] 48.7 49.0 50.7 51.2 51.9 53.0 54.1 55.6 56.2 56.7 57.3 58.9 59.0 61.0 64.0
[31] 64.1 65.5 66.8 66.8 67.9 67.9 68.7 68.9 69.1 69.4 69.8 70.6 71.0 73.6 73.6
[46] 74.3 74.4 75.7 76.7 76.9 77.0 77.3 78.9 79.2 79.4 79.7 80.0 81.4 81.7 82.4
[61] 82.8 82.9 82.9 84.2 84.3 85.0 86.5 86.5 87.6 87.7 87.7 87.7 87.9 87.9 88.0
[76] 88.3 88.4 88.7 89.2 89.9 90.0 90.3 90.3 90.4 90.9 91.0 91.0 91.6 91.9 91.9
[91] 92.5 92.5 92.6 92.6 92.7 92.9 93.0 94.2 94.6 95.7 95.8 96.2 96.5 96.8 96.8
[106] 96.9 96.9 97.2 97.2 97.3 97.7 97.7 97.8 98.1 98.2 98.5 98.5 98.7 98.7 98.8
[121] 98.8 99.3 99.3 99.4 99.4 99.5 99.5 99.6 99.6 99.6 99.7 99.7 99.7 99.8 99.9
[136] 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9 99.9
[151] 99.9 99.9 99.9 99.9
```

To reorder the rows of a data frame to correspond to the sorted order of one of the variables in the data frame, the order function can be used. This function returns a set of indices which are in the proper order to rearrange the data frame appropriately:

```
> sworld = world[order(world$literacy),]
> head(sworld)
            country gdp income literacy military
22 Burkina Faso 1100 1258 12.8 64200000
103 Niger 800 865 14.4 33300000
89 Mali 900 1024 19.0 22400000
29 Chad 1200 1555 25.5 101300000
121 Sierra Leone 500 842 29.6 13200000
14 Benin 1100 1094 33.6 96500000
```

To sort by descending values of a variable, pass the decreasing=TRUE argument to sort or order.

When you're first working with a data frame, it can be helpful to get some preliminary information about the variables. One easy way to do this is to pass the data frame to the summary function, which understands what a data frame is, and will give separate summaries for each of the variables:

```
> summary(world)
\begin{tabular}{|c|c|c|c|}
\hline country & gdp & income & literacy \\
\hline Length:154 & Min. : 500 & Min. : 569 & Min. : 12.80 \\
\hline Class : character & 1st Qu.: 1825 & 1st Qu.: 2176 & 1st Qu.:69.17 \\
\hline Mode :character & Median : 4900 & Median : 5930 & Median :88.55 \\
\hline & Mean : 9031 & Mean : 10319 & Mean :81.05 \\
\hline & 3rd Qu.:11700 & 3rd Qu.:15066 & 3rd Qu.:98.42 \\
\hline & Max. :55100 & Max. :63609 & Max. :99.90 \\
\hline
\end{tabular}
    military
    Min. :6.500e+06
    1st Qu.:5.655e+07
    Median :2.436e+08
    Mean :5.645e+09
    3rd Qu.:1.754e+09
    Max. :3.707e+11
```

Another useful way to view the properties of a variable is with the stem function, which produces a text-base stem-and-leaf diagram. Each observation for the variable is represented by a number in the diagram showing that observation's value:

```
> stem(world$gdp)
```

The decimal point is 4 digit(s) to the right of the $\mid$

0 | 11111111111111111111111111112222222222222222222333333333334444444
0 | 5555555555566666666677777778889999

```
| | 000111111223334
1 | 66788889
2 | 0022234
2 | 7778888999
| | 00013
3 | 88
|
|
|
5 |
```

Graphical techniques are often useful when exploring a data frame. While we'll look at graphics in more detail later, the functions boxplot, hist, and plot combined with the density function are often good choices. Here are examples:

```
> boxplot(world$gdp,main='Boxplot of GDP')
> hist(world$gdp,main='Histogram of GDP')
> plot(density(world$gdp),main='Density of GDP')
```




Suppose we want to add some additional information to our data frame, for example the continents in which the countries can be found. Very often we have information from different sources and it's very important to combine it correctly. The URL http://www.stat.berkeley.edu/s133/data/conts.txt contains the information about the con-
tinents. Here are the first few lines of that file:

```
country,cont
Afghanistan,AS
Albania,EU
Algeria,AF
American Samoa,OC
Andorra,EU
```

In R, the merge function allows you to combine two data frames based on the value of a variable that's common to both of them. The new data frame will have all of the variables from both of the original data frames. First, we'll read in the continent values into a data frame called conts:

```
conts = read.csv('http://www.stat.berkeley.edu/classes/s133/data/conts.txt',na.string='.
```

To merge two data frames, we simply need to tell the merge function which variable(s) the two data frames have in common, in this case country:

```
world1 = merge(world,conts,by='country')
```

Notice that we pass the name of the variable that we want to merge by, not the actual value of the variable itself. The first few records of the merged data set look like this:

| head(world1) |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  | country | gdp | income | literacy | military | ont |
| 1 | Albania | 4500 | 4937 | 98.7 | $5.6500 \mathrm{e}+07$ | EU |
| 2 | Algeria | 5900 | 6799 | 69.8 | $2.4800 \mathrm{e}+09$ | AF |
| 3 | Angola | 1900 | 2457 | 66.8 | $1.8358 \mathrm{e}+08$ | AF |
| 4 | Argentina | 11200 | 12468 | 97.2 | $4.3000 \mathrm{e}+09$ | SA |
| 5 | Armenia | 3900 | 3806 | 99.4 | $1.3500 \mathrm{e}+08$ | AS |
|  | Australia | 28900 | 29893 | 99.9 | $1.6650 \mathrm{e}+10$ | OC |

We've already seen how to count specific conditions, like how many countries in our data frame are in Europe:

```
> sum(world1$cont == 'EU')
[1] 34
```

It would be tedious to have to repeat this for each of the continents. Instead, we can use the table function:

```
> table(world1$cont)
```

AF AS EU NA OC SA
47413415412

We can now examine the variables taking into account the continent that they're in. For example, suppose we wanted to view the literacy rates of countries in the different continents. We can produce side-by-side boxplots like this:

```
> boxplot(split(world1$literacy,world1$cont))
```



Now let's concentrate on plots involving two variables. It may be surprising, but R is smart enough to know how to "plot" a dataframe. It actually calls the pairs function, which will produce what's called a scatterplot matrix. This is a display with many little graphs showing the relationships between each pair of variables in the data frame. Before we can call plot, we need to remove the character variables (country and cont) from the data using negative subscripts:

```
> plot(world1[,-c(1,6)])
```

The resulting plot looks like this:


As we'd expect, gdp (Gross Domestic Product) and income seem to have a very consistent relationship. The relation between literacy and income appears to be interesting, so we'll examine it in more detail, by making a separate plot for it:

```
> with(world,plot(literacy,income))
```

The first variable we pass to plot (literacy in this example) will be used for the x -axis, and the second (income) will be used on the y-axis. The plot looks like this:


In many cases, the most interesting points on a graph are the ones that don't follow the usual relationships. In this case, there are a few points where the income is a bit higher than we'd expect based on the other countries, considering the rate of literacy. To see which countries they represent, we can use the identify function. You call identify with the same arguments as you passed to plot; then when you click on a point on the graph with the left mouse button, its row number will be printed on the graph. It's usually helpful to have more than just the row number, so identify is usually called with a labels= argument. In this case, the obvious choice is the country name. The way to stop identifying points depends on your operating system; on Windows, right click on the plot and choose "Stop"; on Unix/Linux click on the plot window with the middle button. Here's the previous graph after some of the outlier points are identified:


### 2.9 Adding Color to Plots

Color is often refered to as the third dimension of a 2-dimensional plot, because it allows us to add extra information to an ordinary scatterplot. Consider the graph of literacy and income. By examining boxplots, we can see that there are differences among the distributions of income (and literacy) for the different continents, and it would be nice to display some of that information on a scatterplot. This is one situation where factors come in very handy. Since factors are stored internally as numbers (starting at 1 and going up to the number of unique levels of the factor), it's very easy to assign different observations different colors based on the value of a factor variable.

To illustrate, let's replot the income vs. literacy graph, but this time we'll convert the continent into a factor and use it to decide on the color of the points that will be used for each country. First, consider the world1 data frame. In that data frame, the continent is stored in the column (variable) called cont. We convert this variable to a factor with the factor function. First, let's look at the mode and class of the variable before we convert it to a factor:

```
> mode(world1$cont)
[1] "character"
> class(world1$cont)
[1] "character"
> world1$cont = factor(world1$cont)
```

In many situations, the cont variable will behave the same as it did when it was a simple character variable, but notice that its mode and class have changed:

```
> mode(world1$cont)
[1] "numeric"
> class(world1$cont)
[1] "factor"
```

Having made cont into a factor, we need to choose some colors to represent the different continents. There are a few ways to tell R what colors you want to use. The easiest is to just use a color's name. Most colors you think of will work, but you can run the colors function without an argument to see the official list. You can also use the method that's commonly use by web designers, where colors are specified as a pound sign (\#) followed by 3 sets of hexadecimal digits providing the levels of red, green and blue, respectively. Using this scheme, red is represented as '\#FF0000', green as '\#00FF00', and blue as '\#0000FF'. To see how many unique values of cont there are, we can use the levels function, since it's a factor. (For non-factors, the unique function is available, but it may give the levels in an unexpected order.)

```
> levels(world1$cont)
[1] "AF" "AS" "EU" "NA" "OC" "SA"
```

There are six levels. The first step is to create a vector of color values:

```
mycolors = c('red','yellow','blue','green','orange','violet')
```

To make the best possible graph, you should probably be more careful when choosing the colors, but this will serve as a simple example.

Now, when we make the scatterplot, we add an additional argument, col=, which is a vector of the same length as the number of pairs of points that we're plotting - the color in each position corresponds to the color that will be used to draw that point on the graph. Probably the easiest way to do that is to use the value of the factor cont as a subscript to the mycolors vector that we created earlier. (If you don't see why this does what we want, please take a look at the result of mycolors [world1\$cont]).
with(world1, plot(literacy,income,col=mycolors[cont]))

There's one more detail that we need to take care of. Since we're using color on the graph, we have to provide some way that someone viewing the graph can tell which color represents which continent, i.e. we need to add a legend to the graph. In R, this is done with the legend command. There are many options to this command, but in it's simplest form we just tell R where to put the legend, whether we should show points or lines, and what colors they should be. A title for the legend can also be added, which is a good idea in this example, because the meaning of the continent abbreviations may not be immediately apparent. You can specify $x$ - and $y$-coordinates for the legend location or you can use one of several shortcuts like "topleft" to do things automatically. (You may also want to look at the locator command, that lets you decide where to place your legends interactively). For our example, the following will place a legend in an appropriate place; the title command is also used to add a title to the plot:

```
with(world1,legend('topleft',legend=levels(cont),col=mycolors,pch=1,title='Continent'))
title('Income versus Literacy for Countries around the World')
```

Here's what the plot looks like:


### 2.10 Taking More Control Over Graphics

Although consulting the help file for a particular plotting function will often yield useful information, the R graphics system relies on a general method for setting a variety of graphical parameters through the par function. You should definitely familiarize yourself with the capabilities of this function before trying to customize any graphics. Two parameters that you will probably want to use are xlim= and ylim=. These parameters each accept a vector of length two, showing the minimum and maximum values that will be displayed on the x and y-axes, respectively. For example, suppose we are investigating the relationship between income and military spending in the world1 data frame:

```
> plot(world1$income,world1$military)
```



The problem is that the large outlier for military spending makes it very difficult to see the relationships among the other points. To resolve this problem, we can replot the graph, using the ylim= parameter to restrict the $y$-axis from 0 to $1 \mathrm{e}+11$ :
plot(world1\$income, world1\$military, ylim=c (0,1e11))


Many other graphics parameters exist to control things like the size and spacing of axis labels, the number of tick marks on the axes, the size of your plot and many other details.

| Code | Value |
| :--- | :--- |
| $\% \mathrm{~d}$ | Day of the month (decimal number) |
| $\% \mathrm{~m}$ | Month (decimal number) |
| $\% \mathrm{~b}$ | Month (abbreviated) |
| $\% \mathrm{~B}$ | Month (full name) |
| $\% \mathrm{y}$ | Year (2 digit) |
| $\% \mathrm{Y}$ | Year (4 digit) |

### 2.11 Using Dates in R

Dates on computers have been the source of much anxiety, especially at the turn of the century, when people felt that many computers wouldn't understand the new millenium. These fears were based on the fact that certain programs would store the value of the year in just 2 digits, causing great confusion when the century "turned over". In R, dates are stored as they have traditionally been stored on Unix computers - as the number of days from a reference date, in this case January 1, 1970, with earlier days being represented by negative numbers. When dates are stored this way, they can be manipulated like any other numeric variable (as far as it makes sense). In particular, you can compare or sort dates, take the difference between two dates, or add an increment of days, weeks, months or years to a date. The class of such dates is Date and their mode is numeric. Dates are created with as.Date, and formatted for printing with format (which will recognize dates and do the right thing.)

Because dates can be written in so many different formats, $R$ uses a standard way of providing flexibility when reading or displaying dates. A set of format codes, some of which are shown in the table below, is used to describe what the input or output form of the date looks like. The default format for as.Date is a four digit year, followed by a month, then a day, separated by either dashes or slashes. So conversions like this happen automatically:

```
> as.Date('1915-6-16')
[1] "1915-06-16"
> as.Date('1890/2/17')
[1] "1890-02-17"
```

The formatting codes are as follows:
(For a complete list of the format codes, see the R help page for the strptime function.)
As an example of reading dates, the URL http://www.stat.berkeley.edu/classes/s133/data/movies.txt contains the names, release dates, and box office earnings for around 700 of the most popular movies of all time. The first few lines of the input file look like this:

Rank|name|box|date
1|Titanic|\$600.788|December 19, 1997
2|Avatar|\$594.472|December 18, 2009
3|The Dark Knight|\$529.143|July 18, 2008
As can be seen, the fields are separated by vertical bars, so we can use read.delim with the appropriate sep= argument.

```
> movies = read.delim('http://www.stat.berkeley.edu/classes/s133/data/movies.txt',
+ sep='|',stringsAsFactors=FALSE)
> head(movies)
    Rank name box date
1 1 Titanic $600.788 December 19, 1997
2 2 Avatar $594.472 December 18, 2009
3 The Dark Knight $529.143 July 18, 2008
44 Star Wars: Episode IV - A New Hope $460.998 May 25, 1977
5 5 Shrek 2 $436.471 May 19, 2004
6 E.T. the Extra-Terrestrial $433.005 June 11, 1982
```

The first step in using a data frame is making sure that we know what we're dealing with. A good first step is to use the sapply function to look at the mode of each of the variables:

```
> sapply(movies,mode)
    rank name box date
    "numeric" "character" "character" "character"
```

Unfortunately, the box office receipts (box) are character, not numeric. That's because R doesn't recognize a dollar sign (\$) as being part of a number. (R has the same problem with commas.) We can remove the dollar sign with the sub function, and then use as.numeric to make the result into a number:

```
> movies$box = as.numeric(sub('\\$','',movies$box))
```

To convert the character date values to R Date objects, we can use as.Date with the appropriate format: in this case it's the month name followed by the day of the month, a comma and the four digit year. Consulting the table of format codes, this translates to '\%B $\% \mathrm{~d}, \mathrm{~F}^{\prime}$ :

```
> movies$date = as.Date(movies$date,'%B %d, %Y')
> head(movies$date)
[1] "1997-12-19" "2009-12-18" "2008-07-18" "1977-05-25" "2004-05-19"
[6] "1982-06-11"
```

The format that R now uses to print the dates is the standard Date format, letting us know that we've done the conversion correctly. (If we wanted to recover the original format, we could use the format function with a format similar to the one we used to read the data.)

Another way to create dates is with the ISOdate function. This function accepts three numbers representing the year, month and day of the date that is desired. So to reproduce the last date in the previous vector, we could use

```
> lastdate = ISOdate(2002,5,3)
> lastdate
```

[1] "2002-05-03 12:00:00 GMT"

Notice that, along with the date, a time is printed. That's because ISOdate returns an object of class POSIXt, not Date. To make a date like this work properly with objects of class Date, you can use the as.Date function.

Once we've created an $R$ Date value, we can use the functions months, weekdays or quarters to extract those parts of the date. For example, to see which day of the week these very popular movies were released, we could use the table function combined with weekdays:

```
> table(weekdays(movies$date))
    Friday Monday Saturday Sunday Thursday Tuesday Wednesday
        738 13 10% 9
```

Notice that the ordering of the days is not what we'd normally expect. This problem can be solved by creating a factor that has the levels in the correct order:

```
> movies$weekday = factor(weekdays(movies$date),
+ levels = c('Monday','Tuesday','Wednesday','Thursday','Friday','Saturday','Sunday'),
```

Now we can use weekday to get a nicer table:

```
> table(movies$weekday)
    Monday Tuesday Wednesday Thursday Friday Saturday Sunday
        13 44 165 
```

Similarly, if we wanted to graphically display a chart showing which month of the year the popular movies were released in, we could first create an ordered factor, then use the barplot function:

```
> movies$month = factor(months(movies$date),levels=c('January','February','March','April
> barplot(table(movies$month))
```



To do a similar thing with years, we'd have to create a new variable that represented the year using the format function. For a four digit year the format code is $\% \mathrm{Y}$, so we could make a table of the hit movies by year like this:

```
> table(format(movies$date,'%Y'))
1938 1939 1940 1942 1946 1950 1953 1955 1956 1959 1961 1963 1964 1965 1967 1968
    1
1969 1970 1971 1972 1973 1974 1975 1976 1977 1978 1979 1980 1981 1982 1983 1984
    1 5
1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000
    11
2001 2002 2003 2004 2005 2006 2007 2008 2009
    47
```


### 2.12 Data Summaries

We've looked at a few graphical techniques for exploring data, and now we're going to turn to a numerical one. Consider the question "Which day of the week has the highest average box office for hit movies released on that day?". As a first step in answering that question, it would be helpful to look at the mean box office receipts for each of the days. If you look for a function to do that specific task, you probably wouldn't find one, because R takes the more general approach of providing a function that will allow you to calculate anything you want from vectors of values broken down by groups. In fact, there are a variety of ways to do this. The one we're going to look at is called aggregate. You pass aggregate a vector or data frame containing the variables you want to summarize, a list of the groups to summarize by, and the function you'd like to use for your summaries. That way, a single function can perform many tasks, and, as we'll see when we learn to write functions, it even allows $R$ to do things that the developers of R never imagined. For now, we'll stick to some built in functions, like mean. To find the means for the box office receipts for each day of the week, we could use a call to aggregate like this:

```
> aggregate(movies$box,movies['weekday'],mean)
    weekday x
1 Monday 126.7766
2 Tuesday 104.8419
3 Wednesday 127.1272
4 Thursday 104.0686
5 Friday 102.6522
6 Saturday 82.2441
7 Sunday 103.0268
```

The same thing could be done to calculate other statistics, like median, min, max, or any statistic that returns a single scalar value for each group. Another nice feature of aggregate is that it if the first argument is a data frame, it will calculate the statistic for each column of the data frame. If we passed aggregate both the rank and box, we'd get two columns of summaries:

```
> aggregate(movies[,c('rank','box')],movies['weekday'],mean)
    weekday rank box
> aggregate(movies[,c('Rank','box')],movies['weekday'],mean)
        weekday Rank box
1 Monday 443.1538 126.7766
2 Tuesday 511.7037 104.8419
3 Wednesday 455.0116 127.1272
4 Thursday 560.5122 104.0686
5 Friday 520.0766 102.6522
6 Saturday 596.1000 82.2441
7 Sunday 497.6667 103.0268
```

To add a column of counts to the table, we can create a data frame from the table function, and merge it with the aggregated results:

```
> dat = aggregate(movies[,c('Rank','box')],movies['weekday'],mean)
> cts = as.data.frame(table(movies$weekday))
> head(cts)
    Var1 Freq
1 Monday 13
2 Tuesday 27
3 Wednesday }17
4 Thursday 41
5 Friday 744
6 Saturday 10
```

To make the merge simpler, we rename the first column of cts to weekday.

```
> names(cts)[1] = 'weekday'
> res = merge(cts,dat)
> head(res)
    weekday Freq Rank box
1 Friday 744 520.0766 102.6522
2 Monday 13 443.1538 126.7766
3 Saturday 10 596.1000 82.2441
4 Sunday 12 497.6667 103.0268
5 Thursday 41 560.5122 104.0686
6 Tuesday 27 511.7037 104.8419
```

Finally, we can order the columns as follows:

| > res $[$ order (res $\$$ weekday), |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: |
| weekday |  |  |  |  |
| 2 | Monday | 13 | 443.1538 | 126.7766 |
| 6 | Tuesday | 27 | 511.7037 | 104.8419 |
| 7 | Wednesday | 172 | 455.0116 | 127.1272 |
| 5 | Thursday | 41 | 560.5122 | 104.0686 |
| 1 | Friday | 744 | 520.0766 | 102.6522 |
| 3 | Saturday | 10 | 596.1000 | 82.2441 |
| 4 | Sunday | 12 | 497.6667 | 103.0268 |

### 2.13 Functions

As you've already noticed, functions play an important role in R. A very attractive feature of $R$ is that you can write your own functions which work exactly the same as the ones that are part of the official $R$ release. In fact, if you create a function with the same name as one
that's already part of R, it will override the built-in function, and possibly cause problems. For that reason, it's a good idea to make sure that there's not already another function with the name you want to use. If you type the name you're thinking of, and R responds with a message like "object "xyz" not found" you're probably safe.

There are several reasons why creating your own functions is a good idea.

1. If you find yourself writing the same code over and over again as you work on different problems, you can write a function that incorporates whatever it is you're doing and call the function, instead of rewriting the code over and over.
2. All of the functions you create are saved in your workspace along with your data. So if you put the bulk of your work into functions that you create, $R$ will automatically save them for you (if you tell R to save your workspace when your quit.)
3. It's very easy to write "wrappers" around existing functions to make a custom version that sets the arguments to another function to be just what you want. R provides a special mechanism to "pass along" any extra arguments the other function might need.
4. You can pass your own functions to built-in $R$ functions like aggregate, by, apply, sapply, lapply, mapply, sweep and other functions to efficiently and easy perform customized tasks.

Before getting down to the details of writing your own functions, it's a good idea to understand how functions in $R$ work. Every function in $R$ has a set of arguments that it accepts. You can see the arguments that built-in functions take in a number of ways: viewing the help page, typing the name of the function in the interpreter, or using the args function. When you call a function, you can simply pass it arguments, in which case they must line up exactly with the way the function is designed, or you can specifically pass particular arguments in whatever order you like by providing the with names using the name=value syntax. You also can combine the two, passing unnamed arguments (which have to match the function's definition exactly), followed by named arguments in whatever order you like. For example, consider the function read.table. We can view its argument list with the command:

```
> args(read.table)
function (file, header = FALSE, sep = "", quote = "\")", dec = ".",
    row.names, col.names, as.is = !stringsAsFactors, na.strings = "NA",
    colClasses = NA, nrows = -1, skip = 0, check.names = TRUE,
    fill = !blank.lines.skip, strip.white = FALSE, blank.lines.skip = TRUE,
    comment.char = "#", allowEscapes = FALSE, flush = FALSE,
    stringsAsFactors = default.stringsAsFactors(), encoding = "unknown")
NULL
```

This argument list tells us that, if we pass unnamed arguments to read.table, it will interpret the first as file, the next as header, then sep, and so on. Thus if we wanted to
read the file my.data, with header set to TRUE and sep set to ', ', any of the following calls would be equivalent:

```
read.table('my.data',TRUE,',')
read.table(sep=',',TRUE,file='my.data')
read.table(file='my.data',sep=',',header=TRUE)
read.table('my.data',sep=',', header=TRUE)
```

Notice that all of the arguments in the argument list for read.table have values after the name of the argument, except for the file argument. This means that file is the only required argument to read.table; any of the other arguments are optional, and if we don't specify them the default values that appear in the argument list will be used. Most R functions are written so the the first few arguments will be the ones that will usually be used so that their values can be entered without providing names, with the other arguments being optional. Optional arguments can be passed to a function by position, but are much more commonly passed using the name=value syntax, as in the last example of calling read.table.

Now let's take a look at the function read.csv. You may recall that this function simply calls read.table with a set of parameters that makes sense for reading comma separated files. Here's read.csv's function definition, produced by simply typing the function's name at the R prompt:

```
function (file, header = TRUE, sep = ",", quote = "\"", dec = ".",
    fill = TRUE, comment.char = "", ...)
read.table(file = file, header = header, sep = sep, quote = quote,
    dec = dec, fill = fill, comment.char = comment.char, ...)
<environment: namespace:utils>
```

Pay special attention to the three periods (...) in the argument list. Notice that they also appear in the call to read.table inside the function's body. The three dots mean all the arguments that were passed to the function that didn't match any of the previous arguments in the argument list. So if you pass anything other than file, header, sep, quote, dec, or fill to read.csv, it will be part of the three dots; by putting the three dots at the end of the argument list in the call to read.table, all those unmatched arguments are simply passed along to read.table. So if you make a call to read.csv like this:
read.csv(filename,stringsAsFactors=FALSE)
the stringsAsFactors=FALSE will get passed to read.table, even though it wasn't explicitly named in the argument list. Without the three dots, R will not accept any arguments that aren't explicitly named in the argument list of the function definition. If you want to intercept the extra arguments yourself, you can include the three dots at the end of the argument list when you define your function, and create a list of those arguments inside the function body by refering to list (...).

Suppose you want to create a function that will call read.csv with a filename, but which will automatically set the stringsAsFactors=FALSE parameter. For maximum flexibility,
we'd want to be able to pass other arguments (like na.strings=, or quote=) to read.csv, so we'll include the three dots at the end of the argument list. We could name the function read.csv and overwrite the built-in version, but that's not a good idea, if for no other reason than the confusion it would cause if someone else tried to understand your programs! Suppose we call the function myread.csv. We could write a function definition as follows:

```
> myread.csv = function(file,stringsAsFactors=FALSE,...){
+ read.csv(file,stringsAsFactors=stringsAsFactors,...)
+ }
```

Now, we could simply use
thedata $=$ myread.csv(filename)
to read a comma-separated file with stringsAsFactors=FALSE. You could still pass any of read.table's arguments to the function (including stringsAsFactors=TRUE if you wanted), and, if you ask R to save your workspace when you quit, the function will be available to you next time you start $R$ in the same directory.

### 2.14 Functions

When you create a function, it defines a separate environment and the variables you create inside your function only exist in that function environment; when you return to where you called the function from, those variables no longer exist. You can refer to other objects that are in the calling environment, but if you make any changes to them, the changes will only take place in the function environment. To get information back to the calling environment, you must pass a return value, which will be available through the functions name. R will automatically return the last unassigned value it encounters in your function, or you can place the object you want to return in a call to the return function. You can only return a single object from a function in R; if you need to return multiple objects, you need to return a list containing those objects, and extract them from the list when you return to the calling environment.

As a simple example of a function that returns a value, suppose we want to calculate the ratio of the maximum value of a vector to the minimum value of the vector. Here's a function definition that will do the job:
maxminratio $=$ function $(x) \max (x) / \min (x)$
Notice for a single line function you don't need to use brackets (\{\}) around the function body, but you are free to do so if you like. Since the final statement wasn't assigned to a variable, it will be used as a return value when the function is called. Alternatively, the value could be placed in a call to the return function. If we wanted to find the max to min ratio for all the columns of the matrix, we could use our function with the apply function:
apply(mymat, 2 , maxminratio)
The 2 in the call to apply tells it to operate on the columns of the matrix; a 1 would be used to work on the rows.

Before we leave this example, it should be pointed out that this function has a weakness what if we pass it a vector that has missing values? Since we're calling min and max without the na.rm=TRUE argument, we'll always get a missing value if our input data has any missing values. One way to solve the problem is to just put the na.rm=TRUE argument into the calls to min and max. A better way would be to create a new argument with a default value. That way, we still only have to pass one argument to our function, but we can modify the na.rm= argument if we need to.

```
maxminratio \(=\) function( \(x, n a . r m=T R U E) \max (x, n a . r m=n a . r m) / \min (x, n a . r m=n a . r m)\)
```

If you look at the function definitions for functions in R, you'll see that many of them use this method of setting defaults in the argument list.

As another example of a function, recall the graph of income versus literacy with different colored points for the different continents. If we were working with the datasets like the world1 dataset and wanted to create a variety of plots, we could write a function like this:

```
worldplotter = function(data,xvar,yvar,cvar,colors,ltitle=cvar,legendloc='topleft'){
    colorvar = factor(data[,cvar])
    with(data,plot(data[,xvar],data[,yvar],col=colors[colorvar],xlab=xvar,ylab=yvar))
    with(data,legend(legendloc,legend=levels(colorvar),col=colors,pch=1,title=ltitle))
}
```

Now we could produce the income versus literacy graph by calling:

```
worldplotter(world1,'literacy','income','cont',c('red','blue','green','orange','yellow',
```

By changing the arguments, a variety of plots can be produced.
As your functions get longer and more complex, it becomes more difficult to simply type them into an interactive R session. To make it easy to edit functions, R provides the edit command, which will open an editor appropriate to your operating system. When you close the editor, the edit function will return the edited copy of your function, so it's important to remember to assign the return value from edit to the function's name. If you've already defined a function, you can edit it by simply passing it to edit, as in
minmaxratio $=$ edit (minmaxratio)
You may also want to consider the fix function, which automates the process slightly.
To start from scratch, you can use a call to edit like this:

```
newfunction = edit(function(){})
```


### 2.15 Sizes of Objects

Before we start looking at character manipulation, this is a good time to review the different functions that give us the size of an object.

1. length - returns the length of a vector, or the total number of elements in a matrix (number of rows times number of columns). For a data frame, returns the number of columns.
2. dim - for matrices and data frames, returns a vector of length 2 containing the number of rows and the number of columns. For a vector, returns NULL. The convenience functions nrow and ncol return the individual values that would be returned by dim.
3. nchar - for a character string, returns the number of characters in the string. Returns a vector of values when applied to a vector of character strings. For a numeric value, nchar returns the number of characters in the printed representation of the number.

### 2.16 Character Manipulation

While it's quite natural to think of data as being numbers, manipulating character strings is also an important skill when working with data. We've already seen a few simple examples, such as choosing the right format for a character variable that represents a date, or using table to tabulate the occurences of different character values for a variable. Now we're going to look at some functions in R that let us break apart, rearrange and put together character data.

One of the most important uses of character manipulation is "massaging" data into shape. Many times the data that is available to us, for example on a web page or as output from another program, isn't in a form that a program like R can easily interpret. In cases like that, we'll need to remove the parts that R can't understand, and organize the remaining parts so that R can read them efficiently.

Let's take a look at some of the functions that R offers for working with character variables:

- paste The paste function converts its arguments to character before operating on them, so you can pass both numbers and strings to the function. It concatenates the arguments passed to it, to create new strings that are combinations of other strings. paste accepts an unlimited number of unnamed arguments, which will be pasted together, and one or both of the arguments sep= and collapse=. Depending on whether the arguments are scalars or vectors, and which of sep= and collapse= are used, a variety of different tasks can be performed.

1. If you pass a single argument to paste, it will return a character representation:
```
> paste('cat')
[1] "cat"
> paste(14)
[1] "14"
```

2. If you pass more than one scalar argument to paste, it will put them together in a single string, using the sep= argument to separate the pieces:
```
> paste('stat',133,'assignment')
[1] "stat 133 assignment"
```

3. If you pass a vector of character values to paste, and the collapse= argument is not NULL, it pastes together the elements of the vector, using the collapse= argument as a separator:
```
> paste(c('stat',133,'assignment'),collapse=' ')
[1] "stat 133 assignment"
```

4. If you pass more than one argument to paste, and any of those arguments is a vector, paste will return a vector as long as its' longest argument, produced by pasting together corresponding pieces of the arguments. (Remember the recycling
rule which will be used if the vector arguments are of different lengths.) Here are a few examples:
```
> paste('x',1:10,sep='')
    [1] "x1" "x2" "x3" "x4" "x5" "x6" "x7" "x8" "x9" "x10"
> paste(c('x','y'),1:10,sep='')
    [1] "x1" "y2" "x3" "y4" "x5" "y6" "x7" "y8" "x9" "y10"
```

- grep The grep function searches for patterns in text. The first argument to grep is a text string or regular expression that you're looking for, and the second argument is usually a vector of character values. grep returns the indices of those elements of the vector of character strings that contain the text string. Right now we'll limit ourselves to simple patterns, but later we'll explore the full strength of commands like this with regular expressions.
grep can be used in a number of ways. Suppose we want to see the countries of the world that have the world 'United' in their names.
> grep('United', world1\$country)
[1] 144145
grep returns the indices of the observations that have 'United' in their names. If we wanted to see the values of country that had 'United' in their names, we can use the value=TRUE argument:

```
> grep('United',world1$country,value=TRUE)
[1] "United Arab Emirates" "United Kingdom"
```

Notice that, since the first form of grep returns a vector of indices, we can use it as a subscript to get all the information about the countries that have 'United' in their names:

```
> world1[grep('United',world1$country),]
    country gdp income literacy military cont
144 United Arab Emirates 23200 23818 77.3 1600000000 AS
145 United Kingdom 27700 28938 99.9 42836500000 EU
```

grep has a few optional arguments, some of which we'll look at later. One convenient argument is ignore.case=TRUE, which, as the name implies will look for the pattern we specified without regard to case.

- strsplit strsplit takes a character vector, and breaks each element up into pieces, based on the value of the split= argument. This argument can be an ordinary text string, or a regular expression. Since the different elements of the vector may have different numbers of "pieces", the results from strsplit are always returned in a list. Here's a simple example:

```
> mystrings = c('the cat in the hat','green eggs and ham','fox in socks')
> parts = strsplit(mystrings,' ')
> parts
[[1]]
[1] "the" "cat" "in" "the" "hat"
[[2]]
[1] "green" "eggs" "and" "ham"
[[3]]
[1] "fox" "in" "socks"
```

While we haven't dealt much with lists before, one function that can be very useful is sapply; you can use sapply to operate on each element of a list, and it will, if possible, return the result as a vector. So to find the number of words in each of the character strings in mystrings, we could use:

```
> sapply(parts,length)
```

[1] 543

- substring The substring function allows you to extract portions of a character string. Its first argument is a character string, or vector of character strings, and its second argument is the index (starting with 1) of the beginning of the desired substring. With no third argument, substring returns the string starting at the specified index and continuing to the end of the string; if a third argument is given, it represents the last index of the original string that will be included in the returned substring. Like many functions in $R$, its true value is that it is fully vectorized: you can extract substrings of a vector of character values in a single call. Here's an example of a simple use of substring

```
> strings = c('elephant','aardvark','chicken','dog','duck','frog')
> substring(strings,1,5)
[1] "eleph" "aardv" "chick" "dog" "duck" "frog"
```

Notice that, when a string is too short to fully meet a substringing request, no error or warning is raised, and substring returns as much os the string as is there.

Consider the following example, extracted from a web page. Each element of the character vector data consists of a name followed by five numbers. Extracting an individual field, say the field with the state names is straight forward:

$$
\begin{array}{rllllll}
>\text { data }=c(\text { "Lyndhurst } & \text { Ohio } & 199.02 & 15,074 & 30 & 5 & 25 ", \\
& \text { "Southport Town New York } & 217.69 & 11,025 & 24 & 4 & 20 ",
\end{array}
$$

```
            "Bedford Massachusetts 221.20 12,658 28 0 28")
> states = substring(data,16,28)
> states
```

```
[1] "Ohio " "New York " "Massachusetts"
```

```
[1] "Ohio " "New York " "Massachusetts"
```

It is possible to extract all the fields at once, at the cost of a considerably more complex call to substring:

```
> starts = c(1, 16, 30, 38,46,50,54)
> ends = c(14,28,35,43,47,50,55)
> ldata = length(data)
> lstarts = length(starts)
> x = substring(data,rep(starts,rep(ldata,lstarts)),rep(ends,rep(ldata,lstarts)))
> matrix(x,ncol=lstarts)
```



Like many functions in R, substring can appear on the left hand side of an assignment statement, making it easy to change parts of a character string based on the positions they're in. To change the third through fifth digits of a set of character strings representing numbers to 99 , we could use:

```
> nums = c('12553','73911','842099','203','10')
> substring(nums,3,5) = '99'
> nums
[1] "12993" "73991" "849999" "209" "10"
```

- tolower, toupper These functions convert their arguments to all upper-case characters or all lower-case characters, respectively
- sub, gsub These functions change a regular expression or text pattern to a different set of characters. They differ in that sub only changes the first occurence of the specified pattern, while gsub changes all of the occurences. Since numeric values in R cannot contain dollar signs or commas, one important use of gsub is to create numeric variables from text variables that represent numbers but contain commas or dollars. For example, in gathering the data for the world dataset that we've been using, I extracted the information about military spending from http://en.wikipedia.org/wiki/List_of_countries_by_military_e Here's an excerpt of some of the values from that page:

```
> values = c('370,700,000,000','205,326,700,000','67,490,000,000')
```

> as.numeric(values)

```
[1] NA NA NA
Warning message:
NAs introduced by coercion
```

The presence of the commas is preventing R from being able to convert the values into actual numbers. gsub easily solves the problem:
> as.numeric(gsub(',','', values))
[1] 37070000000020532670000067490000000

### 2.17 Working with Characters

As you probably noticed when looking at the above functions, they are very simple, and, quite frankly, it's hard to see how they could really do anything complex on their own. In fact, that's just the point of these functions - they can be combined together to do just about anything you would want to do. As an example, consider the task of capitalizing the first character of each word in a string. The toupper function can change the case of all the characters in a string, but we'll need to do something to separate out the characters so we can get the first one. If we call strsplit with an empty string for the splitting character, we'll get back a vector of the individual characters:

```
> str = 'sherlock holmes'
> letters = strsplit(str,'')
> letters
[[1]]
    [1] "s" "h" "e" "r" "l" "o" "c" "k" " " "h" "o" "l" "m" "e" "s"
> theletters = letters[[1]]
```

Notice that strsplit always returns a list. This will be very useful later, but for now we'll extract the first element before we try to work with its output.

The places that we'll need to capitalize things are the first position in the vector or letters, and any letter that comes after a blank. We can find those positions very easily:

```
> wh = c(1,which(theletters == , ') + 1)
> wh
[1] 1 10
```

We can change the case of the letters whose indexes are in wh, then use paste to put the string back together.

```
> theletters[wh] = toupper(theletters[wh])
> paste(theletters,collapse='')
[1] "Sherlock Holmes"
```

Things have gotten complicated enough that we could probably stand to write a function:

```
maketitle = function(txt){
    theletters = strsplit(txt,'')[[1]]
    wh = c(1,which(theletters == , ') + 1)
    theletters[wh] = toupper(theletters[wh])
    paste(theletters,collapse='')
}
```

Of course, we should always test our functions:

```
> maketitle('some crazy title')
```

[1] "Some Crazy Title"

Now suppose we have a vector of strings:

```
> titls = c('sherlock holmes','avatar','book of eli','up in the air')
```

We can always hope that we'll get the right answer if we just use our function:

```
> maketitle(titls)
[1] "Sherlock Holmes"
```

Unfortunately, it didn't work in this case. Whenever that happens, sapply will operate on all the elements in the vector:

```
> sapply(titls,maketitle)
    sherlock holmes avatar book of eli up in the air
"Sherlock Holmes" "Avatar" "Book Of Eli" "Up In The Air"
```

Of course, this isn't the only way to solve the problem. Rather than break up the string into individual letters, we can break it up into words, and capitalize the first letter of each, then combine them back together. Let's explore that approach:

```
> str = 'sherlock holmes'
> words = strsplit(str,' ')
> words
[[1]]
[1] "sherlock" "holmes"
```

Now we can use the assignment form of the substring function to change the first letter of each word to a capital. Note that we have to make sure to actually return the modified string from our call to sapply, so we insure that the last statement in our function returns the string:

```
> sapply(words[[1]],function(w){substring(w,1,1) = toupper(substring(w, 1, 1));w})
    sherlock holmes
"Sherlock" "Holmes"
```

Now we can paste the pieces back together to get our answer:

```
> res = sapply(words[[1]],function(w){substring(w,1,1) = toupper(substring(w,1,1));w})
> paste(res,collapse=' ')
[1] "Sherlock Holmes"
```

To operate on a vector of strings, we'll need to incorporate these steps into a function, and then call sapply:

```
mktitl = function(str){
    words = strsplit(str,' ')
    res = sapply(words[[1]],function(w){substring(w,1,1) = toupper(substring(w,1,1));w})
    paste(res,collapse=' ')
}
```

We can test the function, making sure to use a string different than the one we used in our initial test:

```
> mktitl('some silly string')
[1] "Some Silly String"
```

And now we can test it on the vector of strings:

```
> titls = c('sherlock holmes','avatar','book of eli','up in the air')
> sapply(titls,mktitl)
    sherlock holmes avatar book of eli up in the air
"Sherlock Holmes" "Avatar" "Book Of Eli" "Up In The Air"
```

How can we compare the two methods? The R function system.time will report the amount of time any operation in R uses. One important caveat - if you wish to assign an expression to a value in the system.time call, you must use the "<-" assignment operator, because the equal sign will confuse the function into thinking you're specifying a named parameter in the function call. Let's try system.time on our two functions:

```
> system.time(one <- maketitle(titls))
    user system elapsed
        0 0 0
> system.time(two <- mktitl(titls))
    user system elapsed
    0.000 0.000 0.001
```

For such a tiny example, we can't really trust that the difference we see is real. Let's use the movie names from a previous example:

```
> movies = read.delim('http://www.stat.berkeley.edu/classes/s133/data/movies.txt',
+ sep='|',stringsAsFactors=FALSE)
> nms = tolower(movies$name)
```

```
> system.time(one <- maketitle(nms))
    user system elapsed
    0.000 0.000 0.001
> system.time(two <- mktitl(nms))
    user system elapsed
    0.008 0.000 0.007
```

It looks like the first method is better than the second. Of course, if they don't get the same answer, it doesn't really matter how fast they are. In $R$, the all.equal function can be used to see if things are the same:

```
> all.equal(one,two)
```

[1] TRUE

### 2.18 Reading Data into R

Let's review the methods of reading data into $R$ :

1. scan - Reads vectors of data which all have the same mode, for example all numbers or all character strings. Each element needs to be separated from the others by one or more blanks, or the sep= argument can be used to specify a different separator. If the first argument to scan is a file, it will read from that file; if the first argument is empty, it reads data from the terminal, ended by a completely blank line. By default, scan expects to see numbers - if you're using it to read strings, use the what=' ' argument.

For example, scan be used to create a vector of color names, as an alternative to using the c function:

```
> mycolors = scan(,what='')
1: red blue yellow green orange
6:
Read 5 items
> mycolors
[1] "red" "blue" "yellow" "green" "orange"
```

scan can also be used to create numeric matrices, by passing the call to scan to the matrix function. Suppose the file mat. dat looks like this:
$\begin{array}{lll}7 & 191215\end{array}$
89174
521297
1294013

We could read this matrix into R as follows:

```
> mymat = matrix(scan('mat.dat'),ncol=4,byrow=TRUE)
Read 16 items
> mymat
\begin{tabular}{lrrrr} 
& {\([, 1]\)} & {\([, 2]\)} & {\([, 3]\)} & {\([, 4]\)} \\
{\([1]\),} & 7 & 19 & 12 & 15 \\
{\([2]\),} & 8 & 9 & 17 & 4 \\
{\([3]\),} & 52 & 12 & 9 & 7 \\
{\([4]\),} & 12 & 9 & 40 & 13
\end{tabular}
```

Note the use of byrow=TRUE to overide R's default of reading matrices by columns.
2. read.table, read.delim, read.csv These functions all allow us to create data frames, where different columns (variables) can be of different modes. read.table is the basic
function, and read.csv is a wrapper that sets the separator to a comma, and assumes the first line of the file being read contains the variable names (header=TRUE). read.delim is similar to read.csv, but uses a tab as a separator (sep=' t '). The first, and only required, argument to these functions is a filename or URL. Some other potentially useful arguments include:

- stringsAsFactors= Setting this argument to FALSE prevents R from converting character data into factors.
- na.string= This argument is useful if missing values in your file are represented by something other than NA or NaN, or if you want to make sure that strings like NA or NaN are not treated as missing values
- skip= This argument allows you to specify the number of lines in your file that should be ignored before reading the data.
- fill=TRUE If there are an unequal number of values on some lines, this option will pad the shorter lines with missing values. Make sure you understand the nature of your data before using this option.

If you have problems reading your data, the count.fields function can be useful in finding which lines have the wrong number of values. For example, recall the world data set that we've used previously. If we wanted to check that there were the same number of fields in each line, we could do the following:

```
> flds = count.fields('http://www.stat.berkeley.edu/classes/s133/data/world.txt',se
> table(flds)
flds
    5
1 5 5
```

This shows that all 155 records have 5 comma-separated fields. If there were records that didn't match the others, the which function could be used to find their line numbers.
3. readLines The previous functions all were trying to extract pieces of the input data into separate variables, and will always be the main tool for creating vectors, matrices, and data frames. But if we're just processing text, say, from a web page or from the output of some other computer program, the data won't be arranged in the way that scan or read.table need. In cases like this, we simply want to read the text into $R$ in a way that we can manipulate it to our needs. The R function that does this is readLines. The readLines function accepts a URL or file as its first argument, and it returns a vector with as many elements as there are lines from the input source. Unlike scan or read.table, readLines simply extracts the text from its input source and returns each line as a character string. So whenever we're confronted with "unorganized" data, readLines is the function that will read it into $R$ so that we can
manipulate it further. (There's also a similar function called readline that will read exactly one line from standard input.)
One sometimes useful argument to pass to readLines is the $n=$ argument. With its default of -1 , all of the lines in the input will be read; if you provide a number that's greater than 0 , readLines will read in only that many lines.
4. Connections In addition to reading files, R provides a set of functions known as connections. (Type "?connections" in R to learn about all the possibilities.) One very handy type of connection is the textConnection. This allows you to paste text into an $R$ session, just as if it came from a file. For example, recall the previous example of reading a file with scan to create a matrix. We can reproduce that example without needing a file, by cutting and pasting the data into a call to textConnection:

```
> thedata = textConnection('7 19 12 15
+ 8 9174
+ 521297
+ 1294013
+ ')
> mymat = matrix(scan(thedata),ncol=4,byrow=TRUE)
Read 16 items
> mymat
\begin{tabular}{lrrrr} 
& {\([, 1]\)} & {\([, 2]\)} & {\([, 3]\)} & {\([, 4]\)} \\
{\([1]\),} & 7 & 19 & 12 & 15 \\
{\([2]\),} & 8 & 9 & 17 & 4 \\
{\([3]\),} & 52 & 12 & 9 & 7 \\
{\([4]\),} & 12 & 9 & 40 & 13
\end{tabular}
```

This makes it very easy to run examples that you may find online, and saves the trouble of creating a file when you just need to read in a small amount of data.

## Chapter 3

## Regular Expressions

### 3.1 Regular Expressions

Regular expressions are a method of describing patterns in text that's far more flexible than using ordinary character strings. While an ordinary text string is only matched by an exact copy of the string, regular expressions give us the ability to describe what we want in more general terms. For example, while we couldn't search for email addresses in a text file using normal searches (unless we knew every possible email address), we can describe the general form of an email address (some characters followed by an "@" sign, followed by some more characters, a period, and a few more characters. through regular expressions, and then find all the email addresses in the document very easily.

Another handy feature of regular expressions is that we can "tag" parts of an expression for extraction. If you look at the HTML source of a web page (for example, by using View¿Source in a browser, or using download.file in R to make a local copy), you'll notice that all the clickable links are represented by HTML like:

```
<a href="http://someurl.com/somewhere">
```

It would be easy to search for the string href= to find the links, but what if some webmasters used something like

```
<a href = 'http://someurl.com/somewhere'>
```

Now a search for href= won't help us, but it's easy to express those sorts of choices using regular expressions.

There are a lot of different versions of regular expressions in the world of computers, and while they share the same basic concepts and much of the same syntax, there are irritating differences among the different versions. R offers us three versions of regular expressions: the basic ones (which we'll be using in class and all the examples in these notes), extended regular expressions, and perl regular expressions. (perl is a scripting language whose creator, Larry Wall, developed some attractive extensions to the basic regular expression syntax.) The differences are laid out in very terse language on the $R$ help page for regex and regexpr, and, since regular expressions are a somewhat challenging topic, there are many valuable resources on the internet.

Before we start, one word of caution. We'll see that the way that regular expressions work is that they take many of the common punctuation symbols and give them special meanings. Because of this, when you want to refer to one of these symbols literally (that is, as simply a character like other characters), you need to precede those symbols with a backslash ( $\backslash$ ). But backslashes already have a special meaning in character strings; they are used to indicate control characters, like tab ( $\backslash \mathrm{t}$ ), and newline $(\backslash \mathrm{n})$. The upshot of this is that when you want to type a backslash to keep $R$ from misinterpreting certain symbols, you need to precede it with two backslashes in the input. By the way, the characters for which this needs to be done are:

$$
\sim \$+? *()[]\{ \} \mid \
$$

| Modifier | Meaning |
| :--- | :--- |
| $*$ | zero or more |
| $?$ | zero or one |
| + | one or more |
| $\{\mathrm{n}\}$ | exactly n occurences |
| $\{\mathrm{n}\}$, | at least n occurences |
| $\{\mathrm{n}, \mathrm{m}\}$ | between n and m occurences |

To reiterate, when any of these characters is to be interpreted literally in a regular expression, they must be preceded by two backslashes when they are passed to functions in R. If you're not sure, it's almost always safe to add a backslash (by typing two backslashes) in front of a character - if it's not needed, it will be ignored.

Regular expressions are constructed from three different components: literal characters, which will only be matched by the identical literal character, character classes, which are matched by more than one characters, and modifiers which operate on characters, character classes, or combinations of the two. A character class consists of an opening square bracket ([), one or more characters, and a closing square bracket (]), and is matched by any of the characters between the brackets. If the first character inside the brackets is the caret ( $\sim$ ), then the character class is matched by anything except the other characters between the brackets. Ranges are allowed in character classes and one of the most important examples is [0-9], a character class matched by any of the digits from 0 to 9 . Other ranges of characters include $[\mathrm{a}-\mathrm{z}]$, all the lower case letters, and $[\mathrm{A}-\mathrm{Z}]$, all the uppercase letters.

The period (.) represents the wildcard character. Any character (except for the newline character) will be matched by a period in a regular expression; when you literally want a period in a regular expression you need to precede it with a backslash.

Many times you'll need to express the idea of the beginning or end of a line or word in a regular expression. For example, you may be looking for a line number at the beginning of a line, or only be interested in searching for a string if it's at the end of a line. The carat ( ${ }^{\wedge}$ ) represents the beginning of a line in a regular expression, and the dollar sign (\$) represents the end of a line. To specify that the regular expression you're looking for is a word (i.e. it's surrounded by white space, punctuation or line beginnings and endings), surround the regular expression with escaped angle brackets ( $\backslash<$ and $\backslash>$ ).

One of the most powerful features in regular expressions is being able to specify that you're interested in patterns which may be variable. In the previous example regarding extracting links through the href= argument, we'd like to be able to find a reference no matter how many spaces there are between the href and the $=$. We also might want to account for the fact that quotes around the url are sometimes omitted. There are a few characters that act as modifiers to the part of the regular expression that precedes them, summarized in the table below.

The first three modifiers in the above table are the most important ones; the others are used much less often. Let's return to the idea of looking for email addresses. Here's a regular expression that will match most email addresses: $\left[-\mathrm{A}-\mathrm{Za}-\mathrm{zO}-9_{-} . \%\right]+@\left[-\mathrm{A}-\mathrm{Za}-\mathrm{zO}-9_{-} . \%\right]+\backslash .[\mathrm{A}-\mathrm{Za}-\mathrm{z}]+$
. In words we could read the regular expression as "one or more occurences of the characters between the brackets literally followed by an @-sign, followed by one or more characters between the brackets, literally followed by a period, and completed by one or more letters from among A-Z and a-z. You can simplify things by specifying ignore.case=TRUE to many $R$ functions that deal with regular expressions; in that case you would only have to put either $\mathrm{A}-\mathrm{Z}$ or $\mathrm{a}-\mathrm{z}$ in the character class, and it would still match both upper or lower case letters.

If we use the regular expression in a call to grep, it will find all of the elements in a character vector that contain an email address:

```
> chk = c('abc noboby@stat.berkeley.edu','text with no email',
+ 'first me@mything.com also you@yourspace.com')
> grep('[-A-Za-z0-9_.%]+@[-A-Za-z0-9_.%]+\\.[A-Za-z]+', chk)
[1] }1
```

Since regular expressions in R are simply character strings, we can save typing by storing regular expressions in variables. For example, if we say:

```
> emailpat = '[-A-Za-z0-9_.%]+@[-A-Za-z0-9_.%]+\\.[A-Za-z]+'
```

then we can use the R variable emailpat in place of the full regular expression. (If you use this technique, be sure to modify your stored variable when you change your regular expression.)

To actually get to the regular expressions, we can use the gregexpr function, which provides more information about regular expression matches. First, let's see what the output from gregexpr looks like:

```
> gregout = gregexpr(emailpat,chk)
> gregout
[[1]]
[1] 5
attr(,"match.length")
[1] 24
[[2]]
[1] -1
attr(,"match.length")
[1] -1
[[3]]
[1] 7 27
attr(,"match.length")
[1] 14 17
```

First, notice that, since there may be a different number of regular expressions found in different lines, gregexpr returns a list. In each list element is a vector of starting points
where regular expressions were found in the corresponding input string. In addition, there is additional information stored as an attribute, which is part of the value, but which doesn't interfere if we try to treat the value as if it was simply a vector. The match.length attribute is another vector, of the same length as the vector of starting points, telling us how long each match was. Concentrating on the first element, we can use the substring function to extract the actual address as follows:

```
> substring(chk[1],gregout[[1]],gregout[[1]] + attr(gregout[[1]],'match.length') - 1)
[1] "noboby@stat.berkeley.edu"
```

To make it a little easier to use, let's make a function that will do the extraction for us:

```
getexpr = function(s,g)substring(s,g,g + attr(g,'match.length') - 1)
```

Now it's a little easier to get what we're looking for:

```
> getexpr(chk[2],gregout[[2]])
[1] ""
> getexpr(chk[3],gregout[[3]])
[1] "me@mything.com" "you@yourspace.com"
```

To use the same idea on an entire vector of character strings, we could either write a loop, or use the mapply function. The mapply function will repeatedly call a function of your choice, cycling through the elements in as many vectors as you provide to the function. To use our getexpr function with mapply to extract all of the email addresses in the chk vector, we could write:

```
> emails = mapply(getexpr,chk,gregout)
> emails
$"abc noboby@stat.berkeley.edu"
[1] "noboby@stat.berkeley.edu"
$"text with no email"
[1] ""
$"first me@mything.com also you@yourspace.com"
[1] "me@mything.com" "you@yourspace.com"
```

Notice that mapply uses the text of the original character strings as names for the list it returns; this may or may not be useful. To remove the names, use the assignment form of the names function to set the names to NULL

```
> names(emails) = NULL
> emails
[[1]]
[1] "noboby@stat.berkeley.edu"
```

[[2]]
[1] ""

```
[[3]]
[1] "me@mything.com als" "you@yourspace.com"
```

The value that mapply returns is a list, the same length as the vector of input strings (chk in this example), with an empty string where there were no matches. If all you wanted was a vector of all the email addresses, you could use the unlist function:

```
> unlist(emails)
[1] "noboby@stat.berkeley.edu" ""
[3] "me@mything.com" "you@yourspace.com"
```

The empty strings can be removed in the usual way:

```
emails = emails[emails != '']
```

or
emails = subset(emails,emails != '')
Suppose we wanted to know how many emails there were in each line of the input text (chk). One idea that might make sense is to find the length of each element of the list that the getexpr function returned:

```
> emails = mapply(getexpr,chk,gregout)
> names(emails) = NULL
> sapply(emails,length)
```

The problem is that, in order to maintain the structure of the output list, mapply put an empty (length 0) string in the second position of the list, so that length sees at least one string in each element of the list. The solution is to write a function that modifies the length function so that it only returns the length if there are some characters in the strings for a particular list element. (We can safely do this since we've already seen that there will always be at least one element in the list. We can use the if statement to do this:

```
> sapply(emails,function(e)if(nchar(e[1]) > 0)length(e) else 0)
[1] 1 0 2
```


### 3.2 How matches are found

Regular expressions are matched by starting at the beginning of a string and seeing if a possible match might begin there. If not, the next character in the string is examined, and so on; if the end of the string is reached, then no match is reported.

Let's consider the case where there is a potential match. The regular expression program remembers where the beginning of the match was and starts checking the characters to the right of that location. As long as the expression continues to be matched, it will continue, adding more characters to the matched pattern until it reaches a point in the string where the regular expression is no longer matched. At that point, it backs up until things match again, and it checks to see if the entire regular expression has been matched. If it has, it reports a match; otherwise it reports no match.

While the specifics of this mechanism will rarely concern you when you're doing regular expression matches, there is one important point that you should be aware of. The regular expression program is always going to try to find the longest match possible. This means if you use the wildcard character, ., with the "one or more" modifier, *, you may get more than you expected.

Suppose we wish to remove HTML markup from a web page, in order to extract the information that's on the page. All HTML markup begins with a left angle bracket (<) and ends with a right angle bracket ( $>$ ), and has markup information in between. Before diving in and trying to remove the markup, let's make sure we can find it correctly. An obvious (but ill-advised) choice for the regular expression is <.*>. In words it means "a literal left angle bracket, followed by one or more of any character, followed by a literal right angle bracket". Let's see how effective it is:

```
> htmls = c('This is an image: <IMG SRC="img/rxb.gif">',
+ '<a href="somepage.html">click here</a>')
> grep('<.*>',htmls)
[1] 1 2
```

We've matched both pieces, but what have we really got? We can apply our mapply-based solution to see the actual strings that were matched:

```
> getexpr = function(s,g)substring(s,g,g + attr(g,'match.length') - 1)
> matches = mapply(getexpr,htmls,gregexpr('<.*>',htmls))
> names(matches) = NULL
> matches
[1] "<IMG SRC=\"img/rxb.gif\">"
[2] "<a href=\"somepage.html\">click here</a>"
```

The first match worked fine, but the second match went right past the end of the first piece of markup, and included the second piece in it. For this reason, regular expressions are said to be greedy - they will always try to find the longest pattern that satisfies the match. Fixing problems like this is pretty easy - we just have to think about what we really want
to match. In this case, we don't want zero or more occurences of anything; what we want is zero or more occurences of anything except a right angle bracket. As soon as we see the first right angle bracket after the left angle bracket we want to stop. Fortunately, it's very easy to express ideas like this with negated character classes. In this case, we simply replace the period with [^>]:

```
> matches = mapply(getexpr,htmls,gregexpr('<[^>]*>',htmls))
> names(matches) = NULL
> matches
[[1]]
[1] "<IMG SRC=\"img/rxb.gif\">"
[[2]]
[1] "<a href=\"somepage.html\">" "</a>"
```

The two pieces of markup in the second element of htmls are now correctly found.
Another way to solve the problem of greedy regular expressions is to use a feature of regular expressions invented by Larry Wall, the creator of perl. His idea was to use the question mark (?) after an asterisk $(*)$ or plus sign $((+))$ to indicate that you want a nongreedy match, that is, to search for the smallest string which will match the pattern. So an alternative to the solution shown above is:

```
> matches = mapply(getexpr,htmls,gregexpr('<.*?>',htmls,perl=TRUE))
```


### 3.3 Tagging and Backreferences

Consider again the problem of looking for email addresses. The regular expression that we wrote is exactly what we want, because we don't care what's surrounding the email address. But in many cases, the only way we can find what we want is to specify the surroundings of what we're looking for. Suppose we wish to write a program that will find all of the links (URLs that can be reached by clicking some text on the page) of a web page. A line containing a link may look something like this:

```
<a href="http://www.stat.berkeley.edu">UC Berkeley Stat Dept Home Page</a><br />
```

Finding the links is very easy; but our goal here is to extract the links themselves. Notice that there's no regular expression that can match just the link; we need to use some information about the context in which it's found, and when we extract the matched expression there will be extra characters that we really don't want. To handle this problem, parentheses can be used to surround parts of a regular expression that we're really interested in, and tools exist to help us get those parts separated from the overall expression. In $R$, the only functions that can deal with these tagged expressions are sub and gsub, so to take take advantage of them, you may have to first extract the regular expressions with the methods we've already seen, and then apply sub or gsub. To illustrate, let's compose a simple regular expression to
find links. I don't need to worry about the case of the regular expression, because the grep, sub, gsub and gregexpr functions all support the ignore. case= argument. Notice that I've surrounded the part we want ( $\left[\wedge^{\prime \prime} \gg\right]+$ ) in parentheses. This will allow me to refer to this tagged expression as $\backslash 1$ in a call to gsub. (Additional tagged expressions will be refered to as $\backslash 2, \backslash 3$, etc.) Using this pattern, we can first find all the chunks of text that have our links embedded in them, and then use gsub to change the entire piece to just the part we want:

```
> link = '<a href="http://www.stat.berkeley.edu">UC Berkeley Stat Dept Home Page</a><br
> gregout = gregexpr('href *= *["\']?([^"\'>]+)["\']? *>',link,ignore.case=TRUE)
> thematch = mapply(getexpr,link,gregout)
> gsub('href *= *["\']?([`"\'>]+)["\']? *>','\\1',thematch,ignore.case=TRUE)
[1] "http://www.stat.berkeley.edu"
```


### 3.4 Getting Text into R

Up until now, we've been working with text that's already been formatted to make it easy for R to read, and scan or read.table (and its associated wrapper functions) have been sufficient to take care of things. Now we want to treat our input as raw text; in other words, we don't want R to assume that the data is in any particular form. The main function for taking care of this in $R$ is readLines. In the simplest form, you pass readLines the name of a URL or file that you want to read, and it returns a character vector with one element for each line of the file or url, containing the contents of each line. An optional argument to readLines specifies the number of lines you want to read; by default it's set to -1 , which means to read all available lines. readLines removes the newline at the end of each line, but otherwise returns the text exactly the way it was found in the file or URL.
readLines also accepts connections, which are objects in $R$ that represent an alternative form of input, such as a pipe or a zipped file. Take a look at the help file for connections for more information on this capability.

For moderate-sized problems that aren't too complex, using readLines in its default mode (reading all the lines of input into a vector of character strings) will usually be the best way to solve your problem, because most of the functions you'll use with such data are vectorized, and can operate on every line at once. As a simple example, suppose we wanted to get the names of all the files containing notes for this class. A glance at the page http://www.stat.berkeley.edu/classes/s133/schedule.html indicates that all the online notes can be found on lines like this one:
<tr><td> Jan 23 </td><td> <a href="Unix.html">Introduction to UNIX</td></tr>
We can easily extract the names of the note files using the sub function (since there is only one link per line, we don't need to use gsub, although we could).

The first step is to create a vector of character strings that will represents the lines of the URL we are trying to read. We can simply pass the URL name to readLines:

```
> x = readLines('http://www.stat.berkeley.edu/classes/s133/schedule.html')
```

Next, we can write a regular expression that can find the links. Note that the pattern that we want (i.e. the name of the file referenced in the link) has been tagged with parentheses for later extraction. By using the caret ( $\sim$ ) and dollar sign ( $\$$ ) we can describe our pattern as an entire line - when we substitute the tagged expression for the pattern we'll have just what we want. I'll also add the basename of the files so that they could be, for example, entered into a browser.

```
> baseurl = 'http://www.stat.berkeley.edu/classes/s133'
> linkpat = '^.*<td> *<a href=["\'](.*)["\']>.*$'
> x = readLines('http://www.stat.berkeley.edu/classes/s133/schedule.html')
> y = grep(linkpat,x,value=TRUE)
> paste(baseurl,sub(linkpat,'\\1',y),sep='/')
    [1] "http://www.stat.berkeley.edu/classes/s133/Intro.html"
    [2] "http://www.stat.berkeley.edu/classes/s133/OS.html"
    [3] "http://www.stat.berkeley.edu/classes/s133/Unix.html"
    [4] "http://www.stat.berkeley.edu/classes/s133/R-1a.html"
    [5] "http://www.stat.berkeley.edu/classes/s133/R-2a.html"
    [6] "http://www.stat.berkeley.edu/classes/s133/R-3a.html"
```

As an example of how to extract information from a web page, consider the task of extracting the spring baseball schedule for the Cal Bears from http://calbears.cstv.com/sports/m-basebl/sched/cal-m-basebl-sched.html.

### 3.5 Reading a web page into $R$

Read the contents of the page into a vector of character strings with the readLines function:

```
> thepage = readLines('http://calbears.cstv.com/sports/m-basebl/sched/cal-m-basebl-sched
```

Note: When you're reading a web page, make a local copy for testing; as a courtesy to the owner of the web site whose pages you're using, don't overload their server by constantly rereading the page. To make a copy from inside of R, look at the download.file function. You could also save a copy of the result of using readLines, and practice on that until you've got everything working correctly.

Now we have to focus in on what we're trying to extract. The first step is finding where it is. If you look at the web page, you'll see that the title "Opponent / Event" is right above the data we want. We can locate this line using the grep function:

```
> grep('Opponent / Event',thepage)
[1] }35
```

If we look at the lines following this marker, we'll notice that the first date on the schedule can be found in line 400, with the other information following after:

```
> thepage[400:407]
```

[1] " <tr id=\"990963\" title=\"2009,1,21,16,00,00\" valign=\"TOP\" bgcolor=\"\#d1d1
[2] " "
[3] " <td class=\"row-text\">02/21/09</td>"
[4] " "
[5] " <td class=\"row-text\">vs. UC Riverside</td>"
[6] " "
[7] " <td class=\"row-text\">Berkeley, Calif.</td>"
[8] " "

Based on the previous step, the data that we want is always preceded by the HTML tag "<td class="row-text">", and followed by "</td>". Let's grab all the lines that have that pattern:

```
> mypattern = '<td class="row-text">([^<]*)</td>'
> datalines = grep(mypattern,thepage[400:length(thepage)],value=TRUE)
```

I used value=TRUE, so I wouldn't have to worry about the indexing when I restricted myself to the lines from 400 on. Also notice that I've already tagged the part that I want, in preparation to the final call to gsub.

Now that I've got the lines where my data is, I can use grexpr, then getexpr (from the previous lecture), and gsub to extract the information without the HTML tags:

```
> getexpr = function(s,g)substring(s,g,g+attr(g,'match.length')-1)
> gg = gregexpr(mypattern,datalines)
> matches = mapply(getexpr,datalines,gg)
> result = gsub(mypattern,'\\1',matches)
> names(result) = NULL
> result[1:10]
    [1] "02/21/09" "vs. UC Riverside" "Berkeley, Calif." "1:00 p.m. PT"
    [5] "02/22/09" "vs. Vanderbilt" "Berkeley, Calif." "1:00 p.m. PT"
[9] "02/23/09" "vs. Vanderbilt"
```

It seems pretty clear that we've extracted just what we wanted - to make it more usable, we'll convert it to a data frame and provide some titles. Since it's hard to describe how to convert a vector to a data frame, we'll use a matrix as an intermediate step. Since there are four pieces of information (columns) for each game (row), a matrix is a natural choice:

```
> schedule = as.data.frame(matrix(result,ncol=4,byrow=TRUE))
> names(schedule) = c('Date','Opponent','Location','Result')
> head(schedule)
    Date Opponent Location Result
1 02/21/09 vs. UC Riverside Berkeley, Calif. 1:00 p.m. PT
2 02/22/09 vs. Vanderbilt Berkeley, Calif. 1:00 p.m. PT
3 02/23/09 vs. Vanderbilt Berkeley, Calif. 1:00 p.m. PT
4 02/25/09 at Santa Clara Santa Clara, Calif. 6:00 p.m. PT
5 02/27/09 at Long Beach State Long Beach, Calif. 6:30 p.m. PT
6 02/28/09 at Long Beach State Long Beach, Calif. 2:00 p.m. PT
```


### 3.6 Another Example

At http://www.imdb.com/chart is a box-office summary of the ten top movies, along with their gross profits for the current weekend, and their total gross profits. We would like to make a data frame with that information. As always, the first part of the solution is to read the page into $R$, and use an anchor to find the part of the data that we want. In this case, the table has column headings, including one for "Rank".

```
> x = readLines('http://www.imdb.com/chart/')
> grep('Rank',x)
```

[1] 114113931651

Starting with line 1141 we can look at the data to see where the information is. A little experimentation shows that the useful data starts on line 1157:

```
> x[1157:1165]
[1] " <td class=\"chart_even_row\">"
[2] " <a href=\"/title/tt0989757/\">Dear John</a> (2010/I)"
```

```
[3] " </td>"
[4] " <td class=\"chart_even_row\" style=\"text-align: right; padding-right: 20px\"
[5] " $30.5M"
[6] " </td>"
[7] " <td class=\"chart_even_row\" style=\"text-align: right\">"
[8] " $30.5M"
[9] " </td>"
```

There are two types of lines that contain useful data: the ones with the title, and the ones that begin with some blanks followed by a dollar sign. Here's a regular expression that will pull out both those lines:

```
> goodlines = '<a href="/title[^>]*>(.*)</a>.*$|^ *\\$'
> try = grep(goodlines,x,value=TRUE)
```

Looking at the beginning of try, it seems like we got what we want:

```
> try[1:10]
```

| [1] | " | <a href=\"/title/tt1001508/\">He's Just Not That Into You</a> (2009)" |
| :---: | :---: | :---: |
| [2] | " | \$27.8M" |
| [3] | " | \$27.8M" |
| [4] | " | <a href=\"/title/tt0936501/\">Taken</a> (2008/I)" |
| [5] | " | \$20.5M" |
| [6] | " | \$53.6M" |
| [7] | " | <a href=\"/title/tt0327597/\">Coraline</a> (2009)" |
| [8] | " | \$16.8M" |
| [9] | " | \$16.8M" |
| [10] | " | <a href=\"/title/tt0838232/\">The Pink Panther 2</a> (2009)" |

Sometimes the trickiest part of getting the data off a webpage is figuring out exactly the part you need. In this case, there is a lot of extraneous information after the table we want. By examining the output, we can see that we only want the first 30 entries. We also need to remove the extra information from the title line. We can use the sub function with a modified version of our regular expression:

```
> try = try[1:30]
> try = sub('<a href="/title[^>]*>(.*)</a>.*$','\\1',try)
> head(try)
[1] " He's Just Not That Into You"
[2] " $27.8M"
[3] " $27.8M"
[4] " Taken"
[5] " $20.5M"
[6] " $53.6M"
```

Once the spaces at the beginning of each line are removed, we can rearrange the data into a 3 -column data frame:

```
> try = sub('^ *','',try)
> movies = data.frame(matrix(try,ncol=3,byrow=TRUE))
> names(movies) = c('Name','Wkend Gross','Total Gross')
> head(movies)
            Name Wkend Gross Total Gross
1 Dear John $30.5M $30.5M
2 Avatar $22.9M $629M
3 From Paris with Love $8.16M $8.16M
4 Edge of Darkness $6.86M $28.9M
5 Tooth Fairy $6.63M $34.5M
6 When in Rome $5.55M $20.9M
```


### 3.7 Dynamic Web Pages

While reading data from static web pages as in the previous examples can be very useful (especially if you're extracting data from many pages), the real power of techniques like this has to do with dynamic pages, which accept queries from users and return results based on those queries. For example, an enormous amount of information about genes and proteins can be found at the National Center of Biotechnology Information website (http://www.ncbi.nlm.nih.gov/), much of it available through query forms. If you're only performing a few queries, it's no problem using the web page, but for many queries, it's beneficial to automate the process.

Here is a simple example that illustrate the concept of accessing dynamic information from web pages. The page http://finance.yahoo.com provides information about stocks; if you enter a stock symbol on the page, (for example aapl for Apple Computer), you will be directed to a page whose URL (as it appears in the browser address bar) is

```
http://finance.yahoo.com/q?s=aapl&x=0&y=0
```

The way that stock symbols are mapped to this URL is pretty obvious. We'll write an R function that will extract the current price of whatever stock we're interested in.

The first step in working with a page like this is to download a local copy to play with, and to read the page into a vector of character strings:

```
> download.file('http://finance.yahoo.com/q?s=aapl&x=0&y=0','quote.html')
trying URL 'http://finance.yahoo.com/q?s=aapl&x=0&y=0'
Content type 'text/html; charset=utf-8' length unknown
opened URL
downloaded 39Kb
> x = readLines('quote.html')
```

To get a feel for what we're looking for, notice that the words "Last Trade:" appear before the current quote. Let's look at the line containing this string:

```
> grep('Last Trade:',x)
25
> nchar(x[25])
[1] }87
```

Since there are over 800 characters in the line, we don't want to view it directly. Let's use gregexpr to narrow down the search:

```
> gregexpr('Last Trade:',x[25])
[[1]]
[1] 411
attr(,"match.length")
[1] 11
```

This shows that the string "Last Trade:" starts at character 411. We can use substr to see the relevant part of the line:

```
substring(x[25],411,500)
[1] "Last Trade:</th><td class=\"yfnc_tabledata1\"><big><b><span id=\"yfs_l10_aapl\">196
```

There's plenty of context - we want the part surrounded by <big><b><span ... and </span>. One easy way to grab that part is to use a tagged regular expression with gsub:

```
> gsub('^.*<big><b><span [`>]*>([^<]*)</span>.*$', \\\1',x[25])
[1] "196.19"
```

This suggests the following function:

```
> getquote = function(sym){
+ baseurl = 'http://finance.yahoo.com/q?s='
+ myurl = paste(baseurl,sym,'&x=0&y=0',sep='')
+ x = readLines(myurl)
+ q = gsub('^.*<big><b><span [`>]*>([^<]*)</span>.*$','\\1',grep('Last Trade:',x,valu
+ as.numeric(q)
+}
```

As always, functions like this should be tested:

```
> getquote('aapl')
[1] 196.19
> getquote('ibm')
[1] 123.21
> getquote('nok')
[1] 13.35
```

These functions provide only a single quote; a little exploration of the yahoo finance website shows that we can get CSV files with historical data by using a URL of the form:

```
http://ichart.finance.yahoo.com/table.csv?s=xxx
```

where xxx is the symbol of interest. Since it's a comma-separated file, We can use read.csv to read the chart.

```
gethistory = function(symbol)
    read.csv(paste('http://ichart.finance.yahoo.com/table.csv?s=',symbol,sep=''))
```

Here's a simple test:

```
> aapl = gethistory('aapl')
> head(aapl)
            Date Open High Low Close Volume Adj.Close
1 2009-02-20 89.40 92.40 89.00 91.20 26780200 91.20
2 2009-02-19 93.37 94.25 90.11 90.64 32945600 90.64
3 2009-02-18 95.05 95.85 92.72 94.37 24417500 94.37
4 2009-02-17 96.87 97.04 94.28 94.53 24209300 94.53
5 2009-02-13 98.99 99.94 98.12 99.16 21749200 99.16
6 2009-02-12 95.83 99.75 95.83 99.27 29185300 99.27
```

Unfortunately, if we try to use the Date column in plots, it will not work properly, since R has stored it as a factor. The format of the date is the default for the as.Date function, so we can modify our function as follows:

```
gethistory = function(symbol){
    data = read.csv(paste('http://ichart.finance.yahoo.com/table.csv?s=',symbol,sep=''))
    data$Date = as.Date(data$Date)
    data
}
```

Now, we can produce plots with no problems:

```
> aapl = gethistory('aapl')
> plot(aapl$Date,aapl$Close,main='Closing price for AAPL',type='l')
```

The plot is shown below:


This suggest a function for plotting any of the variables in the CSV file:

```
plothistory = function(symbol,what){
    match.arg(what,c('Open','High','Low','Close','Volume','Adj.Close'))
    data = gethistory(symbol)
    plot(data$Date,data[,what],main=paste(what,'price for ',symbol),type='l')
    invisible(data)
}
```

This function introduces several features of functions that we haven't seen yet.

- The match. arg function lets us specify a list of acceptable values for a parameter being passed to a function, so that an error will occur if you use a non-existent variable:

```
> plothistory('aapl','Last')
Error in match.arg("what", c("Open", "High", "Low", "Close", "Volume", :
    'arg' should be one of Open, High, Low, Close, Volume, Adj.Close
```

- The invisible function prevents the returned value (data in this case) from being printed when the output of the function is not assigned, but also allows us to assign the output to a variable if we want to use it latter:

```
> plothistory('aapl','Close')
```

will produce a plot without displaying the data to the screen, but

```
> aapl.close = plothistory('aapl','Close')
```

will produce the plot, and store the data in aapl.close.

### 3.8 Another Example

When using google, it's sometimes inconvenient to have to click through all the pages. Let's write a function that will return the web links from a google search. If you type a search time into google, for example a search for 'introduction to r", you'll notice that the address bar of your browser looks something like this:
http://www.google.com/search?q=introduction+to+r\&ie=utf-8\&oe=utf-8\&aq=t\&rls=com.ubuntu:e
For our purposes, we only need the "q=" part of the search. For our current example, that would be the URL
http://www.google.com/search?q=introduction+to+r
Note that, since blanks aren't allowed in URLs, plus signs are used in place of spaces. If we were to click on the "Next" link at the bottom of the page, the URL changes to something like
http://www.google.com/search?hl=en\&safe=active\&client=firefox-a\&rls=com.ubuntu:en-US:uno
For our purposes, we only need to add the \&start= argument to the web page. Since google displays 10 results per page, the second page will have start=10, the next page will have start $=20$, and so on. Let's read in the first page of this search into $R$ :

```
z = readLines('http://www.google.com/search?q=introduction+to+r')
Warning message:
In readLines("http://www.google.com/search?q=introduction+to+r") :
    incomplete final line found on 'http://www.google.com/search?q=introduction+to+r'
```

As always, you can safely ignore the message about the incomplete final line.
Since we're interested in the web links, we only want lines with "href=" in them. Let's check how many lines we've got, how long they are, and which ones contain the href string:

```
> length(z)
[1] 9
> nchar(z)
Error in nchar(z) : invalid multibyte string 3
```

The error message looks pretty bad - fortunately it's very easy to fix. Basically, the error means that, for the computer's current setup, there's a character that isn't recognized. We can force R to recognize every character by issuing the following command:

```
> Sys.setlocale('LC_ALL','C')
[1] "LC_CTYPE=C;LC_NUMERIC=C;LC_TIME=C;LC_COLLATE=C;LC_MONETARY=C;LC_MESSAGES=en_US.UTF-
```

The "UTF-8" means that all characters will now be recognized.

```
> nchar(z)
[1] 
> grep('href *=',z)
[1] 3
```

It's pretty clear that all of the links are on the third line.
Now we can construct a tagged regular expression to grab all the links.

```
> hrefpat = 'href *= *"([^"]*)"'
> getexpr = function(s,g)substring(s,g,g+attr(g,'match.length')-1)
> gg = gregexpr(hrefpat,z[[3]])
> res = mapply(getexpr,z[[3]],gg)
> res = sub(hrefpat,'\\1',res)
> res[1:10]
    [1] "http://images.google.com/images?q=introduction+to+r&um=1&ie=UTF-8&sa=N&hl=en&tab=w
    [2] "http://video.google.com/videosearch?q=introduction+to+r&um=1&ie=UTF-8&sa=N&hl=en&t
    [3] "http://maps.google.com/maps?q=introduction+to+r&um=1&ie=UTF-8&sa=N&hl=en&tab=wl"
    [4] "http://news.google.com/news?q=introduction+to+r&um=1&ie=UTF-8&sa=N&hl=en&tab=wn"
    [5] "http://www.google.com/products?q=introduction+to+r&um=1&ie=UTF-8&sa=N&hl=en&tab=wf
    [6] "http://mail.google.com/mail/?hl=en&tab=wm"
    [7] "http://www.google.com/intl/en/options/"
    [8] "/preferences?hl=en"
    [9] "https://www.google.com/accounts/Login?hl=en&continue=http://www.google.com/search/
[10] "http://www.google.com/webhp?hl=en"
```

We don't want the internal (google) links - we want external links which will begin with "http://". Let's extract all the external links, and then eliminate the ones that just go back to google:

```
> refs = res[grep('^https?:',res)]
> refs = refs[-grep('google.com/',refs)]
> refs[1:3]
    [1] "http://cran.r-project.org/doc/manuals/R-intro.pdf"
    [2] "http://74.125.155.132/search?q=cache:d4-KmcWVA-oJ:cran.r-project.org/doc/manuals/R
    [3] "http://74.125.155.132/search?q=cache:d4-KmcWVA-oJ:cran.r-project.org/doc/manuals/R
```

If you're familiar with google, you may recognize these as the links to google's cached results. We can easily eliminate them:

```
> refs = refs[-grep('cache:',refs)]
> length(refs)
[1] 10
```

We can test these same steps with some of the other pages from this query:

```
> z = readLines('http://www.google.com/search?q=introduction+to+r&start=10')
Warning message:
In readLines("http://www.google.com/search?q=introduction+to+r&start=10") :
    incomplete final line found on 'http://www.google.com/search?q=introduction+to+r&start
> hrefpat = 'href *= *"([^"]*)"'
> getexpr = function(s,g)substring(s,g,g+attr(g,'match.length')-1)
> gg = gregexpr(hrefpat,z[[3]])
> res = mapply(getexpr,z[[3]],gg)
> res = sub(hrefpat,'\\1',res)
> refs = res[grep('^https?:',res)]
> refs = refs[-grep('google.com/',refs)]
> refs = refs[-grep('cache:',refs)]
> length(refs)
```

[1] 10

Once again, it found all ten links. This obviously suggests a function:

```
googlerefs = function(term,pg=0){
    getexpr = function(s,g)substring(s,g,g+attr(g,'match.length')-1)
    qurl = paste('http://www.google.com/search?q=',term,sep='')
    if(pg > 0)qurl = paste(qurl,'&start=',pg * 10,sep='')
    qurl = gsub(' ','+',qurl)
    z = readLines(qurl)
    hrefpat = 'href *= *"([^"]*)"'
    wh = grep(hrefpat,z)
    gg = gregexpr(hrefpat,z[[wh]])
    res = mapply(getexpr,z[[wh]],gg)
    res = sub(hrefpat,'\\1',res)
    refs = res[grep('^https?:',res)]
    refs = refs[-grep('google.com/|cache:',refs)]
    names(refs) = NULL
    refs[!is.na(refs)]
}
```

Now suppose that we want to retreive the links for the first ten pages of query results:
> links = sapply(0:9,function(pg) googlerefs('introduction to r', pg ) )
> links = unlist(links)
> head(links)
[1] "http://cran.r-project.org/doc/manuals/R-intro.pdf"
[2] "http://cran.r-project.org/manuals.html"
[3] "http://www.biostat.wisc.edu/~kbroman/Rintro/"
[4] "http://faculty.washington.edu/tlumley/Rcourse/"
[5] "http://www.stat.cmu.edu/~larry/all-of-statistics/=R/Rintro.pdf"
[6] "http://www.stat.berkeley.edu/~spector/R.pdf"

## Chapter 4

## Graphics

### 4.1 More on Plotting

We've seen the usage of some basic graphics functions in previous lectures, but there are still a few points that should be covered before we study more advanced graphics commands. One issue has to do with multiple lines on a plot. In addition to the high-level plot command, R provides the points and lines functions, which can add new data to a plot. Consider the nationwide Community Health Data, available at the website http://communityhealth.hhs.gov. The data is available in a zip file, which contains a number of CSV files containing information recorded for each county in the USA. One such file, containing information about various risk factors and access to health care in the counties can be found on the class website:http://www.stat.berkeley.edu/classes/s133/data/RISKFACTORSANDACCESSTOCARE.csv. First, we'll read in the data, and look at the first few records:

```
> risk = read.csv('http://www.stat.berkeley.edu/classes/s133/data/RISKFACTORSANDACCESSTC
> head(risk)
    State_FIPS_Code County_FIPS_Code CHSI_County_Name CHSI_State_Name
        1 1 Autauga Alabama
        1 3 Baldwin Alabama
        1 5 Barbour Alabama
        1 7 Bibb Alabama
        1 9 Blount Alabama
        11 Bullock Alabama
    CHSI_State_Abbr Strata_ID_Number No_Exercise CI_Min_No_Exercise
        AL 29 27.8 20.7
        AL 16
        AL 5
        AL 42 -1111.1 -1111.1
            AL 28 33.5 26.3
            AL 75 -1111.1 -1111.1
    CI_Max_No_Exercise Few_Fruit_Veg CI_Min_Fruit_Veg CI_Max_Fruit_Veg Obesity
            34.9 78.6 69.4 87.8 24.5
            31.2 76.2 71.2 81.3 23.6
    -1111.1 -1111.1 
    -1111.1 86.6 77.8 95.4 -1111.1
            40.6 74.6 66.1 83.0
            -1111.1 -1111.1 -1111.1 -1111.1 -1111.1
    CI_Min_Obesity CI_Max_Obesity High_Blood_Pres CI_Min_High_Blood_Pres
            17.3 31.7 29.1 19.2
            19.5 27.6 30.5
            16.2 35.0 -1111.1 
            -1111.1 -1111.1 -1111.1 -1111.1
            17.2 31.2 -1111.1 -1111.1
            -1111.1 -1111.1 
```

| CI_Max_High_Blood_Pres |  | Smoker | CI_Min_Smoker | CI_Max_Smoker | Diabetes |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1 | 39.0 | 26.6 | 19.1 | 34.0 | 14.2 |  |
| 2 | 36.6 | 24.6 | 20.3 | 28.8 | 7.2 |  |
| 3 | -1111.1 | 17.7 | 10.2 | 25.1 | 6.6 |  |
| 4 | -1111.1 | -1111.1 | -1111.1 | -1111.1 | 13.1 |  |
| 5 | -1111.1 | 23.6 | 16.7 | 30.4 | 8.4 |  |
| 6 | -1111.1 | -1111.1 | -1111.1 | -1111.1 | -1111.1 |  |
| CI_Min_Diabetes CI_Max_Diabetes |  |  | Uninsured Elderly_Medicare Disabled_Medicare |  |  |  |
| 1 | 9.1 | 19.3 | 5690 | 4762 |  | 1209 |
| 2 | 5.2 | 9.3 | 19798 | 22635 |  | 3839 |
| 3 | 2.0 | 11.3 | 5126 | 3288 |  | 1092 |
| 4 | 4.7 | 21.5 | 3315 | 2390 |  | 974 |
| 5 | 4.4 | 12.4 | 8131 | 5019 |  | 1300 |
| 6 | -1111.1 | -1111.1 | 2295 | 1433 |  | 504 |
| Prim_Care_Phys_Rate Dentist_Rate Community_Health_Center_Ind HPSA_Ind |  |  |  |  |  |  |
| 1 | 45.3 | 22.6 |  |  | 1 | 2 |
| 2 | 67.0 | 30.8 |  |  | 1 | 2 |
| 3 | 45.8 | 24.6 |  |  | 1 | 2 |
| 4 | 41.8 | 18.6 |  |  | 1 | 1 |
| 5 | 16.2 | 10.8 |  |  | 2 | 1 |
| 6 | 54.3 | 18.1 |  |  | 1 | 1 |

It's clear that the value -1111.1 is being used for missing values, and we'll need to fix that before we work with the data:

```
> risk[risk == -1111.1] = NA
```

Suppose we want to investigate the relationship between Diabetes and Smoking in each of the counties in California. We could create a data set with only California using the subset command, and then plot the two variables of interest:

```
> risk.ca = subset(risk, CHSI_State_Name == 'California')
> plot(risk.ca$Smoker,risk.ca$Diabetes)
```

Here's what the plot looks like:


Now let's say that we wanted to examine the relationship between smoking and diabetes for some other state, say Alabama. We can extract the Alabama data using subset, and then use the points command to add that data to the existing plot. (Unlike plot, points doesn't produce a new plot, it adds to the currently active plot.)

```
> risk.al = subset(risk, CHSI_State_Name == 'Alabama')
> points(risk.al$Smoker,risk.al$Diabetes,col='red')
```

The plot now looks like this:


Clearly there's a problem: some of the Alabama points are off the scale. This demonstrates that when you wish to plot multiple sets of points on the same graph that you have to make sure that the axes are big enough to accomodate all of the data. One very easy way to do this is to call the plot function with the minimums and maximums of all the data using type='n' as one of the arguments. This tells $R$ to set up the axes, but not to actually plot anything. So a better way to plot the two sets of points would be as follows:

```
> plot(range(c(risk.ca$Smoker,risk.al$Smoker),na.rm=TRUE),
+ range(c(risk.ca$Diabetes,risk.al$Diabetes),na.rm=TRUE),
+ type='n',xlab='Smoking Rate',ylab='Diabetes Rate')
> points(risk.ca$Smoker,risk.ca$Diabetes)
> points(risk.al$Smoker,risk.al$Diabetes,col='red')
> legend('topright',c('California','Alabama'),col=c('black','red'),pch=1)
> title('Diabetes Rate vs. Smoking by County')
```

The completed plot looks like this:

## Diabetes Rate vs. Smoking by County



To add a line to a plot, the lines function can be used in place of the points function. The built-in data set Puromycin provides data on concentration and reaction rate of Puromycin on two types of cells, treated and untreated. You can learn more about R's builtin data sets by using the data() function, and then using the usual help facility within R. Since this is a small data set (only 23 rows), we can examine it directly:
> Puromycin

|  | conc | rate | state |
| :--- | ---: | ---: | ---: |
| 1 | 0.02 | 76 | treated |
| 2 | 0.02 | 47 | treated |
| 3 | 0.06 | 97 | treated |
| 4 | 0.06 | 107 | treated |
| 5 | 0.11 | 123 | treated |
| 6 | 0.11 | 139 | treated |
| 7 | 0.22 | 159 | treated |
| 8 | 0.22 | 152 | treated |
| 9 | 0.56 | 191 | treated |
| 10 | 0.56 | 201 | treated |


| 11 | 1.10 | 207 | treated |
| ---: | ---: | ---: | ---: |
| 12 | 1.10 | 200 | treated |
| 13 | 0.02 | 67 | untreated |
| 14 | 0.02 | 51 | untreated |
| 15 | 0.06 | 84 | untreated |
| 16 | 0.06 | 86 | untreated |
| 17 | 0.11 | 98 | untreated |
| 18 | 0.11 | 115 | untreated |
| 19 | 0.22 | 131 | untreated |
| 20 | 0.22 | 124 | untreated |
| 21 | 0.56 | 144 | untreated |
| 22 | 0.56 | 158 | untreated |
| 23 | 1.10 | 160 | untreated |

Since there are two observations at each concentration, we can use the aggregate function to calculate the mean before plotting the data:

```
> Puro = aggregate(list(rate=Puromycin$rate),list(conc=Puromycin$conc,state=Puromycin$st
```

By putting the rate variable in a named list, I insure that the column with the mean will be called "rate". Alternatively, I could rename the column later:

```
> Puro = aggregate(Puromycin$rate,list(conc=Puromycin$conc,state=Puromycin$state),mean)
> names(Puro) [3] = 'rate'
```

Now we can create two data frames, one for the treated cells, and one for the untreated ones:

```
> Puro.treated = subset(Puro,state=='treated')
> Puro.untreated = subset(Puro,state=='untreated')
```

Examination of the data shows that the rate for the treated cells are higher than the untreated cells. Thus, instead of creating an empty plot as in the previous example, I'll just plot the line for the treated cells first:

```
> plot(Puro.treated$conc,Puro.treated$rate,xlab='Rate',ylab='Conc',main='Rate vs. Concen
> lines(Puro.untreated$conc,Puro.untreated$rate,col='blue')
> legend('bottomright',c('Treated','Untreated'),col=c('black','blue'),lty=1)
```

The plot appears below:

Rate vs. Concentration for Puromycin


### 4.2 Multiple Plots on a Page

The mfrow or mfcol arguments to the par function allow you to divide the plotting page into a grid, to accomodate multiple plots on a single page. The layout of the plot is determined by a vector of length 2 , specifying the number of rows and columns in the grid. The difference between mfrow and mfcol concerns the order in which the plots are drawn. When using mfrow, plots are drawn across the rows, while mfcol draws the plot down the columns.

As an example, consider the builtin airquality data set, which contains various air quality measures for a five month period in New York. We can get an idea of what the data is like by using the summary function:

```
> summary(airquality)
    Ozone Solar.R Wind
Min. : 1.00 Min. : 7.0 Min. : 1.700 Min. :56.00
1st Qu.: 18.00 1st Qu.:115.8 1st Qu.: 7.400 1st Qu.:72.00
Median : 31.50 Median :205.0 Median : 9.700 Median :79.00
```

```
Mean : 42.13 Mean :185.9 Mean : 9.958 Mean :77.88
3rd Qu.: 63.25 3rd Qu.:258.8 3rd Qu.:11.500 3rd Qu.:85.00
Max. :168.00 Max. :334.0 Max. :20.700 Max. :97.00
NA's : 37.00 NA's : 7.0
    Month Day
Min. :5.000 Min. : 1.00
1st Qu.:6.000 1st Qu.: 8.00
Median :7.000 Median :16.00
Mean :6.993 Mean :15.80
3rd Qu.:8.000 3rd Qu.:23.00
Max. :9.000 Max. :31.00
```

Suppose we want to plot histograms of each of the first four variables, side by side with a plot of the variable over time. The first step is to convert the Month and Date variables into $R$ Date variables:

```
> airquality$date = as.Date(ISOdate(1973,airquality$Month,airquality$Day))
```

Rather than typing in the plotting commans repeatedly, we can write a function to make the plots for each variable:

```
twoplot = function(var) \{
    plot(density (airquality[,var], na.rm=TRUE), main=paste('Density of', var))
    plot(airquality\$date, airquality[,var], type='l', main=paste(var,'vs. time'), ylab=var)
\}
```

Since we'll be plotting the first four variables, we'll want a $4 \times 2$ grid, and we'll want to plot by rows. Thus, we issue the following command:

```
> par(mfrow=c(4,2))
```

We can use sapply to call our twoplot function for each of the variables:

```
> sapply(names(airquality) [1:4],twoplot)
    Ozone Solar.R Wind Temp
[1,] 1216 1216 1216 1216
[2,] 1247 1247 1247 1247
[3,] 1277 1277 1277 1277
[4,] 1308 1308 1308 1308
[5,] 1339 1339 1339 1339
[6,] 1369 1369 1369 1369
```

Here's the plot:


As can be seen, the default for multiple plots leaves quite a bit of space between the plots. The graphics parameter that controls this is called mar. The value that determines the spacing is a vector of length 4 , with the number of lines of space on the bottom, left, top, and right of the plots. We can find the current value of graphics parameters by passing the name of the parameter to par:

```
> par('mar')
[1] 5.1 4.1 4.1 2.1
```

Let's remove one line from each of the top and bottom, and replot the series of graphs:

```
> par(mar=c(4.1,4.1,3.1,2.1),mfrow=c(4,2))
> sapply(names(airquality) [1:4],twoplot)
    Ozone Solar.R Wind Temp
[1,] 1216 1216 1216 1216
[2,] 1247 1247 1247 1247
[3,] 1277 1277 1277 1277
[4,] 1308 1308 1308 1308
[5,] 1339 1339 1339 1339
```


## [6,] $1369 \quad 136913691369$

The plot is shown below:


After plotting multiple plots, you can restore R's normal behaviour of plotting each plot on a separate page by resetting mfrow as follows:
> $\operatorname{par}(\operatorname{mfrow}=c(1,1))$

### 4.3 More on Barplots

We briefly looked at barplots when we examined the day of the week on which popular movies opened. You may recall that we passed the result of a call from the table function to barplot. This idea can be extended to create side-by-side or stacked barplots. As an alternative to using table, we can produce a matrix with the values we wish to plot. By providing dimnames for this matrix, barplot will be able to appropriately label the plot.

Once again consider the risk data set we used earlier. To simplify the plot, the different states in the data set can be grouped into regions, using the built-in state.name and state.region objects:

```
> risk = merge(risk,data.frame(state=state.name,region=state.region),by.x='CHSI_State_Na
```

Suppose we're interested in comparing the average smoking, diabetes, and obesity rates for the different regions. First, we use the aggregate function to find the averages of the variables, broken down by regions:

```
> mns = aggregate(risk[,c('Smoker','Diabetes','Obesity')],risk['region'],mean,na.rm=TRU
> mns
    region Smoker Diabetes Obesity
1 Northeast 22.62537 7.161972 22.13430
2 South 25.15847 8.754302 25.71493
3 North Central 22.28592 7.318565 24.16283
4 West 19.50740 6.349167 21.01306
```

If we try to pass this data frame to barplot, we'll get an error, since barplot needs a matrix. In addition, the column that identifies the different groups (in this case region), needs to be part of the row names, not a variable in the data frame itself. These two steps create the row names, and eliminate the region column from the data frame:

```
> row.names(mns) = mns$region
> mns$region = NULL
```

If we were to use the following statement to create the barplot:

```
> barplot(as.matrix(mns))
```

we'd find that the bars were representing the variables, not the regions. To fix this, we simply pass the transpose of the matrix to barplot:

```
> barplot(t(as.matrix(mns)))
```

Here's what the plot looks like:


This is known as a stacked barplot, and while it's useful for some kinds of data, I don't find it appropriate for this type of data. By passing the beside=TRUE argument to barplot, we can produce a side-by-side barchart, which I find more useful. The legend=TRUE argument helps to identify the bars:

```
> barplot(t(as.matrix(mns)),beside=TRUE,legend=TRUE)
```

Here's the result:


### 4.4 Mapping

We've looked at some data about different countries around the world, but so far we haven't taken advantage of the fact that the data has a geographic origin (other than trying to see if relationships were different among different continents by using color to represent continent in scatterplots.) The R library maps gives us the ability to use different colors to represent values of variables on actual maps of the world or the United States. A current concern in the United States has to do with the number of people without health insurance. Since this continues to be of great concern, it would be interesting to see if there are geographic patterns to the rate of ininsured adults in the different states.

The data for this example comes from the swivel.com website, and can be downloaded from the class website from http://www.stat.berkeley.edu/classes/s133/data/insurance.csv.

```
> library(maps)
> ins = read.csv('http://www.stat.berkeley.edu/classes/s133/data/insurance.csv',stringsA
> head(ins)
            State Employer Individual Medicaid Medicare Other.Public Uninsured
\begin{tabular}{lrllllll}
1 & Alabama & 0.54 & 0.03 & 0.15 & 0.13 & 0.01 & 0.14 \\
2 & Alaska & 0.52 & 0.04 & 0.16 & 0.06 & 0.05 & 0.17 \\
3 & Arizona & 0.47 & 0.05 & 0.16 & 0.13 & 0.01 & 0.18 \\
4 & Arkansas & 0.47 & 0.06 & 0.15 & 0.14 & 0.02 & 0.17 \\
5 & California & 0.48 & 0.07 & 0.16 & 0.09 & 0.01 & 0.18 \\
6 & Colorado & 0.59 & 0.07 & 0.07 & 0.08 & 0.02 & 0.16
\end{tabular}
```

The first step in preparing a map (after loading the maps library) is determining a variable to use to provide color to the different regions. In this case we'll use the Uninsured variable. Our goal will be to break the data up into four groups, based on the value of the Uninsured variable, and then to color in each state in the map using a color based on the groups.

To create the four groups based on values of Uninsured, we can use the cut function. If we pass cut a variable and a number of groups, it will divide the range of the variable by that number, and assign each variable to one of the groups. Depending on how the variable is distributed, there may be more observations in one group than the other. Alternatively, we can provide cut with a breaks= argument, giving one more value than the number of groups we want, and it will assign the values to groups based on the ranges that the breaks define. Thus, if different values of the variable being used to determine the ranges have special meanings, the grouping can be customized using this argument. A final alternative is to guarantee nearly equal-sized groups by using quantiles of the variable in question as the breaks. The include.lowest=TRUE argument should be included to make sure that the smallest value gets properly classified. To create four equal-sized groups for the Uninsured variable, we could use the following call to cut:

```
> ugroups = cut(ins$Uninsured,quantile(ins$Uninsured,(0:4)/4),include.lowest=TRUE)
> head(ugroups)
```

[1] (0.13,0.17] (0.13,0.17] (0.17,0.24] (0.13,0.17] (0.17,0.24] (0.13,0.17]
Levels: [0.08,0.11] (0.11,0.13] (0.13,0.17] (0.17,0.24]
Notice that cut produces a factor by default; to suppress this, use the labels=FALSE argument. The factor, since it contains information about the actual values, will turn out to be quite useful.

The maps library provides three databases: "world", "state", and "county". For each identifier in the database, there is information on what polygons need to be drawn to create an outline of the area in question. For example, the entry identified by california in the state database would contain the information about California's borders in the form of polygon coordinates which the polygon function will draw when we ask for a map of California. While the help page for the map function implies that we can pass a vector of region names and colors directly to map, things are complicated by the fact that some states can't be plotted by a single polygon, and map gets confused about the proper colors to use when it needs to draw more than one polygon for a state.

One way around the problem is to create multiple entries in a vector of colors for those states that have more than one polygon. To do this, we need to look at the region names stored inside the database. We can get a vector of region names by calling map with the names=TRUE and plot=FALSE arguments:
> map.names $=$ map('state', names=TRUE, plot=FALSE)
The regions which represent multiple polygons for a single state will always contain semicolons:

```
> grep(':',map.names,value=TRUE)
    [1] "massachusetts:martha's vineyard" "massachusetts:main"
    [3] "massachusetts:nantucket" "michigan:north"
    [5] "michigan:south" "new york:manhattan"
    [7] "new york:main" "new york:staten island"
    [9] "new york:long island" "north carolina:knotts"
[11] "north carolina:main" "north carolina:spit"
[13] "virginia:chesapeake" "virginia:chincoteague"
[15] "virginia:main" "washington:san juan island"
[17] "washington:lopez island" "washington:orcas island"
[19] "washington:whidbey island" "washington:main"
```

To properly connect our data with these region names, we first create a vector of state names corresponding to the regions in the data base:
$>$ map.states $=\operatorname{sub}\left({ }^{\prime}\left(\left[{ }^{\wedge}:\right] *\right): . *^{\prime}, \prime \backslash \backslash 1^{\prime}\right.$, map. names $)$
Now we can use the match function to see which observations in the ins dataframe correspond to the regions in the database. Since the database uses all lower case, I'll use the tolower function to convert the state names in the ins data frame to lower case:

```
> which.state = match(map.states,tolower(ins$State))
```

Now that we know how the state names line up with the region names, we can create a vector of colors to properly create our map:

```
> mycolors = c('gray','white','pink','red')
> thecolors = mycolors[ugroups[which.state]]
```

This process is complicated enough that it might be worth making a function to give us the proper vector of groupings. Here's such a function, created by putting together the steps we just followed:

```
mapgroups = function(db,myregions,mygroups,tolower=TRUE){
    map.names = map(db,names=TRUE,plot=FALSE)
    map.regions = gsub('^([^:]*):.*$', \\\1',map.names)
    if(tolower)myregions = tolower(myregions)
    which.region = match(map.regions,myregions)
    mygroups[which.region]
}
```

(I've included the tolower= argument because not all the map databases use lower case.) Using this function (or the step-by-step approach that led to it), we can now make our plot:

```
> mycolors = c('gray','white','pink','red')
> thecolors = mycolors[mapgroups('state',ins$State,ugroups)]
> map('state',col=thecolors,fill=TRUE)
```

Plots like this should always have a legend:

```
> title('Uninsured Rates by State')
> legend('bottomleft',legend=levels(ugroups),fill=mycolors,cex=.8)
```

The map is pictured below.

## Uninsured Rates by State



There are a variety of functions in R which will help us choose colors that will be useful for plotting. Some of the functions you might want to investigate include rainbow, heat.colors, topo.colors, as well as the color.gradient function in the plotrix library, the colorpanel function in the gplots library. and the functions in the RColorBrewer library. Let's look at another example, also from swivel.com, concerning rates of childhood obesity. A copy of the dataset is available on the class website.

```
> obesity = read.csv('http://www.stat.berkeley.edu/classes/s133/data/obesity.csv')
```

Before preceding, it turns out that the state names in this data set have some embedded blanks:

```
> head(as.character(obesity$State))
[1] " Alabama " " Alaska " " Arizona " " Arkansas " " California "
[6] " Colorado "
```

Left uncorrected, this would make our mapgroups function fail to find any matching states in the map data base, and when we plot the map, there would be no colors. If you think you're doing everything right, but there are no colors on the map, check to make sure that the state names are correct.

Naturally fixing something like this is not a problem:

```
> obesity$State = gsub('^ +',',,obesity$State)
> obesity$State = gsub(' +$',',,obesity$State)
```

Now we can proceed with producing the map. We'll use the Childhood.Obesity.Rate variable for the example, and a color scheme generated by the heat.colors function:

```
> mycolors = rev(heat.colors(4))
> ogroups = cut(obesity$Childhood.Obesity.Rate,
+ quantile(obesity$Childhood.Obesity.Rate,(0:4)/4),include.lowest=TRUE)
> thecolors = mycolors[mapgroups('state',obesity$State,ogroups)]
> map('state',col=thecolors,fill=TRUE)
> title('Childhood Obesity Rates by State')
> legend('bottomleft',legend=levels(ogroups),fill=mycolors,cex=.8)
```

The map appears below:

Childhood Obesity Rates by State


As an example of using the county maps, we can use another one of the Community Health data sets, this one concerned with demographics. It's located at http://www.stat.berkeley.edu/classes/s133

The first step is to read the data into $R$. We'll concentrate on the variable Hispanic, which gives the percentage of Hispanics in each county.

```
> demo = read.csv('http://www.stat.berkeley.edu/classes/s133/data/DEMOGRAPHICS.csv')
> summary(demo$Hispanic)
    Min. 1st Qu. Median Mean 3rd Qu. Max.
    0.000 1.100 2.300 7.018 6.300 97.500
```

Next we need to see how the county names are stored in the county map database:

```
> nms = map('county', names=TRUE,plot=FALSE)
> head(nms)
[1] "alabama,autauga" "alabama,baldwin" "alabama,barbour" "alabama,bibb"
[5] "alabama,blount" "alabama,bullock"
```

We need to combine the state and county information in our data set so that it matches up with the format used in the database. We could either call tolower now, or leave it to our mapgroups function:

```
> head(subset(demo,select=c(CHSI_State_Name,CHSI_County_Name)))
    CHSI_State_Name CHSI_County_Name
1 Alabama Autauga
2 Alabama Baldwin
3 Alabama Barbour
4 Alabama Bibb
5 Alabama Blount
6 Alabama Bullock
> thecounties = paste(demo$CHSI_State_Name,demo$CHSI_County_Name,sep=',')
```

Based on the summary information above, we can cut the Hispanic variable at $1,2,5$, and 10 . Then we can create a pallete of blues using the brewer .pal function from the RColorBrewer package.

```
> hgroups = cut(demo$Hispanic,c(0,1,2,5,10,100))
> table(hgroups)
hgroups
    (0,1] (1,2] (2,5] (5,10] (10,100]
        678 770 778 356 558
> library(RColorBrewer)
> mycolors = brewer.pal(5,'Blues')
> thecolors = mycolors[mapgroups('county',thecounties,hgroups)]
> map('county',col=thecolors,fill=TRUE)
> legend('bottomleft',levels(hgroups),fill=mycolors,cex=.8)
> title('Percent Hispanic by County')
```

The cex=. 8 argument reduces the text size to $80 \%$ of the default size, to prevent the legend from running into the map. The map looks like this:

Percent Hispanic by County


In previous examples, we created equal sized groups using the quantile function. Let's see if it will make a difference for this example:

```
> hgroups1 = cut(demo$Hispanic,quantile(demo$Hispanic,(0:5)/5))
> table(hgroups1)
hgroups1
\begin{tabular}{rrrrr}
\((0,1]\) & \((1,1.7]\) & \((1.7,3.2]\) & \((3.2,8.7]\) & \((8.7,97.5]\) \\
678 & 597 & 627 & 618 & 620
\end{tabular}
```

The rest of the steps are the same as before:

```
> mycolors = brewer.pal(5,'Blues')
> thecolors = mycolors[mapgroups('county',thecounties,hgroups1)]
> map('county',col=thecolors,fill=TRUE)
> legend('bottomleft',levels(hgroups1),fill=mycolors,cex=.8)
> title('Percent Hispanic by County')
```

The plot, which is very similar to the previous plot, appears below:

Percent Hispanic by County


As a final example of working with maps, let's revisit the world data set that we've used in other examples. Suppose we want to create a map showing literacy rates around the world. First we need to decide on a grouping. The summary function is useful in helping us decide:

```
> world = read.csv('http://www.stat.berkeley.edu/classes/s133/data/world2.txt',na.string
> summary(world$literacy)
    Min. 1st Qu. Median Mean 3rd Qu. Max.
    12.80 69.10 88.40 80.95 98.50 99.90
```

Let's create four levels: less than 50use cut to create these levels and label them at the same time:
litgroups $=$ cut(world\$literacy, breaks=c $(0,50,70,95,100)$,include.lowest=TRUE,labels=c('<5
We can use the mapgroups function to come up with the correct colors, noticing that the region names in the world database are not in lower case:

```
> mycolors = topo.colors(4)
> litcolors = mycolors[mapgroups('world',world$country,litgroups,tolower=FALSE)]
> map('world',col=litcolors,fill=TRUE)
> title('World Literacy Rates')
> legend('left',legend=levels(litgroups),fill=mycolors,cex=.9)
```

World Literacy Rates


The map appears below
An alternative which is useful when you only want to use part of a database is to eliminate missing values from the vector of colors and the corresponding regions from the full list of regions, and pass those vectors directly to map. Applying this idea to the previous example, we could have gotten the same plot with statements like this:

```
> omit = is.na(litcolors)
> useregions = map('world',names=TRUE,plot=FALSE)[!omit]
> map('world',regions=useregions,col=litcolors[!omit],fill=TRUE)
```


### 4.5 The Lattice Plotting Library

The graphics we've been using up until now are sometimes known as "traditional" graphics in the R community, because they are the basic graphics components that have been part of the $S$ language since its inception. To review, this refers to the high-level functions like plot, hist, barplot, plot, pairs, and boxplot, the low-level functions like points, lines, and legend, and the graphics parameter system accessed through the par function. There's another entire set of graphics tools available through the lattice library. Originally developed as the trellis library, the implementation in R is known as lattice, although the name "trellis" persists in some functions and documentation. All of the functions in the lattice library use the formula interface that we've seen in classification and modeling functions instead of the usual list of $x$ and $y$ values. Along with other useful features unique to each function, all of the lattice functions accept a data= argument, making it convenient to work with dataframes; by specifying the data frame name via this argument, you can refer to the variables in the data frame without the data frame name. They also accept a subset= argument, similar to the second argument to the subset function, to allow selection of only certain cases when you are creating a plot. Finally, the lattice plotting functions can produce what are known as conditioning plots. In a conditioning plot, several graphs, all with common scaling, are presented in a single display. Each of the individual plots is constructed using observations that have a particular value of a variable (known as the conditioning variable), allowing complex relationships to be viewed more easily. To illustrate the idea, let's revisit the income versus literacy graph that we looked at when we first started studying graphics. The lattice equivalent of the traditional plot command is xyplot. This function accepts a plotting formula, and has some nice convenience functions not available in the regular plot command. For example, the groups= argument allows specifying a grouping variable; observations with different levels of this variable will be plotted with different colors. The argumentauto.key=TRUE automatically shows which colors represent which groups. So we could create our graph with the single statement:

```
> library(lattice)
> world = read.csv('http://www.stat.berkeley.edu/classes/s133/data/world2.txt',comment='
> xyplot(income ~ literacy,data=world,groups=cont,auto.key=TRUE)
```

The plot is shown below.


If you wish to finetune the appearance of lattice plots, you can modify most aspects of lattice plots through the command trellis.par.set, and you can display the current values of options with the command trellis.par.get. To explore possible modifications of the trellis (lattice) environment, take a look at the output from

```
> names(trellis.par.get())
```

Any of the listed parameters can be changed through the trellis.par.set() command.
To illustrate the idea of a conditioning plot, let's create a scatter plot like the previous one, but, instead of using color to distinguish among the continents, we'll use the continent as a conditioning variable, resulting in a separate scatter plot for each continent. To use a conditioning variable in any of the lattice commands, follow the formula with a vertical bar (I) and the name of the conditioning variable. To get xyplot to display the value of the conditioning variable, it helps if it's a factor:

```
> world$cont = factor(world$cont)
> xyplot(income ~ literacy | cont,data=world)
```

The plot is shown below:


### 4.6 Customizing the Panel Function

One of the basic concepts of lattice plots is the idea of a panel. Each separate graph that is displayed in a multi-plot lattice graph is known as a panel, and for each of the basic types of lattice plots, there's a function called panel.plottype, where plottype is the type of plot in question. For example, the function that actually produces the individual plots for xyplot is called panel. xyplot. To do something special inside the panels, you can pass your own panel function to the lattice plotting routines using the panel= argument. Generally, the first thing such a function would do is to call the default panel plotting routine; then additional operations can be performed with functions like panel.points, panel.lines, panel.text. (See the help page for panel.functions to see some other possibilities.) For example, in the income versus literacy plot, we might want to show the best regression line that goes through the points for each continent, using the panel.lmline function. Here's how we could construct and call a custom panel function:

```
> mypanel = function(x,y,...){
+ panel.xyplot(x,y,\ldots)
+ panel.lmline(x,y)
+ }
xyplot(income ~ literacy | cont,data=world,panel=mypanel)
```

The plot is shown below.


As another example, consider again the Community Health Data risk and access to care data set. We want to see if there is a relationship between the number of physicians in a state, and the rate of Diabetes in that state. We'll read it in as before, aggregate it, and merge it with the state regions.

```
> risk = read.csv('http://www.stat.berkeley.edu/classes/s133/data/RISKFACTORSANDACCESSTC
> risk[risk==-1111.1] = NA
> avgs = aggregate(risk[,c('Diabetes','Prim_Care_Phys_Rate')],risk['CHSI_State_Name'
],mean,na.rm=TRUE)
> avgs = merge(avgs,data.frame(state.name,region=state.region),by.x='CHSI_State_Name',by
```

Notice that I used the variable number instead of the name in the call to merge. Let's first use color to represent the different regions.

```
> xyplot(Diabetes~Prim_Care_Phys_Rate,groups=region,data=avgs,auto.key=TRUE,main='Diabet
```

Here's the plot:


Alternatively, we could place each region in a separate panel, and display the best fit regression line:

```
> mypanel = function(x,y,...){
+ panel.xyplot(x,y,...)
+ panel.lmline(x,y)
+ }
> xyplot(Diabetes~Prim_Care_Phys_Rate|region,data=avgs,main='Diabetes vs. Physician Rate
```

The plot appears below:


By default, the lattice functions display their panels from bottom to top and left to right, similar to the way points are drawn on a scatterplot. If you'd like the plots to be displaying going from top to bottom, use the as.table=TRUE argument to any of the lattice plotting functions.

The lattice library is actually flexible enough to produce separate plots for each state:

[^0]
## Diabetes vs. Physician Rate by Region



Looking at the plot, we should make some elements of the plot smaller, namely the titles on the strips and the points themselves:

This results in the following plot:


Finally, let's suppose that we want to break up the plots into two pages, each with 25 plots in a $5 \times 5$ arrangement. To get exactly 50 states, we'll use the subset= argument of the lattice functions to remove Alaska (for which there's no data), and the layout= argument to arrange the plots the way we want, and the page= argument to call a function at the end of each page:

```
> xyplot(Diabetes~Prim_Care_Phys_Rate|CHSI_State_Name,data=risk,main='Diabetes vs. Physi
```

You can run this example to see the two pages.
Now that we've seen some of the basics of how the lattice library routines work, we'll take a look at some of the functions that are available. Remember that there are usually similar alternatives available among the traditional graphics functions, so you can think of these as additional choices that are available, and not necessarily the only possibility for producing a particular type of plot.

### 4.7 Univariate Displays

Univariate displays are plots that are concerned with the distribution of a single variable, possibly comparing the distribution among several subsamples of the data. They are especially useful when you are first getting acquainted with a data set, since you may be able to identify outliers or other problems that could get masked by more complex displays or analyses.

### 4.7.1 dotplot

A simple but surprisingly useful display for small to moderate amounts of univariate data is the dotplot. Each observation's value for a variable is plotted as a dot along a line that spans the range of the variable's value. In the usual case, there will be several such lines, one for each level of a grouping variable, making it very easy to spot differences in the variable's distribution for different groups.

To illustrate, we'll use a a data set from a wine recognition experiment where a number of chemical and other measurements were taken on wines from three cultivars. The data is available at http://www.stat.berkeley.edu/classes/s133/data/wine.data; information about the variables is at http://www.stat.berkeley.edu/classes/s133/data/wine.names Suppose we are interested in comparing the alcohol level of wines from the three different cultivars:

```
> wine = read.csv('http://www.stat.berkeley.edu/classes/s133/data/wine.data',header=FALS
> names(wine) = c("Cultivar", "Alcohol", "Malic.acid", "Ash", "Alkalinity.ash",
+ "Magnesium", "Phenols", "Flavanoids", "NF.phenols", "Proanthocyanins",
+ "Color.intensity","Hue","OD.Ratio","Proline")
> wine$Cultivar = factor(wine$Cultivar)
> dotplot(Cultivar~Alcohol,data=wine,ylab='Cultivar')
```

The plot is shown below.


### 4.7.2 bwplot

The bwplot produces box/whisker plots. Unfortunately, notched boxplots are not currently available using bwplot. To create a box/whisker plot of Alcohol for the three cultivars, we can use the same formula we passed to dotplot:
> bwplot(Alcohol~Cultivar, data=wine, xlab='Cultivar', ylab='Alcohol')

The plot is shown below.


For both dotplot and bwplot, if you switch the roles of the variables in the formula, the orientation of the plot will change. In other words, the lines in the dotplot will be displayed vertically instead of horizontally, and the boxplots will be displayed horizontally instead of vertically.

As a second example, consider the literacy rates for the different continents in the world data set. We can compare these rates using the following command:

```
> bwplot(literacy~cont,data=world,main='Literacy Rates by Continent')
```

The plot is shown below

## Literacy Rates by Continent



### 4.7.3 densityplot

As its name implies, this function produces smoothed plots of densities, similar to passing a call to the density function to the plot function. To compare multiple groups, it's best to create a conditioning plot:

```
> densityplot(~Alcohol|Cultivar,data=wine)
```

Notice that, for plots like this, the formula doesn't have a left hand side. The plot is shown below:


As another example of a custom panel function, suppose we wanted to eliminate the points that are plotted near the x -axis and replace them with what is known as a rug a set of tickmarks pointing up from the x -axis that show where the observations were. In practice, many people simply define panel functions like this on the fly. After consulting the help pages for panel.densityplot and panel.rug, we could replace the points with a rug as follows:

```
> densityplot(~Alcohol|Cultivar,data=wine,panel=function(x,...){
+ panel.densityplot(x,plot.points=FALSE)
+ panel.rug(x=x)
+ })
```

Of course, if you find it easier or more convenient to define a custom panel function separate from the call to the plotting function, you can use that method. Here's the result:


## Chapter 5

## Databases, MySQL and SQLite

## 5.1 barchart

A bar chart is like a histogram for categorical data. The barchart function expects its input data frame to already have the numbers of observations for each grouping tabulated. For the simplest case of a single variable with no conditioning variable, you can use a call to table on the right hand side of the tilda to produce a vertical bar chart:

```
> barchart(~}\mathrm{ table(cont),data=world)
```

The plot is shown below.


For more complex barcharts, a data frame containing the counts to be plotted needs to be constructed. This can be done easily using the table in conjunction with as.data.frame. To illustrate, we'll return to the movies data set which has the release dates and box office receipts for some of the all-time most popular movies. Suppose we want to see if the distribution of the day of the week the movies opened on has changed over time. First, we'll read the data and create a grouping variable for different time periods:

```
> movies = read.delim('http://www.stat.berkeley.edu/classes/s133/data/movies.txt',as.is=
> movies$box = as.numeric(sub('\\$','',movies$box))
```

```
> movies$date = as.Date(movies$date,'%B %d, %Y')
> movies$year = as.numeric(format(movies$date,'%Y'))
> movies$weekday = factor(weekdays(movies$date),
+ levels=c('Monday','Tuesday','Wednesday','Thursday','Friday','Saturday','Sunday'
> movies$yrgrp = cut(movies$year,c(1936,1980,1985,1990,1995,2000,2006,2011),
+ labels=c('1937-1979','1980-1984','1985-1990','1991-1995','1996-2000','2001-2006
> counts = as.data.frame(table(yrgrp=movies$yrgrp,weekday=movies$weekday))
> barchart(Freq~}\mp@subsup{}{~}{~
```

The plot is shown below.


If the roles of Freq and weekday were reversed in the previous call to barchart, the bars would be drawn horizontally instead of vertically.

### 5.2 3-D Plots: cloud

The three-dimensional analog of the two-dimensional xyplot in the lattice library is cloud. By using a conditioning variable, cloud can allow us to consider the relationship of four
variables at once. To illustrate, here's conditioning plot showing the relationship among four variables from the wine data frame:
cloud(Alcohol ~ Color.intensity + Malic.acid|cut(Hue, 4), data=wine)
The plot is shown below:


One important point about lattice graphics is that they operate slightly differently from R's traditional graphics. When you type a lattice command at the top level R session, it's R's automatic printing that actually displays the plot. So if you're calling a lattice function in a function or source file, you'll need to surround the call with a call to the print function, or store the result of the lattice plot in a variable, and print that variable.

### 5.3 Spreadsheets

Spreadsheets, in particular the "xls" format used by Microsoft Excel, are one of the most common (if not the most common) methods for transfering data from one organization to
another. When you download or receive a spreadsheet, it's often a good idea to make sure that it really is a spreadsheet. Comma-separated files, which are easily read into spreadsheet programs, are often erroneously labeled "spreadsheets" or "Excel files", and may even have an incorrect extension of ".xls". In addition, Excel spreadsheets are often used to hold largely textual information, so simply finding a spreadsheet that appears to contain data can be misleading. Furthermore, many systems are configured to use a spreadsheet program to automatically open files with an extension of ".csv", further adding to the confusion.

For many years, the only reliable way to read an Excel spreadsheet was with Microsoft Excel, which is only available on Windows and Mac OS computers; users on UNIX were left with no option other than finding a different computer. In the last few years, a number of programs, notably gnumeric and OpenOffice.org (usually available through the ooffice command) have been developed through careful reverse engineering to allow Unix users the ability to work with these files. To insure its advantage in the marketplace, Microsoft doesn't publish a detailed description of exactly how it creates its spreadsheet files. There are often "secret" ways of doing things that are only known to the developers within Microsoft. Reverse engineering means looking at the way a program handles different kinds of files, and then trying to write a program that imitates what the other program does. The end result of all this is that there are several ways to get the data from spreadsheet files into R .

Spreadsheets are organized as a collection of one or more sheets, stored in a single file. Each of the sheets represents a rectangular display of rows and columns, not unlike a data frame. Unfortunately, people often embed text, graphics and pictures into spreadsheets, so it's not a good idea to assume that a spreadsheet has the consistent structure of a data frame or matrix, even if portions of it do appear to have that structure. In addition, spreadsheets often have a large amount of header information (more than just a list of variable names), sometimes making it challenging to figure out the correct variable names to use for the different columns in the spreadsheet.

Our main concern will be in getting the information from the spreadsheet into R: we won't look at how to work with data within Excel.

If you are simply working with a single Excel spreadsheet, the easiest way to get it into $R$ is to open the spreadsheet with any compatible program, go to the File menu, and select Save As. When the file selector dialog appears, notice that you will be given an option of different file format choices, usually through a drop down menu. Choose something like "Tab delimited text", or "CSV (Comma separated values)". If any of the fields in the spreadsheet contain commas, tab delimited is a better choice, but generally it doesn't matter which one you use. Now, the file is (more or less) ready to be read into R, using read.csv or read.delim. A very common occurence is for fields stored in a spreadsheet to contain either single or double quotes, in which case the quote= argument can be used to make sure R understands what you want. Spreadsheets often arrange their data so that there are a different number of valid entries on different lines, which will confuse read.table; the fill= argument may be of use in these cases. Finally, as mentioned previously, there are often multiple descriptive lines of text at the top of a spreadsheet, so some experimentation with the skip= argument to read.table may be necessary. Alternatively, you can simply delete those lines from the file
into which you save the tab- or comma-delimited data.

As you can see, this is a somewhat time-consuming process which needs to be customized for each spreadsheet. It's further complicated by the fact that it only handles one sheet of a multi-sheet spreadsheet; in those cases the process would need to be repeated for each sheet. If you need to read a number of spreadsheets, especially ones where you need to access the data from more than one sheet, you need to use a more programmable solution.

R provides several methods to read spreadsheets without having to save them as tabor comma-delimited files. The first is the read.xls function in the gdata library. This function uses a Perl program (included as part of the library), that converts the spreadsheet to a comma-separated file, and then uses read.csv to convert it to a data frame. In order for this library to work, perl must also be installed on the computer that's running R. perl will be installed on virtually any Unix-based computer (including Mac OSX), but will most likely not be on most Windows computers (although once perl is installed on a Windows system, the read.xls function will work with no problems). However there is a Windowsonly package, xlsReadWrite, available from CRAN which can both read and write Excel files. (On other platforms, the dataframes2xls package provides a write.xls function.)

Another method utilizes a facility known as ODBC (Open DataBase Connectivity), which is a method that allows different programs that handle data to communicate with each other. The ODBC interface uses a query language known as SQL, which we'll study later, so for now I'll just describe the use of read.xls. (Remember, for just one or two data tables from a spreadsheet, saving as a tab- or comma-delimited file and using the correct read.table variant will usually be the easiest route. )

Since read.xls does nothing more than convert the spreadsheet to comma-separated form and then call read.csv, the guidelines for using it are very similar to the normal use of read.csv. The most useful feature of read.xls is that it accepts an optional sheet= argument, allowing multiple sheets from a spreadsheet file to be automatically read.

As a simple example, consider a spreadsheet with listings for the top 200 educational institutions in the US with respect to the number of postdoctoral students, which I found at http://mup.asu.edu/Top200-III/2_2005_top200_postdoc.xls

Here's a view of how the data looks in the UNIX gnumeric spreadsheet:


Here are the first few lines of the file created when I use File- ¿Save As, and choose the CSV format:

```
"The Top 200 Institutions--Postdoctoral Appointees
(2005)",,,, ,
,,,,,
"Top 50 Institutions
in Postdoctoral Appointees
(2005)","Number of Postdocs","National Rank","Control Rank",,"Institutional
Control"
"Harvard University",4384,1,1,,Private
"Johns Hopkins University",1442,2,2,,Private
"Stanford University",1259,3,3,,Private
"University of California - Los Angeles",1094,4,1,,Public
"Yale University",1012,5,4,,Private
"University of California - San Francisco",1003,6,2, ,Public
"University of Washington - Seattle",963,7,3,,Public
"University of California - San Diego",886,8,4,,Public
"Massachusetts Institute of Technology",851,9,5,,Private
"University of Pennsylvania",815,10,6,,Private
"Columbia University",793,11,7,,Private
"University of California - Berkeley",774,12,5,,Public
```

While the data itself looks fine, it's unlikely that the header information will be of much use. Since there are 7 header lines, I could use the following statements to read the data into R:

```
> fromcsv = read.csv('2_2005_top200_postdoc.csv',header=FALSE,skip=7,stringsAsFactors=FA
> dim(fromcsv)
[1] 206 6
> head(fromcsv)
```

    V1 V2 V3 V4 V5 V6
    1 Harvard University 43841 NA Private
$2 \quad$ Johns Hopkins University 144222 NA Private
3
4 University of California - Los Angeles 109441 NA Public
5 Yale University 101254 NA Private
6 University of California - San Francisco 100362 NA Public

The fifth column can be removed (take a look at the spreadsheet to see why), and we should supply some names to the spreadsheet. One problem with this spreadsheet is that it repeats its header information several times part way through the spreadsheet. These lines will have to be removed manually. The can be identified by the fact that the sixth variable should be either Public or Private, and could be eliminated as follows:

```
> fromcsv = fromcsv[fromcsv$V6 %in% c('Public','Private'),]
```

The fifth variable can be removed by setting it to NULL, and the columns can be named.

```
> fromcsv$V5 = NULL
> names(fromcsv) = c('Institution','NPostdocs','Rank','ControlRank','Control')
```

Finally, a check of the columns shows that, because of the header problem, the numeric variables explicitly need to be converted:

```
> sapply(fromcsv,class)
Institution NPostdocs Rank ControlRank Control
"character" "character" "character" "character" "character"
> fromcsv[,c(2,3,4)] = sapply(fromcsv[,c(2,3,4)],as.numeric)
```

A similar procedure could be carried out with read.xls, although it might take some experimentation with skip= to make things work properly. The only other difference between read.xls and read.csv for this example is that a space mysteriously appeared at the end of one of the variables when using read.xls:

```
library(gdata)
fromreadxls = read.xls('2_2005_top200_postdoc.xls',stringsAsFactors=FALSE,header=FALSE,
fromreadxls = fromreadxls[-1,-c(1,6)]
fromreadxls$V7 = sub(' $','',fromreadxls$V7)
fromreadxls = fromreadxls[fromreadxls$V7 %in% c('Public','Private'),]
fromreadxls[,c(2,3,4)] = sapply(fromreadxls[,c(2,3,4)],as.numeric)
names(fromreadxls) = c('Institution','NPostdocs','Rank','ControlRank','Control')
```


### 5.4 Writing Spreadsheets

As with reading a spreadsheet, one option for writing a spreadsheet is to write out a commaor tab-separated file, and to use a spreadsheet program to read it and then save it as a ".xls" file. The write.csv, and write.table functions are useful in this regard. For example, we could create a comma-seperated version of the world data frame as follows:

```
> write.csv(world,file='world.csv')
```



Here's the result of reading the csv file with a spreadsheet program:
The File->Save As menu would allow saving the spreadsheet in an appropriate format.
To automate the process of writing spreadsheets, the Windows-only xlsReadWrite package provides a write.xls function; for other operating systems, this function is provided by the dataframe2xls package.

### 5.5 Databases

A database is a collection of data, usually with some information (sometimes called metadata) about how the data is organized. But many times when people refer to a database, they mean a database server, which is similar to a web server, but responds to requests for data instead of web pages.

By far the most common type of database server is known a a relational database management system (RDBMS), and the most common way of communicating with such a database is a language known as SQL, which is an acronym for Structured Query Language. Some examples of database systems that use SQL to communicate with an RDBMS include Oracle, Sybase, Microsoft SQL Server, SQLite, MySQL and Postgres. While there is an SQL standard, each database manufacturer provides some additional features, so SQL that works with one database is not guaranteed to work on another. We'll try to stick to aspects of SQL that should be available on most SQL based systems.

A Database consists of one or more tables, which are generally stored as files on the computer that's running the DBMS. A table is a rectangular array, where each row represents an observation, and each column represents a variable. Most databases consists of several tables, each containing information about one aspect of the data. For example, consider a database to hold information about the parts needed to build a variety of different products. One way to store the information would be to have a data table that had the part id, its description, the supplier's name, and the cost of the part. An immediate problem with this is scheme concerns how we could store information about the relation between products and parts. Furthermore, if one supplier provided many different parts, redundant information about suppliers would be repeated many times in the data table. In the 1970s when database technology was first being developed, disk and memory space were limited and expensive, and organizing data in this way was not very efficient, especially as the size of the data base increased. In the late 1970s, the idea of a relational database was developed by IBM, with the first commercial offering coming from a company which is now known as Oracle. Relational database design is governed by a principle known as normalization. While entire books are devoted to the subject, the basic idea of normalization is to try and remove redundancy as much as possible when creating the tables that make up a data base. Continuing the parts example, a properly normalized database to hold the parts information would consist of four tables. The first would contain a part id to uniquely identify the part, its description, price and an id to identify the supplier. A second table would contain the supplier codes and any other information about the supplier. A third table would contain product ids and descriptions, while the final table would have one record for each part used in each product, stored as pairs of product id and part id. The variables that link together the different databases are refered to as keys, or sometimes foreign keys. Clearly, making sure that there are keys to link information from one table to another is critical to the idea of a normalized data base. This allows large amounts of information to be stored in manageably sized tables which can be modified and updated without having to change all of the information in all of the tables. Such tables will be efficient in the amount of disk and memory resources that they need, which was critical at the time such databases were developed. Also critical to this scheme is a fast and efficient way of joining together these tables so that queries like "Which suppliers are used for product xyz?" or "What parts from Acme Machine Works cost between $\$ 2$ and $\$ 4$ " or "What is the total cost of the parts needed to make product xyz?". In fact, for many years the only programs that were capable of combining data from multiple sources were RDBMSs.

We're going to look at the way the SQL language is used to extract information from RDBMSs, specifically the open source SQLite data base (http://sqlite.org) (which doesn't require a database server), and the open source MySQL data base (http://www.mysql.com) which does. In addition we'll see how to do typical database operations in R, and how to access a database using SQL from inside of R.

One of the first questions that arises when thinking about databases is "When should I use a database?" There are several cases where a database makes sense:

1. The only source for the data you need may be an existing database.
2. The data you're working with changes on a regular basis, especially if it can potentially be changed by many people. Database servers (like most other servers) provide concurrency, which takes care of problems that might otherwise arise if more than one person tries to access or modify a database at the same time.
3. Your data is simply too big to fit into the computer's memory, but if you could conveniently extract just the parts you need, you'd be able to work with the data. For example, you may have hundreds of variables, but only need to work with a small number at at time, or you have tens of thousands of observations, but only need to work with a few thousand at a time.

One of the most important uses of databases in the last ten years has been as back ends to dynamic web sites. If you've ever placed an order online, joined an online discussion community, or gotten a username/password combination to access web resources, you've most likely interacted with a database. In addition both the Firefox and Safari browsers us SQLite databases to store cookies, certificates, and other information.

There are actually three parts to a RDBMS system: data definition, data access, and privelege management. We're only going to look at the data access aspect of databases; we'll assume that a database is already available, and that the administrator of the database has provided you with access to the resources you need. You can communicate with a database in at least three different ways:

1. You can use a command line program that will display its results in a way similar to the way R works: you type in a query, and the results are displayed.
2. You can use a graphical interface (GUI) that will display the results and give you the option to export them in different forms, such as a comma-separated data file. One advantage to these clients is that they usually provide a display of the available databases, along with the names of the tables in the database and the names of the columns within the tables.
3. You can use a library within $R$ to query the database and return the results of the query into an R data frame. For use with MySQL library, the RMySQL library is available for download from CRAN; for SQLite, the RSQLite package is available. When you install either, the DBI library, which provides a consistent interface to different databases, will also be installed.

It's very important to understand that SQL is not a programming language - it's said to be a declarative language. Instead of solving problems by writing a series of instructions or putting together programming statements into functions, with SQL you write a single statement (query) that will return some or all of the records from a database. SQL was designed to be easy to use for non-programmers, allowing them to present queries to the database in a language that is more similar to a spoken language than a programming language. The main tool for data access is the select statement. Since everything needs to be done with this single statement, descriptions of its syntax can be quite daunting.

For example, here's an example that shows some of the important features of the select statement:

```
SELECT columns or computations
    FROM table
    WHERE condition
    GROUP BY columns
    HAVING condition
    ORDER BY column [ASC | DESC]
    LIMIT offset,count;
```

(The keywords in the above statement can be typed in upper or lower case, but I'll generally use upper case to remind us that they are keywords.) MySQL is case sensistive to table and column names, but not for commands. SQLite is not case sensitive at all. SQL statements always end with a semi-colon, but graphical clients and interfaces in other languages sometimes don't require the semi-colon. Fortunately, you rarely need to use all of these commands in a single query. In fact, you may be able to get by knowing just the command that returns all of the information from a table in a database:

```
SELECT * from table;
```


### 5.6 Working with Databases

When you're not using a graphical interface, it's easy to get lost in a database considering that each database can hold multiple tables, and each table can have multiple columns. Three commands that are useful in finding your way around a database are:

| MySQL | SQLite |
| :--- | :--- |
| SHOW DATABASES; | . databases |
| SHOW TABLES IN database; | .tables |
| SHOW COLUMNS IN table; | pragma table_info(table) |
| DESCRIBE table; | .schema table |

For use as an example, consider a database to keep track of a music collection, stored as an SQLite database in the file albums.db. We can use the commands just shown to see how the database is organized. Here, I'm using the UNIX command-line client called sqlite3:

```
springer.spector$ sqlite3 albums.db
SQLite version 3.4.2
Enter ".help" for instructions
sqlite> .mode column
sqlite> .header on
sqlite> .tables
Album Artist Track
sqlite> .schema Album
CREATE TABLE Album
```

```
( alid INTEGER,
aid REAL,
title TEXT
);
CREATE INDEX jj on Album(alid);
sqlite> .schema Artist
CREATE TABLE Artist
( aid REAL,
name TEXT
);
CREATE INDEX ii on Artist(aid);
sqlite> .schema Track
CREATE TABLE Track
( alid INTEGER,
aid REAL,
title TEXT,
filesize INTEGER,
bitrate REAL,
length INTEGER
);
```

Studying these tables we can see that the organization is as follows: each track in the Track table is identified by an artist id (aid) and an album id (alid). To get the actual names of the artists, we can link to the Artist database through the aid key; to get the names of the albums, we can link to the Album table through the alid key. These keys are integers, which don't take up very much space; the actual text of the album title or artist's name is stored only once in the table devoted to that purpose. (This is the basic principle of normalization that drives database design.) The first thing to notice in schemes like this is that the individual tables won't allow us to really see anything iteresting, since they just contain keys, not actual values; to get interesting information, we need to join together multiple tables. For example, let's say we want a list of album titles and artist names. We want to extract the Name from the Artist table and combine it with Title from the Album table, based on a matching value of the aid variable:

```
sqlite> .width 25 50
sqlite> SELECT Artist.name, Album.title FROM Artist, Album WHERE Artist.aid = Album.aid;
name title
-------------------------
Tubby Hayes Orchestra 100% Proof
Jimmy McGriff 100% Pure Funk
Jimmy McGriff A Bag Full Of Blues
Jimmy McGriff A Bag Full Of Soul
Jimmy McGriff Cherry
Jimmy McGriff Countdown
```

```
Jimmy McGriff Electric Funk
Jimmy McGriff I've Got A New Woman
```

Queries like this are surprisingly fast - they are exactly what the database has been designed and optimized to acheive.

There are a few conveniences that you can use in SQL to save typing and improve the appearance of the output. You can use the AS keyword to provide an alternative name for a database for use within a query, or to rename a column so that it will display with a different heading. The previous query could have been written:

```
sqlite> SELECT ar.name AS Artist, al.title AS 'Album Name'
    ...> FROM Artist AS ar, Album AS al
    ...> WHERE ar.aid = al.aid LIMIT 200,10;
Artist Album Name
------------------------- --------------------------------------------------------
Dizzy Gillespie 1945-1950 Small Groups
Dizzy Gillespie Absolutely The Best Dizzy Gillespie
Dizzy Gillespie A Musical Safari
Dizzy Gillespie Dizzys Big 4
Dizzy Gillespie Gene Norman Presents Dizzy Gillespie and His Big B
Dizzy Gillespie Have Trumpet, Will Exite!
Dizzy Gillespie In Paris
Dizzy Gillespie It Don't Mean A Thing
Dizzy Gillespie It Happened One Night
Dizzy Gillespie New Wave
```

Note the new headings that appear in the output. The LIMIT keyword allows you to display just some of the results. Given a single number, it prints that many lines starting from the beginning; given two numbers it starts at the first number and prints as many records as specified in the second number. Combining two data sets in this way is a very common operation, known as an inner join. An alternative way of expressing the query we're looking at would be as follows:

```
SELECT ar.name AS Artist, al.title AS 'Album Name'
        FROM Artist AS ar inner join Album AS al
        using(aid);
```

When the two tables being joined share exactly one common column (key), the operation is sometimes known as a natural join. Since this is the case with the Album and Artist tables, yet another way to express the query is

SELECT ar.name AS Artist, al.title AS 'Album Name' FROM Artist AS ar natural join Album AS al;

Note that if the key used to join two tables does not have the same name in each of the tables, you must use the previous method that specifies the matching condition in the WHERE clause.

SQL provides some convenient facilities for aggregating values based on counts, sums, averages and minimums and maximums, through the COUNT, SUM, AVG, MIN and MAX functions. To find the number of records that match a certain condition, the expression COUNT (*) can be used. For example, to find the number of observations in the Track data set, we could use:

```
sqlite> SELECT COUNT(*) from Track;
```

49337
To count how many tracks were longer than 1000, we could use

```
sqlite> SELECT COUNT(*) from Track WHERE length > 1000;
160
```

To find the track with the longest length in the Track table, we could try:

```
sqlite> SELECT MAX(length) from Track;
MAX(length)
8754
```

This gives us the length of the maximum track, but not its title. The easiest way to get around this is to use a subquery. In SQL, a subquery is a SELECT statement surrounded by parentheses. You can use the values returned by the subquery in WHERE or HAVING clauses. So to find the track with the maximum length, we could use

```
sqlite> SELECT title,length FROM Track WHERE length = (SELECT max(length) FROM Track);
title length
------------------------- ------------------------------------------------------------
The Governor 8754
```

Of course, this query would be more useful if we knew the name of the album and artist that the track came from:

```
sqlite> .width 20 25 25 5
sqlite> SELECT tr.title,al.title,ar.name,tr.length
    ...> FROM Track as tr, Album as al, Artist as ar
    ...> WHERE tr.alid = al.alid and tr.aid = al.aid and ar.aid = al.aid
    ...> AND length = (SELECT max(length) FROM Track);
title title name lengt
-------------------- ------------------------ ---------------------------------
The Governor What You Hear Is What You Melvin Sparks Band 8754
```

When you construct queries like this, it's extremely important to list all of the WHERE conditions that need to be satisfied to avoid getting meaningless duplicate records.

As another example of a subquery, suppose we want to count how many albums we have for each artist, and then tabulate how many artists there are with one album, two albums, three albums, and so on. The first part is fairly easy:

```
sqlite> SELECT aid,count(aid) FROM Album GROUP BY aid limit 100;
aid count(aid)
---------------------
2.0 1
3.0 1
4.0 1
```

We can use this result as a subquery to see the distribution of albums per artist:

```
mysql> SELECT ct,count(ct) FROM
    -> (SELECT aid,count(aid) AS ct FROM Album GROUP BY aid)
    -> GROUP by ct ORDER by ct;
ct count(ct)
1 2061
2 291
3 123
4 61
5 48
6 35
7 27
```

When using subqueries in this way, some databases may require that the subquery is given an alias. In such a case, a query like the following could be used:

```
SELECT ct,count(ct) FROM
    (SELECT aid,count(aid) AS ct FROM Album GROUP BY aid) AS x
    GROUP by ct ORDER by ct;
```


### 5.7 Using SQL for Aggregation

One of the most useful features of SQL is that it can summarize large data sets, producing a smaller result set that can be more easily handled by other programs. For example, suppose we are interested in the total length (in seconds) of the tracks on each album. Instead of processing all the tracks outside of the database, we can create a summarized version of the database that has the lengths already summarized. Very few programs can operate on databases as fast as SQL, so operations like this can save lots of processing time. To perform operations like this we can use the GROUP BY clause:

```
sqlite> SELECT alid,SUM(length) AS TotalTime FROM Track GROUP BY alid limit 50;
alid TotalTime
-------------------- ----------------------------
1 2303
2 2092
3 3563
4 2532
5 2501
6 3956
7 2796
8 2344
9 3254
10 4245
```

Once again, the results would probably be more useful with the title of the album and the artist included. In this example, we can also sort them by the total time of the album:


In this particular example, instead of processing the 49000 or so tracks outside of SQL, we've reduced what we have to work with to around 5000 records, which could make the overall processing much faster. Exactly which aggregation functions will be available depends on the database you're using.

For things like partial matching of strings, all flavors of SQL provide the LIKE operator, which allows limited wildcard matching. With the LIKE operator the percent sign (\%) stands for 0 or more characters, and the underscore (_) stands for exactly one. Many modern databases (MySQL included) provide the RLIKE operator, which uses regular expressions. For the remainder of these examples, we'll use the MySQL database running on springer.berkeley.edu. We'll write a regular expression to find all the artists who have exactly three words in their names.

```
springer.spector$ mysql -u stat133 -p albums
Enter password:
Reading table information for completion of table and column names
You can turn off this feature to get a quicker startup with -A
Welcome to the MySQL monitor. Commands end with ; or \g.
Your MySQL connection id is 11
Server version: 5.0.51a-3ubuntu5.4-log (Ubuntu)
Type 'help;' or '\h' for help. Type '\c' to clear the buffer.
mysql> SELECT name FROM Artist
    -> WHERE name RLIKE , [A-Za-z]+ [A-Za-z]+ [A-Za-z]+$';
+----------------------------------+
| name |
+-------------------------------------
| Tubby Hayes Orchestra
| Pepper Adams Quintet
| Henry Red Allen
| Lovie Austin Serenaders |
| Mary Lou Williams
| Spirits of Rhythm
| Hot Lips Page
| Nat King Cole
| John Handy III
```

Note that in order to access the MySQL database, a username and password needed to be used.

If you look at the original definition of the SELECT statement, you'll notice the HAVING clause which we have not yet covered. The basic difference between HAVING and WHERE is that, due to the timing of operations in the database, we can't use computed variables (like

SUM and AVG) in the WHERE clause, but you can in the HAVING clause. Suppose we wanted to find the artists for which there were more than five albums in the database. A first try might be as follows:

```
mysql > SELECT aid,COUNT(aid) as count FROM Album
    -> GROUP BY aid
    -> WHERE count > 5;
ERROR 1064 (42000): You have an error in your SQL syntax; check the manual that correspo
```

MySQL incorrectly reports this as a syntax error, when the real problem is that we're trying to access a computed variable (count) in a WHERE clause instead of a HAVING clause:

```
mysql> SELECT aid,COUNT(aid) as count FROM Album
    -> GROUP BY aid
    -> HAVING count > 5;
+------+-------+
| aid | count |
+------+-------+
| 11 | 6 |
| 17 | 7 |
| 28 | 6 |
| 44 | 8 |
| 81 | 6 |
```

Of course, queries like this are infinitely more useful if the bring in the relevant information from other tables:

```
mysql> SELECT ar.name as Artist,COUNT(al.alid) AS count
    -> FROM Artist as ar, Album as al
    -> WHERE ar.aid = al.aid
    -> GROUP BY al.aid HAVING count > 5;
\begin{tabular}{|c|c|}
\hline Artist & count \\
\hline Abdullah Ibrahim & 6 \\
\hline Ahmad Jamal & 7 \\
\hline Al Cohn & 6 \\
\hline Al Haig & 8 \\
\hline Anita O'Day & 6 \\
\hline Archie Shepp & 6 \\
\hline
\end{tabular}
```


### 5.8 Accessing databases in $\mathbf{R}$

To provide consistent access to different databases, R uses an intermediate layer of communication known as the DBI (Data Base Interface) library. As we've seen before, different commands are necessary to get information about different databases, so the DBI layer provides a set of routines that will work identically for all databases. Some of these routines are described in the following table.

| dbConnect | connect to a database |
| :--- | :--- |
| dbDisconnect | close the connection to a database |
| dbExistsTable | returns TRUE or FALSE |
| dbGetQuery | send a query to the database and get the results |
| dbListTables | shows all the tables in a database |
| dbListFields | shows the names of columns in a database |
| dbSendQuery | send a query to the database and use fetch to get results |
| dbWriteTable | stores a data frame in a database |

To let the DBI layer know what type of database you are using, you pass a string (like 'MySQL' or 'SQLite') to the dbDriver function. This will return an object which can be passed to dbConnect to make a connection to the database. dbConnect returns a connection object which is passed to all the other routines so that they can communicate with the database you are using.

For example, to connect to the albums SQLite database, we'd use the following statements:

```
drv = dbDriver('SQLite')
con = dbConnect(drv,db='albums.db')
```

Since SQLite doesn't require a database server, you can easily create SQLite databases using dbWriteTable. For very large data sets, you can process the data in chunks, using the append= option of dbWriteTable.

To use MySQL, you must have a valid username and password. For the MySQL database running on springer.berkeley.edu, you'd need to use the following statements:

```
drv = dbDriver('MySQL')
con = dbConnect(drv,dbname='albums',user='stat133',pass='T0pSecr3t')
```

If you're using an SCF machine, you'd need to specify a hostname (springer) when connecting; for non-SCF machines, you would set up an SSH tunnel and use a hostname of '127.0.0.1'.

Once you get the connection object from dbConnect you can use it repeatedly to make as many queries as you need, and the functions you use are the same, regardless of the nature of the underlying database.

It's up to you to decide how much of the work you want to do through the database, and how much you'll do in R. For example, suppose we want to find albums in the albums database whose total time (sum of the length variable in the Track table) is between 2400 and 2700 seconds, displayed in descending order of total time.

One approach (after loading the library and making the connection to the database) would be to do all the work in the database. Notice that this may be your only option if the database you're dealing with is too large to fit into $R$.

```
> albums = dbGetQuery(con,statement='SELECT al.title,ar.name,SUM(tr.length) AS tot\
+ FROM Album AS al,Artist AS ar,Track AS tr\
+ WHERE tr.alid = al.alid AND tr.aid = ar.aid AND tr.aid
+ GROUP BY tr.alid\
+ HAVING tot BETWEEN 2400 AND 2700 ORDER BY tot DESC')
> head(albums)
```



Note the use of a single backslash at the end of each line of input to allow typing the query over multiple lines. Alternatively, the entire query could be passed as one long string. The dbGetQuery function gets the results of the query and puts them into a data frame, in this case called albums.

At the other end of the extreme, you could read in the entire database and work with it entirely in R. This may not be the wisest approach, because if the database is too large, you may have problems. Working with the data in this way, however will allow us to see the $R$ equivalent of some of the database operations we've been studying. Once again, I'm assuming that the RMySQL library has been loaded, and a connection object has been obtained through a call to dbConnect.

```
> album = dbGetQuery(con,statement="select * from Album")
> track = dbGetQuery(con,statement="select * from Track")
> artist = dbGetQuery(con,statement="select * from Artist")
```

We now have three data frames in R corresponding to the three data tables in the database. In $R$, the equivalent of an inner join can be carried out with the merge function. You provide merge with the data frames you wish to join, and a character string or vector of character strings with the name(s) of the variables that you wish to join them by. In database terminology, these names are the keys for the join. The merge function will only accept two data frames, but it can be called repeatedly in case there are more than two data frames that need to be merged.

If there are variables with the same name (other than the keys) in the two data frames to be merged, merge will rename them by adding either . x or . y to the end of the name to tell you which data frame that variable came from. An often easier approach is to rename
variables before merging so that all the names (other than the keys) will be unique. In the current example, the variable title is in both the album data frame and the track data frame. Let's rename the title variable in the album data frame to albumname:

```
> names(album)
[1] "alid" "aid" "title" "year"
> names(album)[3] = 'albumname'
```

Now we can merge the album data frame with the artist data frame using aid as a key, and then merge the track data frame with the album data frame using alid as a key.

```
> album = merge(album,artist,by='aid')
> track = merge(track,album,by='alid')
> head(track)
\begin{tabular}{lrcccrrrr} 
& ald & aid.x \\
1 & 1 & 812 & Nice Work If You Can Get It & 4948 & 256 & 158 & 812 \\
2 & 1 & 812 & Makin' Whoopee & 5870 & 256 & 187 & 812 \\
3 & 1 & 812 & People Will Say We're In Love & 6020 & 256 & 192 & 812 \\
4 & 1 & 812 & Baby, What Else Can I Do & 7220 & 256 & 231 & 812 \\
5 & 1 & 812 & I'm Glad There Is You & 5946 & 256 & 190 & 812 \\
6 & 1 & 812 & My Heart Belongs To Daddy & 4998 & 256 & 160 & 812
\end{tabular}
1 Songs In A Mellow Mood Ella Fitzgerald
2 Songs In A Mellow Mood Ella Fitzgerald
3 Songs In A Mellow Mood Ella Fitzgerald
4 Songs In A Mellow Mood Ella Fitzgerald
5 Songs In A Mellow Mood Ella Fitzgerald
6 \text { Songs In A Mellow Mood Ella Fitzgerald}
```

To calculate the total length of tracks, we only need the album and artist names along with the length of each track:

```
> track = track[,c('albumname','name','length')]
```

The rest of the processing is pretty straightforward now that everything is in R:

```
> tot = aggregate(track$length,list(albumname=track$albumname,artist=track$name),sum)
```

The previous command would be very slow, because aggregate considers all possible combinations of albumname and artist, which is very inefficient for data like this. An alternative is to form a single grouping variable and then to break off the artist and album names after aggregation:

```
> track$albart = paste(track$albumname,track$name,sep='\t')
> tot = aggregate(track$length,track['albart'],sum)
> aa = strsplit(tot$albart,'\t')
```

```
> tot$album = sapply(aa,'[',1)
> tot$artist= sapply(aa,'[',2)
> tot$albart = NULL
> use = tot[tot$x > 2400 & tot$x <= 2700,]
> use = use[order(use$x,decreasing=TRUE),]
> head(use)
```

x
19962700
48462700
7182699
32392699
16092698 Gerard Pochonet et son Quartette
31462698
album
I Need Some Money We'll Be Together Again

Pinky \& Zoot

Out Front!

Blues Groove Tiny Grimes \& Coleman Hawkins
artist
Eddie Harris
Joe Pass a J. J. Johnson

Pinky Winters
Lucky Thompson
Jaki Byard

## Chapter 6

## Cluster Analysis

### 6.1 Database Tables and Factors

A different approach illustrates the relationship between factors and the principles of normalization. Since a factor stores each of its levels only once, normalized tables can often be used to form factors in R. Once again, let's assume that we've loaded the RMySQL library and obtained a connection object. This time, I'll trim off the unneeded variables from the track data frame before processing:

```
> album = dbGetQuery(con,statement="select * from Album")
> track = dbGetQuery(con,statement="select * from Track")
> artist = dbGetQuery(con,statement="select * from Artist")
> track = track[,c('aid','alid','length')]
> names(track) = c('artist','album','length')
> track$artist = factor(track$artist,levels=artist$aid,labels=artist$name)
> track$album = factor(track$album,levels=album$alid,labels=album$title)
```

The tables formed in the process of normalizing the database essentially contain the levels and labels of a factor variable in R. Processing the data set is the same as in the previous example:

```
> track$albart = paste(track$album,track$artist,sep='\t')
> tot = aggregate(track$length,track['albart'],sum)
> aa = strsplit(tot$albart,'\t')
> tot$album = sapply(aa,'[',1)
> tot$artist = sapply(aa,'[',2)
> tot$albart = NULL
> use = tot[tot$x > 2400 & tot$x <= 2700,]
> use = use[order(use$x,decreasing=TRUE),]
> head(use)
```



In practice, the most useful solutions would probably fall in between the extreme of doing everything on the database and doing everything in R .

### 6.2 Using SQL in R

If you like using SQL, or you see a handy way to get something done using SQL, you can use the sqldf package to operate on $R$ data frames using SQL. When you pass a query to
the sqldf function, it will identify the data frames involved in the query, create a temporary SQLite database, perform the query, and return the results. For example, consider the task of merging two data frames, based on the value of a variable id:

```
> data1 = data.frame(id=c(1,4,2,3,5),x=c(7,12,19,15,9))
> data2 = data.frame(id=c(2,3,4,1,5),y=c(21,32,29,35,19))
> sqldf('select * from data1 natural join data2')
    id x y
1}1073
2 4 12 29
3}22192
4 3 15 32
5
```


### 6.3 Reading Spreadsheets with the RODBC Library

Now that we've got the basics of SQL down, we can look at a third option for reading spreadsheets into R, the RODBC library. Note that this functionality is only available on Windows and you don't need a copy of Excel on your computer in order for it to work. The ODBC interface provides access to spreadsheets using SQL as a query language. Here's a sample session showing how we could read the spreadsheet from the previous example using RODBC:

```
> library(RODBC)
> con = odbcConnectExcel('2_2000_top200_postdoc.xls')
> tbls = sqlTables(con)
> tbls
tbls
TABLE_CAT TABLE_SCHEM
1 C:\\cygwin\\home\\spector\\2_2000_top200_postdoc <NA>
2 C: \\cygwin\\home\\spector \(\backslash \backslash 2 \_2000 \_\)top200_postdoc <NA>
TABLE_NAME TABLE_TYPE REMARKS
1 'Postdocs -Top 200 \$' TABLE <NA>
2 'Postdocs -Top 200 \$'Print_Titles TABLE <NA>
> qry = paste('select * from ', '[',tbls\$TABLE_NAME[1],']', sep='')
> postdocs = sqlQuery(con,qry,stringsAsFactors=FALSE)
\(>\) head(postdocs)
F1 The Top 200 Institutions--Postdoctoral Appointees_(2005) F3 F4 F5 F6
1 NA <NA> NA NA NA NA
2 NA Top 50 Institutions \(\backslash\) nin Postdoctoral Appointees \(\backslash n(2005)\) NA NA NA NA
3 NA Harvard University 438411 NA
4 NA Johns Hopkins University 144222 NA
5 NA Stanford University 12593 NA
```

```
6 ~ N A
                                    University of California - Los Angeles 1094 4 1 NA
> postdocs = postdocs[3:nrow(postdocs),c(2,3,4,5,7)]
> postdocs = postdocs[postdocs$F7 %in% c('Public','Private'),]
> dim(postdocs)
[1] 203 5
> sapply(postdocs,class)
The Top 200 Institutions--Postdoctoral Appointees_(2005)
                                    "character"
                                    F3
                            "numeric"
                                    F4
                            "numeric"
                                    F5
                                    "numeric"
                                    F7
                            "character"
> names(postdocs) = c('Institution','NPostdocs','Rank','ControlRank','Control')
```

The RODBC interface was able to correctly classify the numeric columns.

### 6.4 Introduction to Cluster Analysis

While we often think of statistics as giving definitive answers to well-posed questions, there are some statistical techniques that are used simply to gain further insight into a group of observations. One such technique (which encompasses lots of different methods) is cluster analysis. The idea of cluster analysis is that we have a set of observations, on which we have available several measurements. Using these measurements, we want to find out if the observations naturally group together in some predictable way. For example, we may have recorded physical measurements on many animals, and we want to know if there's a natural grouping (based, perhaps on species) that distinquishes the animals from another. (This use of cluster analysis is sometimes called "numerical taxonomy"). As another example, suppose we have information on the demographics and buying habits of many consumers. We could use cluster analysis on the data to see if there are distinct groups of consumers with similar demographics and buying habits (market segmentation).

It's important to remember that cluster analysis isn't about finding the right answer it's about finding ways to look at data that allow us to understand the data better. For example, suppose we have a deck of playing cards, and we want to see if they form some natural groupings. One person may separate the black cards from the red; another may break the cards up into hearts, clubs, diamonds and spades; a third person might separate cards with pictures from cards with no pictures, and a fourth might make one pile of aces, one of twos, and so on. Each person is right in their own way, but in cluster analysis, there's really not a single "correct" answer.

Another aspect of cluster analysis is that there are an enormous number of possible ways of dividing a set of observations into groups. Even if we specify the number of groups, the number of possibilities is still enormous. For example, consider the task of dividing 25 observations into 5 groups. ( 25 observations is considered very small in the world of cluster analysis). It turns out there are $2.4 * 10^{15}$ different ways to arrange those observations into 5 groups. If, as is often the case, we don't know the number of groups ahead of time, and we need to consider all possible numbers of groups (from 1 to 25 ), the number is more than $4 * 10^{18}$ ! So any technique that simply tries all the different possibilities is doomed to failure.

### 6.5 Standardization

There are two very important decisions that need to be made whenever you are carrying out a cluster analysis. The first regards the relative scales of the variables being measured. We'll see that the available cluster analysis algorithms all depend on the concept of measuring the distance (or some other measure of similarity) between the different observations we're trying to cluster. If one of the variables is measured on a much larger scale than the other variables, then whatever measure we use will be overly influenced by that variable. For example, recall the world data set that we used earlier in the semester. Here's a quick summary of the mean values of the variables in that data set:

```
> apply(world1[-c(1,6)],2,mean,na.rm=TRUE)
    gdp income literacy military
9.053595e+03 1.025796e+04 8.094902e+01 5.679061e+09
```

Without some sort of standardization, a variable like literacy, measured on a scale of 0 to 100 has no chance of influencing our solution when the other variables are so much larger.

The traditional way of standardizing variables is to subtract their mean, and divide by their standard deviation. Variables standardized this way are sometimes refered to as zscores, and always have a mean of zero and variance of one. In the case of variables that contain outliers (observations that are much bigger or smaller than the vast majority of the data), this sort of standardization may be too severe, scaling down the outlying observations so that they appear to be closer to the others. One alternative is to use the mean absolute deviation in place of the standard deviation; another possibility is to subtract the median and divide by either the interquartile range or the mean absolute deviation. For the common methods of measuring distances (discussed below), centering the data by subtracting the mean or median is not really critical; it's the division by an appropriate scaling factor that's important.

### 6.6 Distance Measures

The most common distance measure, and the default for most programs that perform cluster analysis is the Euclidean distance, which is an extension of the usual notion of the between
two points in a plane. The Euclidean distance between two observations is calculated as the square root of the sum of the squares of the distances between corresponding variables in the two observations being considered. Another widely used measure is the Manhattan distance, so named because it is similar to the distance between two points in a city, where you can only travel along a grid of streets. It's calculated by adding up the absolute value of the differences of the corresponding variables, and is less likely to be influenced by a very large difference between just one of the variables. The Canberra distance is interesting in that it performs its own standardization; absolute values of differences are divided by the absolute value of the sum of the corresponding variables in the two observations. Depending on the values and distributions of the variables in the data set being clustered, these different distance measures may point out different aspects of the structure of the data set.

Special consideration needs to be given to binary variables, that is, variables that take on only one of two values like TRUE or FALSE, especially when they are used in conjunction with continuous variables. Generally there are two types of measures that are used with binary data. Symmetric measures view two observations as being close together if the binary feature is either absent in both or present in both, while asymmetric measures only view the observations as being close if the feature is present for both.

For some clustering methods, the entire distance matrix must be calculated; for other methods, distances are only calculated as needed.

### 6.7 Clustering Techniques

Much of the history of cluster analysis is concerned with developing algorithms that were not too computer intensive, since early computers were not nearly as powerful as they are today. Accordingly, computational shortcuts have traditionally been used in many cluster analysis algorithms. These algorithms have proven to be very useful, and can be found in most computer software.

More recently, many of these older methods have been revisited and updated to reflect the fact that certain computations that once would have overwhelmed the available computers can now be performed routinely. In R, a number of these updated versions of cluster analysis algorithms are available through the cluster library, providing us with a large selection of methods to perform cluster analysis, and the possibility of comparing the old methods with the new to see if they really provide an advantage.

One of the oldest methods of cluster analysis is known as k-means cluster analysis, and is available in R through the kmeans function. The first step (and certainly not a trivial one) when using k -means cluster analysis is to specify the number of clusters ( $k$ ) that will be formed in the final solution. The process begins by choosing $k$ observations to serve as centers for the clusters. Then, the distance from each of the other observations is calculated for each of the $k$ clusters, and observations are put in the cluster to which they are the closest. After each observation has been put in a cluster, the center of the clusters is recalculated, and every observation is checked to see if it might be closer to a different cluster, now that the centers have been recalculated. The process continues until no observations switch clusters.

Looking on the good side, the k -means technique is fast, and doesn't require calculating all of the distances between each observation and every other observation. It can be written to efficiently deal with very large data sets, so it may be useful in cases where other methods fail. On the down side, if you rearrange your data, it's very possible that you'll get a different solution every time you change the ordering of your data. Another criticism of this technique is that you may try, for example, a 3 cluster solution that seems to work pretty well, but when you look for the 4 cluster solution, all of the structure that the 3 cluster solution revealed is gone. This makes the procedure somewhat unattractive if you don't know exactly how many clusters you should have in the first place.

The R cluster library provides a modern alternative to k-means clustering, known as pam, which is an acronym for "Partitioning around Medoids". The term medoid refers to an observation within a cluster for which the sum of the distances between it and all the other members of the cluster is a minimum. pam requires that you know the number of clusters that you want (like k-means clustering), but it does more computation than k-means in order to insure that the medoids it finds are truly representative of the observations within a given cluster. Recall that in the k-means method the centers of the clusters (which might or might not actually correspond to a particular observation) are only recaculated after all of the observations have had a chance to move from one cluster to another. With pam, the sums of the distances between objects within a cluster are constantly recalculated as observations move around, which will hopefully provide a more reliable solution. Furthermore, as a byproduct of the clustering operation it identifies the observations that represent the medoids,
and these observations (one per cluster) can be considered a representative example of the members of that cluster which may be useful in some situations. pam does require that the entire distance matrix is calculated to facilitate the recalculation of the medoids, and it does involve considerably more computation than k-means, but with modern computers this may not be a important consideration. As with k-means, there's no guarantee that the structure that's revealed with a small number of clusters will be retained when you increase the number of clusters.

Another class of clustering methods, known as hierarchical agglomerative clustering methods, starts out by putting each observation into its own separate cluster. It then examines all the distances between all the observations and pairs together the two closest ones to form a new cluster. This is a simple operation, since hierarchical methods require a distance matrix, and it represents exactly what we want - the distances between individual observations. So finding the first cluster to form simply means looking for the smallest number in the distance matrix and joining the two observations that the distance correspnds to into a new cluster. Now there is one less cluster than there are observations. To determine which observations will form the next cluster, we need to come up with a method for finding the distance between an existing cluster and individual observations, since once a cluster has been formed, we'll determine which observation will join it based on the distance between the cluster and the observation. Some of the methods that have been proposed to do this are to take the minimum distance between an observation and any member of the cluster, to take the maximum distance, to take the average distance, or to use some kind of measure that minimizes the distances between observations within the cluster. Each of these methods will reveal certain types of structure within the data. Using the minimum tends to find clusters that are drawn out and "snake"-like, while using the maximum tends to find compact clusters. Using the mean is a compromise between those methods. One method that tends to produce clusters of more equal size is known as Ward's method. It attempts to form clusters keeping the distances within the clusters as small as possible, and is often useful when the other methods find clusters with only a few observations. Agglomerative Hierarchical cluster analysis is provided in R through the hclust function.

Notice that, by its very nature, solutions with many clusters are nested within the solutions that have fewer clusters, so observations don't "jump ship" as they do in k-means or the pam methods. Furthermore, we don't need to tell these procedures how many clusters we want - we get a complete set of solutions starting from the trivial case of each observation in a separate cluster all the way to the other trivial case where we say all the observations are in a single cluster.

Traditionally, hierarchical cluster analysis has taken computational shortcuts when updating the distance matrix to reflect new clusters. In particular, when a new cluster is formed and the distance matrix is updated, all the information about the individual members of the cluster is discarded in order to make the computations faster. The cluster library provides the agnes function which uses essentially the same technique as hclust, but which uses fewer shortcuts when updating the distance matrix. For example, when the mean method of calculating the distance between observations and clusters is used, hclust only uses the
two observations and/or clusters which were recently merged when updating the distance matrix, while agnes calculates those distances as the average of all the distances between all the observations in the two clusters. While the two techniques will usually agree quite closely when minimum or maximum updating methods are used, there may be noticeable differences when updating using the average distance or Ward's method.

## Chapter 7

## XML

For the hierarchial clustering methods, the dendogram is the main graphical tool for getting insight into a cluster solution. When you use hclust or agnes to perform a cluster analysis, you can see the dendogram by passing the result of the clustering to the plot function.

To illustrate interpretation of the dendogram, we'll look at a cluster analysis performed on a set of cars from 1978-1979; the data can be found at http://www.stat.berkeley.edu/classes/s133/data/cars Since the data is a tab-delimited file, we use read.delim:

```
> cars = read.delim('cars.tab',stringsAsFactors=FALSE)
```

To get an idea of what information we have, let's look at the first few records;


It looks like the variables are measured on different scales, so we will likely want to standardize the data before proceeding. The daisy function in the cluster library will automatically perform standardization, but it doesn't give you complete control. If you have a particular method of standardization in mind, you can use the scale function. You pass scale a matrix or data frame to be standardized, and two optional vectors. The first, called center, is a vector of values, one for each column of the matrix or data frame to be standardized, which will be subtracted from every entry in that column. The second, called scale, is similar to center, but is used to divide the values in each column. Thus, to get z-scores, you could pass scale a vector of means for center, and a vector of standard deviations for scale. These vectors can be created with the apply function, that performs the same operation on each row or column of a matrix. Suppose we want to standardize by subtracting the median and dividing by the mean average deviation:

```
> cars.use = cars[,-c(1,2)]
> medians = apply(cars.use,2,median)
> mads = apply(cars.use,2,mad)
> cars.use = scale(cars.use,center=medians,scale=mads)
```

(The 2 used as the second argument to apply means to apply the function to the columns of the matrix or data frame; a value of 1 means to use the rows.) The country of origin and name of the car will not be useful in the cluster analysis, so they have been removed. Notice that the scale function doesn't change the order of the rows of the data frame, so it will be easy to identify observations using the omitted columns from the original data.

First, we'll take a look at a hierarchical method, since it will provide information about solutions with different numbers of clusters. The first step is calculating a distance matrix. For a data set with n observations, the distance matrix will have n rows and n columns; the $(i, j)$ th element of the distance matrix will be the difference between observation $i$ and observation $j$. There are two functions that can be used to calculate distance matrices in $R$; the dist function, which is included in every version of $R$, and the daisy function, which is part of the cluster library. We'll use the dist function in this example, but you should familiarize yourself with the daisy function (by reading its help page), since it offers some capabilities that dist does not. Each function provides a choice of distance metrics; in this example, we'll use the default of Euclidean distance, but you may find that using other metrics will give different insights into the structure of your data.

```
cars.dist = dist(cars.use)
```

If you display the distance matrix in R (for example, by typing its name), you'll notice that only the lower triangle of the matrix is displayed. This is to remind us that the distance matrix is symmetric, since it doesn't matter which observation we consider first when we calculate a distance. R takes advantage of this fact by only storing the lower triangle of the distance matrix. All of the clustering functions will recognize this and have no problems, but if you try to access the distance matrix in the usual way (for example, with subscripting), you'll see an error message. Thus, if you need to use the distance matrix with anything other than the clustering functions, you'll need to use as.matrix to convert it to a regular matrix.

To get started, we'll use the hclust method; the cluster library provides a similar function, called agnes to perform hierarchical cluster analysis.

```
> cars.hclust = hclust(cars.dist)
```

Once again, we're using the default method of hclust, which is to update the distance matrix using what R calls "complete" linkage. Using this method, when a cluster is formed, its distance to other objects is computed as the maximum distance between any object in the cluster and the other object. Other linkage methods will provide different solutions, and should not be ignored. For example, using method=ward tends to produce clusters of fairly equal size, and can be useful when other methods find clusters that contain just a few observations.

Now that we've got a cluster solution (actually a collection of cluster solutions), how can we examine the results? The main graphical tool for looking at a hierarchical cluster solution is known as a dendogram. This is a tree-like display that lists the objects which are clustered along the x -axis, and the distance at which the cluster was formed along the y -axis. (Distances along the x -axis are meaningless in a dendogram; the observations are
equally spaced to make the dendogram easier to read.) To create a dendogram from a cluster solution, simply pass it to the plot function. The result is displayed below.

```
plot(cars.hclust,labels=cars$Car,main='Default from hclust')
```



If you choose any height along the y-axis of the dendogram, and move across the dendogram counting the number of lines that you cross, each line represents a group that was identified when objects were joined together into clusters. The observations in that group are represented by the branches of the dendogram that spread out below the line. For example, if we look at a height of 6 , and move across the x -axis at that height, we'll cross two lines. That defines a two-cluster solution; by following the line down through all its branches, we can see the names of the cars that are included in these two clusters. Since the y-axis represents how close together observations were when they were merged into clusters, clusters whose branches are very close together (in terms of the heights at which they were merged) probably aren't very reliable. But if there's a big difference along the y-axis between the last merged cluster and the currently merged one, that indicates that the clusters formed are probably doing a good job in showing us the structure of the data. Looking at the dendogram for the car data, there are clearly two very distinct groups; the right hand group seems to consist of two more distinct cluster, while most of the observations in the left hand group are clustering together at about the same height For this data set, it looks like either two or three groups might be an interesting place to start investigating. This is not to imply that looking at solutions with more clusters would be meaningless, but the data seems to suggest that two or three clusters might be a good start. For a problem of this size, we can see the names of the cars, so we could start interpreting the results immediately from the
dendogram, but when there are larger numbers of observations, this won't be possible.
One of the first things we can look at is how many cars are in each of the groups. We'd like to do this for both the two cluster and three cluster solutions. You can create a vector showing the cluster membership of each observation by using the cutree function. Since the object returned by a hierarchical cluster analysis contains information about solutions with different numbers of clusters, we pass the cutree function the cluster object and the number of clusters we're interested in. So to get cluster memberships for the three cluster solution, we could use:

```
> groups.3 = cutree(cars.hclust,3)
```

Simply displaying the group memberships isn't that revealing. A good first step is to use the table function to see how many observations are in each cluster. We'd like a solution where there aren't too many clusters with just a few observations, because it may make it difficult to interpret our results. For the three cluster solution, the distribution among the clusters looks good:

```
> table(groups.3)
groups.3
    1 2 3
    8 2010
```

Notice that you can get this information for many different groupings at once by combining the calls to cutree and table in a call to sapply. For example, to see the sizes of the clusters for solutions ranging from 2 to 6 clusters, we could use:

```
> counts = sapply(2:6,function(ncl)table(cutree(cars.hclust,ncl)))
> names(counts) = 2:6
> counts
$"2"
    1 2
1820
$"3"
    1 2 3
    8 20 10
$"4"
    1
    817 3 10
$"5"
```

```
1
811 6 3 10
$"6"
    1
    811 6 3 5 5
```

To see which cars are in which clusters, we can use subscripting on the vector of car names to choose just the observations from a particular cluster. Since we used all of the observations in the data set to form the distance matrix, the ordering of the names in the original data will coincide with the values returned by cutree. If observations were removed from the data before the distance matrix is computed, it's important to remember to make the same deletions in the vector from the original data set that will be used to identify observations. So, to see which cars were in the first cluster for the four cluster solution, we can use:

```
> cars$Car[groups.3 == 1]
[1] Buick Estate Wagon Ford Country Squire Wagon
[3] Chevy Malibu Wagon Chrysler LeBaron Wagon
[5] Chevy Caprice Classic Ford LTD
[7] Mercury Grand Marquis Dodge St Regis
```

As usual, if we want to do the same thing for all the groups at once, we can use sapply:

```
> sapply(unique(groups.3),function(g)cars$Car[groups.3 == g])
[[1]]
[1] Buick Estate Wagon Ford Country Squire Wagon
[3] Chevy Malibu Wagon Chrysler LeBaron Wagon
[5] Chevy Caprice Classic Ford LTD
[7] Mercury Grand Marquis Dodge St Regis
```

[ [2] ]

| [1] Chevette | Toyota Corona | Datsun 510 | Dodge Omni |
| :--- | :--- | :--- | :--- |
| [5] Audi 5000 | Saab 99 GLE | Ford Mustang 4 | Mazda GLC |
| [9] Dodge Colt | AMC Spirit | VW Scirocco | Honda Accord LX |
| [13] Buick Skylark | Pontiac Phoenix | Plymouth Horizon Datsun 210 |  |
| [17] Fiat Strada | VW Dasher | BMW 320i | VW Rabbit |

## [ [3] ]

[1] Volvo 240 GL Peugeot 694 SL Buick Century Special
[4] Mercury Zephyr Dodge Aspen AMC Concord D/L
[7] Ford Mustang Ghia Chevy Citation Olds Omega

We could also see what happens when we use the four cluster solution

```
> groups.4 = cutree(cars.hclust,4)
> sapply(unique(groups.4),function(g)cars$Car[groups.4 == g])
[[1]]
[1] Buick Estate Wagon Ford Country Squire Wagon
[3] Chevy Malibu Wagon Chrysler LeBaron Wagon
[5] Chevy Caprice Classic Ford LTD
[7] Mercury Grand Marquis Dodge St Regis
```

[ [2] ]
[1] Chevette Toyota Corona Datsun 510 Dodge Omni
[5] Ford Mustang 4 Mazda GLC Dodge Colt AMC Spirit
[9] VW Scirocco Honda Accord LX Buick Skylark Pontiac Phoenix
[13] Plymouth Horizon Datsun 210 Fiat Strada VW Dasher
[17] VW Rabbit
[[3]]
[1] Audi 5000 Saab 99 GLE BMW 320i
[ [4]]
[1] Volvo 240 GL Peugeot 694 SL Buick Century Special
[4] Mercury Zephyr Dodge Aspen AMC Concord D/L
[7] Ford Mustang Ghia Chevy Citation Olds Omega
[10] Datsun 810

The new cluster can be recognized as the third group in the above output.
Often there is an auxiliary variable in the original data set that was not included in the cluster analysis, but may be of interest. In fact, cluster analysis is sometimes performed to see if observations naturally group themselves in accord with some already measured variable. For this data set, we could ask whether the clusters reflect the country of origin of the cars, stored in the variable Country in the original data set. The table function can be used, this time passing two arguments, to produce a cross-tabulation of cluster group membership and country of origin:

```
> table(groups.3,cars$Country)
groups.3 France Germany Italy Japan Sweden U.S.
    1 0
```

|  | 2 | 0 | 5 | 1 | 6 | 1 | 7 |
| :--- | :--- | :--- | :--- | :--- | :--- | :--- | :--- |
|  | 3 | 1 | 0 | 0 | 1 | 1 | 7 |

Of interest is the fact that all of the cars in cluster 1 were manufactured in the US. Considering the state of the automobile industry in 1978, and the cars that were identified in cluster 1, this is not surprising.

In an example like this, with a small number of observations, we can often interpret the cluster solution directly by looking at the labels of the observations that are in each cluster. Of course, for larger data sets, this will be impossible or meaningless. A very useful method for characterizing clusters is to look at some sort of summary statistic, like the median, of the variables that were used to perform the cluster analysis, broken down by the groups that the cluster analysis identified. The aggregate function is well suited for this task, since it will perform summaries on many variables simultaneously. Let's look at the median values for the variables we've used in the cluster analysis, broken up by the cluster groups. One oddity of the aggregate function is that it demands that the variable(s) used to divide up the data are passed to it in a list, even if there's only one variable:

```
> aggregate(cars.use,list(groups.3),median)
    Group.1 MPG Weight Drive_Ratio Horsepower Displacement Cylinders
1 1 -0.7945273 1.5051136 -0.9133729 1.0476133 2.4775849 4.7214353
2 2 0.6859228 -0.5870568 0.5269459 -0.6027364 -0.5809970 -0.6744908
3 3 -0.4058377 0.5246039 -0.1686227 0.3587717 0.3272282 2.0234723
```

If the ranges of these numbers seem strange, it's because we standardized the data before performing the cluster analysis. While it is usually more meaningful to look at the variables in their original scales, when data is centered, negative values mean "lower than most" and positive values mean "higher than most". Thus, group 1 is cars with relatively low MPG, high weight, low drive ratios, high horsepower and displacement, and more than average number of cylinders. Group 2 are cars with high gas mileage, and low weight and horsepower; and group 3 is similar to group 1. It may be easier to understand the groupings if we look at the variables in their original scales:

```
> aggregate(cars[,-c(1,2)],list(groups.3),median)
    Group.1 MPG Weight Drive_Ratio Horsepower Displacement Cylinders
1 1 17.30 3.890 
2 2 30.25 2.215 
3 3 20.70
```

It may also be useful to add the numbers of observations in each group to the above display. Since aggregate returns a data frame, we can manipulate it in any way we want:

```
> a3 = aggregate(cars[,-c(1,2)],list(groups.3),median)
> data.frame(Cluster=a3[,1],Freq=as.vector(table(groups.3)),a3[, -1])
    Cluster Freq MPG Weight Drive_Ratio Horsepower Displacement Cylinders
1 1 1 8 17.30 3.890 
2 2 20 30.25 2.215 
3 3 10 20.70 3.105 
```

To see how the four cluster solution differed from the three cluster solution, we can perform the same analysis for that solution:

```
a4 = aggregate(cars[,-c(1,2)],list(groups.4),median)
> data.frame(Cluster=a4[,1],Freq=as.vector(table(groups.4)),a4[,-1])
    Cluster Freq MPG Weight Drive_Ratio Horsepower Displacement Cylinders
1 1 1 8 17.3 3.890 
2 lllllllll
3 3 3 21.5 2.795 
4 lllllllll
```

The main difference seems to be that the four cluster solution recognized a group of cars that have higher horsepower and drive ratios than the other cars in the cluster they came from.

Unlike the hierarchical clustering methods, techniques like k-means cluster analysis (available through the kmeans function) or partitioning around mediods (avaiable through the pam function in the cluster library) require that we specify the number of clusters that will be formed in advance. pam offers some additional diagnostic information about a clustering solution, and provides a nice example of an alternative technique to hierarchical clustering. To use pam, you must first load the cluster library. You can pass pam a data frame or a distance matrix; since we've already formed the distance matrix, we'll use that. pam also needs the number of clusters you wish to form. Let's look at the three cluster solution produced by pam:

```
> library(cluster)
> cars.pam = pam(cars.dist,3)
```

First of all, let's see if the pam solution agrees with the hclust solution. Since pam only looks at one cluster solution at a time, we don't need to use the cutree function as we did with hclust; the cluster memberships are stored in the clustering component of the pam object; like most R objects, you can use the names function to see what else is available. Further information can be found in the help page for pam. object.

```
> names(cars.pam)
[1] "medoids" "id.med" "clustering" "objective" "isolation"
[6] "clusinfo" "silinfo" "diss" "call"
```

We can use table to compare the results of the hclust and pam solutions:

```
> table(groups.3,cars.pam$clustering)
groups.3 1 2 3
    1 8 0 0
    2
    30}001
```

The solutions seem to agree, except for 1 observations that hclust put in group 2 and pam put in group 3. Which observations was it?

```
> cars$Car[groups.3 != cars.pam$clustering]
```

[1] Audi 5000

Notice how easy it is to get information like this due to the power of R's subscripting operations.

One novel feature of pam is that it finds observations from the original data that are typical of each cluster in the sense that they are closest to the center of the cluster. The indexes of the medoids are stored in the id.med component of the pam object, so we can use that component as a subscript into the vector of car names to see which ones were selected:

```
> cars$Car[cars.pam$id.med]
> cars$Car[cars.pam$id.med]
[1] Dodge St Regis Dodge Omni Ford Mustang Ghia
```

Another feature available with pam is a plot known as a silhouette plot. First, a measure is calculated for each observation to see how well it fits into the cluster that it's been assigned to. This is done by comparing how close the object is to other objects in its own cluster with how close it is to objects in other clusters. (A complete description can be found in the help page for silhouette.) Values near one mean that the observation is well placed in its cluster; values near 0 mean that it's likely that an observation might really belong in some other cluster. Within each cluster, the value for this measure is displayed from smallest to largest. If the silhouette plot shows values close to one for each observation, the fit was good; if there are many observations closer to zero, it's an indication that the fit was not good. The sihouette plot is very useful in locating groups in a cluster analysis that may not be doing a good job; in turn this information can be used to help select the proper number of clusters. For the current example, here's the silhouette plot for the three cluster pam solution, produced by the command

```
> plot(cars.pam)
```

| Range of SC | Interpretation |
| :--- | :--- |
| $0.71-1.0$ | A strong structure has been found |
| $0.51-0.70$ | A reasonable structure has been found |
| $0.26-0.50$ | The structure is weak and could be artificial |
| $<0.25$ | No substantial structure has been found |



The plot indicates that there is a good structure to the clusters, with most observations seeming to belong to the cluster that they're in. There is a summary measure at the bottom of the plot labeled "Average Silhouette Width". This table shows how to use the value:

To create a silhouette plot for a particular solution derived from a hierarchical cluster analysis, the silhouette function can be used. This function takes the appropriate output from cutree along with the distance matrix used for the clustering. So to produce a silhouette plot for our 4 group hierarchical cluster (not shown), we could use the following statements:
plot(silhouette(cutree(cars.hclust,4), cars.dist))
As an example of using the agnes function from the cluster package, consider the famous Fisher iris data, available as the dataframe iris in R. First let's look at some of the data:

```
> head(iris)
```

|  | Sepal.Length Sepal. Width Petal.Length Petal.Width | Species |  |  |  |
| :---: | :---: | ---: | ---: | ---: | ---: |
| 1 | 5.1 | 3.5 | 1.4 | 0.2 | setosa |
| 2 | 4.9 | 3.0 | 1.4 | 0.2 | setosa |
| 3 | 4.7 | 3.2 | 1.3 | 0.2 | setosa |
| 4 | 4.6 | 3.1 | 1.5 | 0.2 | setosa |
| 5 | 5.0 | 3.6 | 1.4 | 0.2 | setosa |
| 6 | 5.4 | 3.9 | 1.7 | 0.4 | setosa |

We will only consider the numeric variables in the cluster analysis. As mentioned previously, there are two functions to compute the distance matrix: dist and daisy. It should be mentioned that for data that's all numeric, using the function's defaults, the two methods will give the same answers. We can demonstrate this as follows:

```
> iris.use = subset(iris,select=-Species)
> d = dist(iris.use)
> library(cluster)
> d1 = daisy(iris.use)
> sum(abs(d - d1))
[1] 1.072170e-12
```

Of course, if we choose a non-default metric for dist, the answers will be different:

```
> dd = dist(iris.use,method='manhattan')
> sum(abs(as.matrix(dd) - as.matrix(d1)))
[1] 38773.86
```

The values are very different!
Continuing with the cluster example, we can calculate the cluster solution as follows:

```
> z = agnes(d)
```

The plotting method for agnes objects presents two different views of the cluster solution. When we plot such an object, the plotting function sets the graphics parameter ask=TRUE, and the following appears in your R session each time a plot is to be drawn:

Hit <Return> to see next plot:

If you know you want a particular plot, you can pass the which.plots= argument an integer telling which plot you want.

The first plot that is displayed is known as a banner plot. The banner plot for the iris data is shown below:

## Banner of $\operatorname{agnes}(x=d)$



Agglomerative Coefficient $=0.93$

The white area on the left of the banner plot represents the unclustered data while the white lines that stick into the red are show the heights at which the clusters were formed. Since we don't want to include too many clusters that joined together at similar heights, it looks like three clusters, at a height of about 2 is a good solution. It's clear from the banner plot that if we lowered the height to, say 1.5 , we'd create a fourth cluster with only a few observations.

The banner plot is just an alternative to the dendogram, which is the second plot that's produced from an agnes object:


The dendogram shows the same relationships, and it's a matter of individual preference as to which one is easier to use.

Let's see how well the clusters do in grouping the irises by species:

```
> table(cutree(z,3),iris$Species)
\begin{tabular}{rrrr} 
& setosa & versicolor & virginica \\
1 & 50 & 0 & 0 \\
2 & 0 & 50 & 14 \\
3 & 0 & 0 & 36
\end{tabular}
```

We were able to classify all the setosa and versicolor varieties correctly. The following plot gives some insight into why we were so successful:

```
> splom(~iris,groups=iris$Species,auto.key=TRUE)
```



### 7.1 What is XML?

XML, which is an acronym for extensible markup language, is a way of creating documents that contain structured information. Up until now, most of the data sets that we've considered were easily accomodated by a observations and variables rectangular data structure (like a comma separated file, which translates neatly to a data frame in R), where the number of variables for each observations is the same. Outside of variable names and the actual data values, there was no additional information stored in the data, either in its text form or once it was read into $R$.

One type of data that we've seen that accomodates extra information is the spreadsheet; people often annotate their data will all sorts of useful and maybe-not-so-useful information. But as we've seen, there's no standard structure to these non-data rows of the spreadsheet, so they really just get in our way and require customized processing.

Another example of non-regular data would be the baseball database; players played for varying numbers of seasons, and for varying numbers of teams; they may or may not have attended college, or played in a world series, etc. Databases have traditionally been used for
data like this, but they certainly have their disadvantages: there are many tables, making it necessary to perform lots of joins, and it's easy to lose track of all that information.

One frustrating aspect regarding designing formats for data is that if you go into the design with a specific type of data in mind, you'll build in features that are wonderful for that data, but may be very lacking for other sorts of data. For example, statisticians would want a rich syntax to describe things like repeated measures, missing values, allowable ranges of variables, etc., but these features would not be of much use to a general user. So in some ways, we can think of XML as a compromise that will allow a wide variety of different information to be stored and distributed in a similar way without favoring any particular structure or type of data. The features that I've described can easily be accomodated in an XML document by simply defining new tags to contain this information. Furthermore, XML is designed so that it's alright if there is no extra information in the document other than the data and its' associated tags. This sort of flexibility is one of the most powerful forces behind the development of XML. To see a list of some of the applications for which XML document styles have been proposed, go to http://xml.coverpages.org/xml.html\#applications.

At first glance, XML looks very similar to HTML, but there are important differences. First, HTML is used to describe the desired appearance of information in the browser, not the structure of that information. Second, the set of allowable tags in HTML is fixed; we can't just redefine them at our convenience. HTML is also inconsistent. Tags like h1 and td must have accompanying closing tags (</h1> and </td>), but tags like <br> and <p> don't. Finally, to accomodate all the people creating web pages and all the browsers trying to display them, HTML doesn't lay down strict rules about the way information is put into a web page. These facts about HTML should not be interpreted as saying the HTML is not useful. It's very useful for what it does, but it doesn't give us a consistent, extensible format for accomodating data that preserves its structure.

Here are some of the things that we'll see in XML documents:

- XML documents always begin with

```
<?xml ....?>
```

- Information is identified by tags (i.e. an indentifier surrounded by angle brackets, like

```
<coursename>
    Statistics 133
</coursename>
```

Every opening tag has a corresponding tag, except for the case where there is no information; then a single tag like <sometag/> can be used. The specific names of these tags will vary with each XML document.

- Tags are case sensitive, and opening and closing tags must match exactly.
- No spaces are allowed between the opening angle bracket and the tag name
- Tag names must begin with a letter, and can contain only letters and numbers.
- As in HTML, angle brackets will always be interpreted as parts of tags; to get literal angle brackets in data we need to use \< and \>.
- Additional information can be stored in the tags in the form of attributes. For example, in the previous example, we could have specified the department as:

```
<coursename department='Statistics'>
    Statistics 133
</coursename>
```

or

```
<course>
```

    <name>
            Statistics 133
        </name>
        <department>
            Statistics
        </department>
    </course>

The decision is up to the designer of the particular document.

- Comments can be placed in an XML document by starting with <!-- and ending with -->, and they may appear anywhere in the document.

Documents that conform to these rules are said to be well-formed, and this is the minimum requirement for any XML document. But to be useful, they should also conform to additional rules described in what is known as the Document Type Definitions for a particular document, or the DTD. The DTD describes the allowable tags, what kind of data can be stored within those tags, and what attributes are allowed in the tags. The DTD for a particular document can be provided in the document itself; when a document uses multiple DTDs, the tag name may be prefaced with an identifier followed by a colon to make clear which DTD the tag comes from. The programs that read XML are known as parsers; without a DTD they simply make sure that the document is well-formed; with a DTD they can additionally check to make sure that the data is valid.

### 7.2 A Simple Example

Let's start with a very simple example to introduce the XML library and some of the strategies we'll need to use when working with XML. The example we'll use is a catalog of plants. (You can find the XML document at http://www.stat.berkeley.edu/classes/s133/data/plant_catalog.xml.) Here's what the beginning of the file looks like:

```
<?xml version="1.0" encoding="ISO-8859-1"?>`M
<!-- Edited with XML Spy v2006 (http://www.altova.com) -->^M
<CATALOG>`M
    <PLANT>`M
        <COMMON>Bloodroot</COMMON>^M
        <BOTANICAL>Sanguinaria canadensis</BOTANICAL>^M
        <ZONE>4</ZONE>`M
        <LIGHT>Mostly Shady</LIGHT>`M
        <PRICE>$2.44</PRICE>^M
        <AVAILABILITY>031599</AVAILABILITY>`M
    </PLANT>`M
    <PLANT>`M
        <COMMON>Columbine</COMMON>`M
        <BOTANICAL>Aquilegia canadensis</BOTANICAL>`M
        <ZONE>3</ZONE>`M
        <LIGHT>Mostly Shady</LIGHT>`M
        <PRICE>$9.37</PRICE>^M
        <AVAILABILITY>030699</AVAILABILITY>^M
    </PLANT>`M
```

The main body of the data is enclosed by the CATALOG tag; we'll sometimes refer to this as a node. Within the CATALOG node are several PLANT nodes - each of them contains several pieces of data which are the information we wish to extract. We're going to use the R XML library with what is known as the Document Object Model (DOM), in which R will read the entire XML file into memory, and internally convert it to a tree structure. (There is another model, called SAX (Simple API for XML), which only reads part of the data at a time, but it's more complicated than the DOM model.) All the information about the data and its structure will be stored in a list inside of $R$, but when we print it, it will look very much like the document that we started with. The basic strategy of working with XML files under this model is to keep "tunneling down" into the document structure without disturbing its structure until we come to the end of the node. For example, with the plant catalog, we want to extract the PLANT nodes as XML structures, and then extract the values of the terminal branches of the tree (like COMMON, BOTANICAL, and ZONE) using the xmlValue function. As we explore the structure of the data, we can use the names function to see what nodes exist; at any time, we can print a node, and it will show us a representation like the original XML document so we'll know where to go next.

The first step in reading an XML document into R is loading the XML library. Next, the xmlTreeParse function is called to read the document into memory, and the root of the XML tree is extracted using xmlRoot:

```
> library(XML)
> doc = xmlTreeParse('plant_catalog.xml')
> root = xmlRoot(doc)
```

Let's look at some properties of this root node:

```
> class(root)
[1] "XMLNode" "RXMLAbstractNode" "XMLAbstractNode" "oldClass"
> names(root)
> names(root)
    [1] "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT"
[10] "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT"
[19] "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT"
[28] "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT" "PLANT"
```

In this example, xmlTreeParse read its input from a local file. Other choices are local gzipped files and URLs representing XML documents or gzipped XML documents.

The class of XMLNode indicates that internally, R is storing the object as part of an XML tree. This will be important later when we decide how to process the entire tree. The result of the names function call tells us that the structure of this document is quite simple. Inside the root node, there are 36 PLANT nodes. (For larger documents, it might be prudent to make a table of the names instead of displaying the names directly.) As we've already seen from looking at the document, this is where our data lies, so we'll want to examine one of the plant nodes a little more carefully to figure out how to extract the actual data.

```
> oneplant = root[[1]]
> class(oneplant)
[1] "XMLNode" "RXMLAbstractNode" "XMLAbstractNode" "oldClass"
> oneplant
    <PLANT>
    <COMMON>
    Bloodroot
    </COMMON>
    <BOTANICAL>
    Sanguinaria canadensis
    </BOTANICAL>
    <ZONE>
    4
    </ZONE>
    <LIGHT>
    Mostly Shady
    </LIGHT>
    <PRICE>
    $2.44
    </PRICE>
    <AVAILABILITY>
    031599
    </AVAILABILITY>
```


## </PLANT>

We can see that this single PLANT object is still an XMLnode; its printed representation shows us exactly what we've got. Notice that the individual elements don't have any further tree structure; this means we can use xmlValue to extract the values:

```
> xmlValue(oneplant[['COMMON']])
[1] "Bloodroot"
> xmlValue(oneplant[['BOTANICAL']])
[1] "Sanguinaria canadensis"
```

Of course, we don't want to perform these tasks one by one for each node of the tree. You may recall that when we were confronted with problems like this before, we used the sapply function, which operates on every element of a list. If the object we want to process is an xmlNode , the corresponding function to use is xmlSApply. For example, to get all the common names of all the plants, we can use xmlValue on all the PLANT nodes like this:

```
> commons = xmlSApply(root,function(x)xmlValue(x[['COMMON']]))
> head(commons)
\begin{tabular}{rrr} 
PLANT & PLANT & PLANT \\
"Bloodroot" & "Columbine" & "Marsh Marigold" \\
PLANT & PLANT & PLANT \\
"Cowslip" "Dutchman's-Breeches" & "Ginger, Wild"
\end{tabular}
```

We could repeat the process for each column manually, and then combine things into a data frame, or we can automate the process using lapply and the names of the objects within the plants:

```
> getvar = function(x,var)xmlValue(x[[var]])
> res = lapply(names(root[[1]]),function(var)xmlSApply(root,getvar,var))
> plants = data.frame(res)
> names(plants) = names(root[[1]])
> head(plants)
                    COMMON BOTANICAL ZONE LIGHT PRICE
    Bloodroot Sanguinaria canadensis 4 Mostly Shady $2.44
    Columbine Aquilegia canadensis 3 Mostly Shady $9.37
        Marsh Marigold Caltha palustris 4 Mostly Sunny $6.81
        Cowslip Caltha palustris 4 Mostly Shady $9.90
Dutchman's-Breeches Dicentra cucullaria 3 Mostly Shady $6.44
6 Ginger, Wild Asarum canadense 3 Mostly Shady $9.03
    AVAILABILITY
1 031599
2 030699
3 051799
4 030699
5 012099
6 041899
```


### 7.3 More Complex Example

For more complex documents, a few other tools are useful. To illustrate, we'll look at a file that uses Geographic Markup Language, or GML. This file (which you can find at http://www.stat.berkeley.edu/classes/s133/data/counties.gml contains the x- and y-coordinates of the county centers for each state in the United States. Information like this would be difficult to store in a less structured environment, because each state has a different number of counties. If we were going to read it into a database, we might want to have a separate table for each state; in some programs, we'd have to force it into a rectangular form, even though it wouldn't be that efficient. If we were using a spreadsheet, we might want to put all the information in a single spreadsheet, with a separate heading for each state. In R, a reasonable way to store the data would be in a list, with a separate data frame for each state. Thus, providing the data in a form that could be easily converted to any of those formats is essential, and that's just what XML does for us.

The first steps are the same as the previous example; loading the library, parsing the tree, and extracting the root.

```
> doc = xmlTreeParse('counties.gml')
root = xmlRoot(doc)
```

To see what's in the root, we can get a table of the names found there:

```
> table(names(root))
```

state
51

Let's extract the first state node for further study:

```
> onestate = root[[1]]
> class(onestate)
[1] "XMLNode" "RXMLAbstractNode" "XMLAbstractNode" "oldClass"
> table(names(onestate))
county name
    67 1
```

Here's what the onestate object looks like - I've truncated it so that it only displays a single county, but we can still see the general structure:

```
<state>
    <gml:name abbreviation="AL">ALABAMA</gml:name>
    <county>
        <gml:name>Autauga County</gml:name>
        <gml:location>
```

```
    <gml:coord>
        <gml:X>-86641472</gml : X>
        <gml:Y>32542207</gml:Y>
    </gml:coord>
    </gml:location>
</county>
```

The name element (labeled as gml:name) is just the name of the state. We can extract them from all of the states using xmlSApply:

```
> statenames = xmlSApply(root,function(x)xmlValue(x[['name']]))
> head(statenames)
    state state state state state state
    "ALABAMA" "ALASKA" "ARIZONA" "ARKANSAS" "CALIFORNIA" "COLORADO"
```

Note that in this example there is an attribute in the name tag, namely the state abbreviation. To access these attributes we can use the xmlAttrs function in a fashion similar to xmlValue:

```
> stateabbs = xmlSApply(root,function(x)xmlAttrs(x[['name']]))
> head(stateabbs)
state.abbreviation state.abbreviation state.abbreviation state.abbreviation
    "AL" "AK" "AZ" "AR"
state.abbreviation state.abbreviation
    "CA" "CD"
```

Since there was only one attribute, xmlSApply was used to extract directly into a vector. If there were multiple attributes, then xmlApply would need to be used, since it will return a list of attributes, preserving the structure of the data.

To process the county data further, we need to extract just the county nodes. The xmlElementsByTagName function will extract just the elements that we want:

```
> counties = xmlElementsByTagName(onestate,'county')
```

> class(counties)
[1] "list"
> length(counties)
[1] 67

Notice that extracting the elements in this way results in a list, not an xmlNode. But what's in the list?

```
> onecounty = counties[[1]]
> class(onecounty)
[1] "XMLNode" "RXMLAbstractNode" "XMLAbstractNode" "oldClass"
> names(onecounty)
```

```
[1] "name" "location"
> onecounty
    <county>
        <gml:name>
    Autauga County
    </gml:name>
    <gml:location>
        <gml:coord>
            <gml:X>
            -86641472
            </gml:X>
            <gml:Y>
            32542207
            </gml:Y>
        </gml: coord>
    </gml:location>
    </county>
```

The elements inside the counties list are still xmlNodes. The fact that they are contained in a list simply means that we'll use sapply or lapply to process them instead of xmlSApply or xmlApply. What we really want are the X and Y values within the coord nodes, so let's extract out those nodes from the full list of county nodes:

```
> coords = lapply(counties,function(x)x[['location']][['coord']])
> class(coords)
[1] "list"
> class(coords[[1]])
[1] "XMLNode" "RXMLAbstractNode" "XMLAbstractNode" "oldClass"
> coords[[1]]
    <gml:coord>
        <gml:X>
    -86641472
        </gml:X>
        <gml:Y>
        32542207
        </gml:Y>
    </gml:coord>
```

Since there is only one coord node within the location nodes, I extracted it directly. I could also have used xmlGetElementsByTagName, and used the first element of the resulting list:

```
coords = lapply(counties,function(x)xmlElementsByTagName(x[['location']],'coord')[[1]])
```

Notice that I used lapply to extract the coord nodes. Since xmlNodes are represented internally as lists, I would have lost the structure of the data if I used sapply in this case.

Now we can extract the x and y values using xmlValue:

```
> x = as.numeric(sapply(coords,function(x)xmlValue(x[['X']])))
```

> y = as.numeric(sapply(coords,function(x)xmlValue(x[['Y']])))

That shows the process for extracting the county names and x - and y -coordinates for a single state. Let's summarize the steps in a function, which we can then apply to the root of the tree to get a separate list for each state:

```
onestate = function(state){
    counties = xmlElementsByTagName(state,'county')
    countynames = sapply(counties,function(x)xmlValue(x[['name']]))
    coords = lapply(counties,function(x)x[['location']][['coord']])
    x = as.numeric(sapply(coords,function(x)xmlValue(x[['X']])))
    y = as.numeric(sapply(coords,function(x)xmlValue(x[['Y']])))
    data.frame(county=countynames,}x=x,y=y
}
```

To combine everything together, and create a list with one data frame per state, we can do the following:

```
> res = xmlApply(root,onestate)
> names(res) = xmlSApply(root,function(x)xmlValue(x[['name']]))
```

Although these examples may seem simplistic, there are usable XML formats that are this simple, or even simpler. For example, at the web site http://www.weather.gov/data/current_obs/ there is a description of an XML format used to distribute weather information. Basically, the XML document is available at http://www.weather.gov/data/current_obs/XXXX.xml where XXXX represents the four letter weather station code, usually related to a nearby airport.

A quick look at the data reveals that the format is very simple:

```
> library(XML)
> doc = xmlTreeParse('http://www.weather.gov/data/current_obs/KOAK.xml')
root = xmlRoot(doc)
> names(root)
    [1] "credit" "credit_URL"
    [3] "image" "suggested_pickup"
    [5] "suggested_pickup_period" "location"
    [7] "station_id" "latitude"
    [9] "longitude" "observation_time"
[11] "observation_time_rfc822" "weather"
[13] "temperature_string" "temp_f"
```

| [15] "temp_c" | "relative_humidity" |
| :--- | :--- |
| [17] "wind_string" | "wind_dir" |
| $[19]$ | "wind_degrees" |
| [21] "wind_gust_mph" | "wind_mph" |
| [23] "pressure_mb" | "pressure_string" |
| [25] "dewpoint_string" | "pressure_in" |
| [27] "dewpoint_c" | "heat_index_string" |
| $[29]$ | "heat_index_f" |

Essentially, all the information is in the root node, so it can be extracted with xmlValue:

```
> xmlValue(root[['temp_f']])
[1] "72"
> xmlValue(root[['wind_mph']])
[1] "6.9"
```

To make this easy to use, we can write a function that will allow us to specify a location and some variables that we want information about:

```
getweather = function(loc='KOAK',vars='temp_f'){
    require(XML)
    url = paste('http://www.weather.gov/data/current_obs/',loc,'.xml',sep='')
    doc = xmlTreeParse(url)
    root = xmlRoot(doc)
    sapply(vars,function(x)xmlValue(root[[x]]))
}
```

Let's check to make sure it works with the defaults:

```
> getweather()
temp_f
    "76"
```

That seems to be ok. To make it even more useful, we can create a vector of station names, and use sapply to find weather information for each station:

```
> result = sapply(c('KOAK','KACV','KSDM'),getweather,var=c('temp_f','wind_mph','wind_dir
> data.frame(t(result))
    temp_f wind_mph wind_dir relative_humidity
KOAK 78 9.2 Northwest 35
KACV 58 17.25 North 75
KSDM 85 8.05 West 14
```

sapply has properly labeled all the stations and variables.

## Chapter 8

## Some Programming Examples

### 8.1 Operating on Groups of Data

We've already seen how the aggregate function let's us calculate data summaries for groups in our data. For example, using the world data set, we could find the average value of each variable, broken down by continent:

```
> world = read.csv('http://www.stat.berkeley.edu/classes/s133/data/world2.txt',na.string
> > names(world)
[1] "country" "cont" "gdp" "income" "literacy" "military" "phys"
[8] "un.date"
> aggregate(world[,-c(1,2,8)],world['cont'],mean,na.rm=TRUE)
    cont gdp income literacy military phys
1 AF 2723.404 3901.191 60.52979 356440000 26.31129
2 AS 7778.049 8868.098 84.25122 5006536341 161.83381
3 EU 19711.765 21314.324 98.40294 6311138235 311.18482
4 NA 8946.667 10379.143 85.52000 25919931267 187.08178
5 OC 14625.000 15547.500 87.50000 4462475000 127.63105
6 SA 6283.333 6673.083 92.29167 2137341667 154.81088
```

Since the aggregate function requires the grouping variables to be in a list, I took advantage of the fact that data frames are also lists, and passed a single element (using single brackets) to aggregate. Alternatively, I could have used a list directly:

```
> aggregate(world[,-c(1,2,8)],list(world$cont),mean,na.rm=TRUE)
    Group.1 gdp income literacy military phys
1 AF 2723.404 3901.191 60.52979 356440000 26.31129
2 AS 7778.049 8868.098 84.25122 5006536341 161.83381
3 EU 19711.765 21314.324 98.40294 6311138235 311.18482
4 NA 8946.667 10379.143 85.52000 25919931267 187.08178
5 OC 14625.000 15547.500 87.50000 4462475000 127.63105
6 SA 6283.333 6673.083 92.29167 2137341667 154.81088
```

I would need to name the list element in order for its column in the output to be properly labeled.

Now suppose I'd like to calculate both the mean and the median for each continent:

```
> aggregate(world[,-c(1,2,8)],world['cont'],function(x)c(mean(x),median(x)))
```

Error in aggregate.data.frame(world[, $-c(1,2,8)]$, world["cont"], function(x) c(mean(x)
'FUN' must always return a scalar

In addition, aggregate doesn't provide us with any way of working with multiple variables - it is restricted to operating on single variables at a time, and the function it uses must return a scalar. Because of these restrictions, it always returns a data frame, so after calling aggregate, your data is ready to plot or display with no further manipulations.

There are two approaches to the cases where aggregate won't work. The first, uses the split function that we've seen for making boxplots. First, we'll define a function to return both the mean and the median in a vector:

```
> mmed = function(x)c(mean(x,na.rm=TRUE),median(x,na.rm=TRUE))
```

Next, we'll create a list of data frames, one for each continent, using the split function:

```
> conts = split(world[,-c(1,2,8)],world$cont)
```

As always, we determine our strategy by looking at a single value, in this case the data frame for a single continent. Since we want the mean and median for each column in the data frame, we can use the apply function, passing it a value of 2 to indicate that we want to calculate the statistics for each column:

```
> onecont = conts[[1]]
> apply(onecont,2,mmed)
    gdp income literacy military phys
[1,] 2723.404 3901.191 60.52979 356440000 26.31129
[2,] 1400.000 1813.000 65.50000 101300000 8.68680
```

This output represents exactly the stucture we want, so we'll use lapply to do the same thing for each continent and retain that structure:

```
> res = lapply(conts,function(onecont)apply(onecont,2,mmed))
> length(res)
[1] 6
> names(res)
[1] "AF" "AS" "EU" "NA" "OC" "SA"
> res[[1]]
    gdp income literacy military phys
[1,] 2723.404 3901.191 60.52979 356440000 26.31129
[2,] 1400.000 1813.000 65.50000 101300000 8.68680
> res[[2]]
    gdp income literacy military phys
[1,] 7778.049 8868.098 84.25122 5006536341 161.8338
[2,] 4300.000 4561.000 89.90000 650000000 139.9254
```

To create a data frame with this information we'd need to use rbind to combine each of the elements of res together. For this problem, there are only six columns, so you might take the trouble to type:

```
> answer = rbind(res[[1]],res[[2]],res[[3]], ...
```

but eventually you'll be confronted with a problem for which that strategy will not work for example if there were 20000 data frames we need to bind together! R provides a curious function called do.call which solves these sorts of problems. The first argument to do.call is the function that you want to use, and the second argument is a list of values which will be used as the arguments to that function. In other words, with do.call you don't have to write out all the arguments to a function; you can just take a list with those arguments and make it the second argument to do.call. So to rbind together each of the elements in res, we could use

```
> rres = do.call(rbind,res)
    gdp income literacy military phys
[1,] 2723.404 3901.191 60.52979 356440000 26.31129
[2,] 1400.000 1813.000 65.50000 101300000 8.68680
[3,] 7778.049 8868.098 84.25122 5006536341 161.83381
[4,] 4300.000 4561.000 89.90000 650000000 139.92540
[5,] 19711.765 21314.324 98.40294 6311138235 311.18482
[6,] 18150.000 19804.000 99.70000 1288500000 317.88580
```

Now we have a data frame with a row of means and a row of medians for each continent. But which continent is which? They are in the same order that they were in the res list, that is

```
> names(res)
[1] "AF" "AS" "EU" "NA" "OC" "SA"
```

So we might be tempted to create a column with each continent replaced twice, and then another column alternating with mean and median. Again, for a problem this size, it may be a reasonable approach, but let's see how we can generate these columns more efficiently. $R$ provides another interesting function called expand.grid which will create a data frame with all possible combinations of two vectors, in this case, we could get what we need with

```
> expand.grid(c('Mean','Median'),names(res))
    Var1 Var2
1 Mean AF
2 Median AF
3 Mean AS
4 Median AS
5 Mean EU
6 Median EU
7 Mean NA
8 Median NA
9 Mean OC
10 Median OC
11 Mean SA
```

Let's combine all the pieces to get the final result:

```
> mmed = function(x)c(mean(x,na.rm=TRUE),median(x,na.rm=TRUE))
> conts = split(world[-c(1,2,8)],world$cont)
> res = lapply(conts,function(onecont)apply(onecont,2,mmed))
> data.frame(expand.grid(Stat=c('Mean','Median'),
                            Cont=names(res)),do.call(rbind,res))
    Stat Cont gdp income literacy military phys
1 Mean AF 2723.404 3901.191 60.52979 356440000 26.31129
```

| 2 | Median | AF | 1400.000 | 1813.000 | 65.50000 | 101300000 | 8.68680 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| 3 | Mean | AS | 7778.049 | 8868.098 | 84.25122 | 5006536341 | 161.83381 |
| 4 | Median | AS | 4300.000 | 4561.000 | 89.90000 | 650000000 | 139.92540 |
| 5 | Mean | EU | 19711.765 | 21314.324 | 98.40294 | 6311138235 | 311.18482 |
| 6 | Median | EU | 18150.000 | 19804.000 | 99.70000 | 1288500000 | 317.88580 |
| 7 | Mean | NA | 8946.667 | 10379.143 | 85.52000 | 25919931267 | 187.08178 |
| 8 | Median | NA | 4900.000 | 6753.000 | 87.70000 | 147000000 | 164.40130 |
| 9 | Mean | OC | 14625.000 | 15547.500 | 87.50000 | 4462475000 | 127.63105 |
| 10 | Median | OC | 13700.000 | 14970.000 | 96.40000 | 591500000 | 128.11915 |
| 11 | Mean | SA | 6283.333 | 6673.083 | 92.29167 | 2137341667 | 154.81088 |
| 12 | Median | SA | 5000.000 | 5563.500 | 92.30000 | 742150000 | 126.00035 |

The other way to solve problems like this is with the by function. The by function produces nicely formatted output, but its output can be manipulated if necessary. Here's the basic approach for a problem like this.

```
> byvals = by(world[,-c(1,2,8)],world$cont,function(x)apply(x,2,mmed))
world$cont: AF
    gdp income literacy military phys
[1,] 2723.404 3901.191 60.52979 356440000 26.31129
[2,] 1400.000 1813.000 65.50000 101300000 8.68680
world$cont: AS
    gdp income literacy military phys
[1,] 7778.049 8868.098 84.25122 5006536341 161.8338
[2,] 4300.000 4561.000 89.90000 650000000 139.9254
-------------------------------------------------------------------
world$cont: EU
    gdp income literacy military phys
[1,] 19711.76 21314.32 98.40294 6311138235 311.1848
[2,] 18150.00 19804.00 99.70000 1288500000 317.8858
--------------------------------------------------------------
world$cont: NA
    gdp income literacy military phys
[1,] 8946.667 10379.14 85.52 25919931267 187.0818
[2,] 4900.000 6753.00 87.70 147000000 164.4013
---------------------------------------------------------------
world$cont: OC
            gdp income literacy military phys
[1,] 14625 15547.5 87.5 4462475000 127.6311
[2,] 13700 14970.0 96.4 591500000 128.1191
world$cont: SA
    gdp income literacy military phys
```

```
[1,] 6283.333 6673.083 92.29167 2137341667 154.8109
[2,] 5000.000 5563.500 92.30000 742150000 126.0003
```

Since each piece of the byvals object looks like part of the data frame we want, we can use do.call with rbind:

```
> ans = do.call(rbind,byvals)
> head(ans)
> head(ans)
\begin{tabular}{lrrrrr} 
& gdp & income literacy & military & phys \\
{\([1]\),} & 2723.404 & 3901.191 & 60.52979 & 356440000 & 26.31129 \\
{\([2]\),} & 1400.000 & 1813.000 & 65.50000 & 101300000 & 8.68680 \\
{\([3]\),} & 7778.049 & 8868.098 & 84.25122 & 5006536341 & 161.83381 \\
{\([4]\),} & 4300.000 & 4561.000 & 89.90000 & 650000000 & 139.92540 \\
{\([5]\),} & 19711.765 & 21314.324 & 98.40294 & 6311138235 & 311.18482 \\
{\([6]\),} & 18150.000 & 19804.000 & 99.70000 & 1288500000 & 317.88580
\end{tabular}
```

As before, the continent names are stored in the unbinded object, and we need to identify the lines as mean or median.

```
> answer = data.frame(expand.grid(Stat=c('Mean','Median'),
+ Cont=names(byvals)),ans)
> answer
\begin{tabular}{lrrrrrrr} 
& \multicolumn{2}{c}{ Stat Cont } & gdp & income literacy & military & phys \\
1 & Mean & AF & 2723.404 & 3901.191 & 60.52979 & 356440000 & 26.31129 \\
2 & Median & AF & 1400.000 & 1813.000 & 65.50000 & 101300000 & 8.68680 \\
3 & Mean & AS & 7778.049 & 8868.098 & 84.25122 & 5006536341 & 161.83381 \\
4 & Median & AS & 4300.000 & 4561.000 & 89.90000 & 650000000 & 139.92540 \\
5 & Mean & EU & 19711.765 & 21314.324 & 98.40294 & 6311138235 & 311.18482 \\
6 & Median & EU & 18150.000 & 19804.000 & 99.70000 & 1288500000 & 317.88580 \\
7 & Mean & NA & 8946.667 & 10379.143 & 85.52000 & 25919931267 & 187.08178 \\
8 & Median & NA & 4900.000 & 6753.000 & 87.70000 & 147000000 & 164.40130 \\
9 & Mean & OC & 14625.000 & 15547.500 & 87.50000 & 4462475000 & 127.63105 \\
10 & Median & OC & 13700.000 & 14970.000 & 96.40000 & 591500000 & 128.11915 \\
11 & Mean & SA & 6283.333 & 6673.083 & 92.29167 & 2137341667 & 154.81088 \\
12 & Median & SA & 5000.000 & 5563.500 & 92.30000 & 742150000 & 126.00035
\end{tabular}
```

For data displays like this, it's always helpful to include the number of observations that each summary statistic represents. To do this, we first create a data frame with the counts for each continent, and then merge it with the answer:

```
> cts = as.data.frame(table(world$cont))
> head(cts)
    Var1 Freq
A AF 47
```

| 2 | AS 41 |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 3 EU 34 |  |  |  |  |  |  |  |
| 4 | NA | 15 |  |  |  |  |  |
| 5 | OC | 4 |  |  |  |  |  |
| 6 | SA 1 | 12 |  |  |  |  |  |
| > names (cts) = c ('Cont', 'N') |  |  |  |  |  |  |  |
| > both = merge(answer,cts) |  |  |  |  |  |  |  |
| > both[, c('Stat', 'Cont', 'N', names(answer[-(1:2)]))] |  |  |  |  |  |  |  |
|  | Stat | Cont N | N gdp | income | literacy | military | phys |
| 1 | Mean | AF 47 | $47 \quad 2723.404$ | 3901.191 | 60.52979 | 356440000 | 26.31129 |
| 2 | Median | AF 47 | 471400.000 | 1813.000 | 65.50000 | 101300000 | 8.68680 |
| 3 | Mean | AS 41 | 417778.049 | 8868.098 | 84.25122 | 5006536341 | 161.83381 |
| 4 | Median | AS 41 | 414300.000 | 4561.000 | 89.90000 | 650000000 | 139.92540 |
| 5 | Mean | EU 34 | 3419711.765 | 21314.324 | 98.40294 | 6311138235 | 311.18482 |
| 6 | Median | EU 34 | 3418150.000 | 19804.000 | 99.70000 | 1288500000 | 317.88580 |
| 7 | Mean | NA 15 | 158946.667 | 10379.143 | 85.52000 | 25919931267 | 187.08178 |
| 8 | Median | NA 15 | 154900.000 | 6753.000 | 87.70000 | 147000000 | 164.40130 |
| 9 | Mean | OC 4 | 414625.000 | 15547.500 | 87.50000 | 4462475000 | 127.63105 |
| 10 | Median | OC 4 | 413700.000 | 14970.000 | 96.40000 | 591500000 | 128.11915 |
| 11 | 1 Mean | SA 12 | 126283.333 | 6673.083 | 92.29167 | 2137341667 | 154.81088 |
| 12 | Median | SA 12 | 125000.000 | 5563.500 | 92.30000 | 742150000 | 126.00035 |

As a simpler example, suppose we want to find the correlation coefficient between income and literacy, once again broken down by continent.

```
> conts = split(world,world$cont)
> cors = sapply(conts,function(x)cor(x$income,x$literacy,use='complete.obs'))
cors
AF AS EU NA OC SA
0.4683727 0.2670737 0.2623438 0.6430440 0.7646586 0.6136649
```

To make a data frame, we can combine the names of the vector with the values:

```
> data.frame(Cont=names(cors),Corr=cors)
    Cont Corr
AF AF 0.4683727
AS AS 0.2670737
EU EU 0.2623438
NA NA 0.6430440
OC OC 0.7646586
SA SA 0.6136649
```

Note that the continent names also showed up as rownames in this case.
As another example of do.call, consider the task of sorting a data frame by its first column, then using the second column to break any ties, and so on for each ofthe columns of the data frame. For example:

```
> x = data.frame(matrix(sample(1:5,100,replace=TRUE),ncol=5))
> head(x)
    X1 X2 X3 X4 X5
1
2
3
4
5
6
```

Since a data frame is a list, with each element representing a column, we can order the data frame as follows:


Another interesting R function is Reduce. This function works with any binary function, that is, one which accepts two arguments, and repeatedly applies the binary function until the list is reduced to a single answer. One of the most important uses of Reduce is to merge more than two data frames at a time. Suppose we have three data frames that we wish to merge:

```
> one = data.frame(id=sample(LETTERS[1:10]),a=rnorm(10))
> two = data.frame(id=sample(LETTERS[1:10]),b=rnorm(10))
> three = data.frame(id=sample(LETTERS[1:10]),c=rnorm(10))
```

Of course, we could call merge twice:

```
> both = merge(one,two)
> both = merge(both,three)
```

But what if we had 20 such data frames:

```
> twenty = lapply(letters[1:20],function(i){
+ z = data.frame(id=sample(LETTERS[1:10]),rnorm(10))
+ names(z)[2] = i
+
> twenty[[1]]
id a
D D 1.9112203
2 F -0.7198699
J -0.4290842
4 E 0.7849467
5 B 1.5758446
l I 0.4998762
7 H 0.3568294
A A -0.8567896
9 G -0.7182695
10 C -0.6894396
> twenty[[2]]
        id b
C 2.03416915
J J 0.69535618
E -0.66387813
H -0.25343952
D -1.04782198
G G 1.56147090
7 B -0.28126409
F F -0.30900749
I I 0.52277648
10 A 0.03841634
```

We simply pass Reduce the merge function and the list of data frames, and it does the rest:


| 6 | F | -0.7198699 | -0.30900749 | -1.0955231 | -0.8593922 | 0.1585112 | 0.5434146 |
| ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
|  | g | h | i | j | k | l | m |
| 1 | 1.1469512 | 1.8675396 | -1.0730001 | -0.6306937 | 2.5853058 | 0.2524264 | 0.67496861 |
| 2 | 0.3483675 | 0.6846907 | -1.7896035 | 0.7710611 | 1.9890408 | 0.6174135 | 0.16124957 |
| 3 | -0.9972951 | -0.7140730 | 0.7919375 | 0.3678690 | 1.2336345 | -0.2323708 | -0.52465997 |
| 4 | 0.1179205 | -0.1865189 | -1.0364221 | 0.6013162 | 1.3426701 | -0.3513651 | 0.48844598 |
| 5 | -0.1171988 | -0.1514659 | 0.2650891 | 0.1813734 | 0.9233442 | -1.7945477 | -0.07855065 |
| 6 | -0.2897749 | -0.5888773 | 1.8274135 | -0.3195992 | 0.6230858 | -0.4897521 | -0.49559174 |
|  | n | o | p | q | r | s | t |
| 1 | 0.5551094 | 1.6335976 | -1.6149968 | -0.0601484 | 0.1622304 | 0.1624207 | -1.1408366 |
| 2 | 1.3832478 | -0.8993505 | -0.3657969 | -0.2817061 | 0.2501859 | -0.2096964 | -0.5082768 |
| 3 | -0.7369804 | 0.2675346 | -0.3801290 | 2.2369038 | 1.7701125 | 0.6809073 | -1.1597869 |
| 4 | 1.4028788 | -0.9317347 | 0.1623700 | -2.8401085 | -2.0066582 | -0.5500940 | 1.9968541 |
| 5 | -0.2516113 | -1.1269027 | 2.2224559 | -0.2109566 | 1.6218192 | -0.7154724 | 1.8204627 |
| 6 | 2.0342595 | -0.1864191 | -0.7241448 | 1.4295025 | -2.1206024 | 0.4883462 | -0.1468977 |

Another useful R function is reshape. This function reorganizes data in either the socalled wide or long format. In the wide format, all observations for a single individual are recorded in one row of a data frame, while in the long view, each observation is a separate row, with an additional variable to identify the observation. For example, here is a data set, in long format, representing test scores on several different observations:

```
> data = data.frame(id=rep(1:3,rep(3,3)),time=rep(1:3,3),x=rnorm(9))
> data
    id time x
1 1 1 -0.85519374
2 1 2 -0.60227681
3 1 
4 2 1 0.28097796
5 2 2 -2.20903570
6 2 3 0.08311228
7 3 1 -0.56753562
8 3 2 0.65588709
9 3 3 0.42419294
```

To convert to wide format, the following statements could be used:

```
> reshape(data,idvar='id',timevar='time',v.names='x',direction='wide')
    id x.1 x.2 x.3
1 1 -0.8551937-0.6022768 0.47671168
4 0.2809780 -2.2090357 0.08311228
7 3-0.5675356 0.6558871 0.42419294
```

Notice that not all possible combinations of observations need to be present:

```
> data1 = data[-7,]
> reshape(data1,idvar='id',timevar='time',v.names='x',direction='wide')
    id x.1 x.2 x.3
1 1 -0.8551937-0.6022768 0.47671168
4 2 0.2809780 -2.2090357 0.08311228
8 3 NA 0.6558871 0.42419294
```

The missing observations are represented as NA in the output data frame.
To illustrace the wide-to-long transformation, consider the following data:

```
> data = data.frame(id = rep(1:3),x1=c(1,2,3),x2=c(10,20,30),x3=c(100,200,300))
> data
    id x1 x2 x3
1}11111010
2 2 2 20 200
3 3 3 30 300
> reshape(data,idvar='id',varying=list(c('x1','x2','x3')),direction='long')
    id time x1
1.1 1 1 1
2.1 2 1 2
3.1 3}101
1.2 1 2 10
2.2 2 2 20
3.2 3 2 30
1.3 1 3 100
2.3 2 3 200
3.3 3 3 300
```

The trickiest part is noticing that the names of the three varying variables have to be placed in a list.

As another example of the use of reshape, consider a study looking at the BMI (Body Mass Index) of girls over time, measured for two different races. This data can be found in a tabdelimited file at http://www.stat.berkeley.edu/classes/s133/data/bmi.tab. The variables in the file are ID, RACE, BMI, and VISIT. Suppose we wish to produce a plot of the average BMI versus visit, with separate lines for the two races. We could use xyplot from the lattice package as follows:

```
> bmi = read.delim('http://www.stat.berkeley.edu/classes/s133/data/bmi.tab')
> avgbmi = aggregate(list(BMI=bmi$BMI),list(Race=bmi$RACE,Visit=bmi$VISIT),
+ mean,na.rm=TRUE)
> library(lattice)
> xyplot(BMI~Visit,group=Race,type='l',auto.key=TRUE,
+ main='BMI vs. Visit',data=avgbmi)
```



The plot appears below:
Now suppose we wish to calculate the correlations between the BMIs at the different visits. The cor function expects all of the variables for which we want the correlations to be separate columns in the data frame we pass to the function. We can rearrange the data to make it suitable for calculating the correlations by calling reshape as follows:

```
> bmi1 = reshape(bmi,idvar=c('ID','RACE'),timevar='VISIT',v.names='BMI',
+ direction='wide')
```

We can now calculate the correlations by race:

```
> by(bmi1,bmi1$RACE,function(x)cor(x[,-c(1,2)],use='complete.obs'))
bmi1$RACE: 1
    BMI.0 BMI.2 BMI.3 BMI.4 BMI.5 BMI.6 BMI.7
BMI.0 1.0000000 0.9513181 0.9238520 0.8871666 0.8489529 0.8227992 0.8018502
BMI.2 0.9513181 1.0000000 0.9490917 0.9144459 0.8625492 0.8339581 0.8110637
BMI.3 0.9238520 0.9490917 1.0000000 0.9517413 0.9025264 0.8612542 0.8327787
BMI.4 0.8871666 0.9144459 0.9517413 1.0000000 0.9458218 0.9054674 0.8781602
BMI.5 0.8489529 0.8625492 0.9025264 0.9458218 1.0000000 0.9530917 0.9105118
BMI.6 0.8227992 0.8339581 0.8612542 0.9054674 0.9530917 1.0000000 0.9568980
```

BMI. $7 \quad 0.80185020 .81106370 .83277870 .87816020 .91051180 .95689801 .0000000$ BMI. $8 \quad 0.79684330 .80260110 .81667980 .85408030 .88597620 .93197120 .9630340$ $\begin{array}{lllllllllll}\text { BMI. } 9 & 0.7888784 & 0.7931164 & 0.8042629 & 0.8351485 & 0.8690846 & 0.9107269 & 0.9316619\end{array}$ BMI. 100.76303970 .76901690 .77776770 .81316660 .84303500 .88030340 .8952306

BMI. 8 BMI. 9 BMI. 10
$\begin{array}{lllll}\text { BMI. } 0 & 0.7968433 & 0.7888784 & 0.7630397\end{array}$
$\begin{array}{lllll}\text { BMI. } 2 & 0.8026011 & 0.7931164 & 0.7690169\end{array}$
BMI. $3 \quad 0.81667980 .80426290 .7777677$
BMI. 40.85408030 .83514850 .8131666
BMI. 50.88597620 .86908460 .8430350
BMI. 60.93197120 .91072690 .8803034
BMI. $7 \quad 0.96303400 .93166190 .8952306$
BMI. 81.00000000 .95962250 .9209648
BMI. $9 \quad 0.95962251 .00000000 .9488572$
BMI. 100.92096480 .94885721 .0000000
bmi1\$RACE: 2
$\begin{array}{llllll}\text { BMI. } 0 & \text { BMI. } 2 & \text { BMI. } 3 & \text { BMI. } 4 & \text { BMI. } 5 & \text { BMI. } 6\end{array}$ BMI.7
BMI. $0 \quad 1.00000000 .96282730 .92817800 .90106070 .86467730 .84103840 .8173900$
BMI. $2 \quad 0.96282731 .00000000 .96079640 .93340430 .89404980 .87300590 .8543804$
BMI. $3 \quad 0.92817800 .96079641 .00000000 .96561330 .93007070 .90811400 .8886918$
BMI. $4 \quad 0.90106070 .93340430 .96561331 .00000000 .96052750 .93788500 .9130036$
BMI. $5 \quad 0.86467730 .89404980 .93007070 .96052751 .00000000 .97224810 .9465896$
BMI. $6 \quad 0.84103840 .87300590 .9081140 \quad 0.93788500 .97224811 .00000000 .9751832$
BMI. $7 \quad 0.81739000 .85438040 .8886918 \quad 0.9130036 \quad 0.94658960 .97518321 .0000000$
$\begin{array}{llllllllllll}\text { BMI. } 8 & 0.8051828 & 0.8423513 & 0.8746659 & 0.8979719 & 0.9293276 & 0.9561339 & 0.9769345\end{array}$
BMI. $9 \quad 0.8003754 \quad 0.83897260 .8689569 \quad 0.8868970 \quad 0.91472810 .94102880 .9582904$ BMI. 100.78622790 .82245670 .84643510 .86405170 .88941210 .91575460 .9316408

BMI. 8 BMI. 9 BMI. 10
$\begin{array}{lllll}B M I . O & 0.8051828 & 0.8003754 & 0.7862279\end{array}$
$\begin{array}{lllll}\text { BMI. } 2 & 0.8423513 & 0.8389726 & 0.8224567\end{array}$
BMI. $3 \quad 0.87466590 .86895690 .8464351$
BMI. $4 \quad 0.89797190 .88689700 .8640517$
BMI. $5 \quad 0.92932760 .91472810 .8894121$
BMI. $6 \quad 0.95613390 .94102880 .9157546$
$\begin{array}{llll}\text { BMI. } 7 & 0.9769345 & 0.9582904 & 0.9316408\end{array}$
BMI. 8 1.0000000 0.9767038 0.9460700
BMI. $9 \quad 0.97670381 .00000000 .9675484$
BMI. 10 0.9460700 0.96754841 .0000000
Not surprisingly, there's a very high correlation between the BMI at the different visits for both races.

## Chapter 9

## Classification Analysis

### 9.1 Introduction to Classification Methods

When we apply cluster analysis to a dataset, we let the values of the variables that were measured tell us if there is any structure to the observations in the data set, by choosing a suitable metric and seeing if groups of observations that are all close together can be found. If we have an auxilliary variable (like the country of origin from the cars example), it may be interesting to see if the natural clustering of the data corresponds to this variable, but it's important to remember that the idea of clustering is just to see if any groups form naturally, not to see if we can actually figure out which group an observation belongs to based on the values of the variables that we have.

When the true goal of our data analysis is to be able to predict which of several nonoverlapping groups an observation belongs to, the techniques we use are known as classification techniques. We'll take a look at three classification techniques: kth nearest neighbor classification, linear discrimininant analysis, and recursive partitioning.

## 9.2 kth Nearest Neighbor Classification

The idea behind nearest neighbor classification is simple and somewhat intuitive - find other observations in the data that are close to an observation we're interested, and classify that observation based on the class of its neighbors. The number of neighbors that we consider is where the " $k$ " comes in - usually we'll have to look at several different values of $k$ to determine which ones work well with a particular data set. Values in the range of one to ten are usually reasonable choices.

Since we need to look at all of the distances between one observation and all the others in order to find the neighbors, it makes sense to form a distance matrix before starting a nearest neighbor classification. Each row of the distance matrix tells us the distances to all the other observations, so we need to find the k smallest values in each row of the distance matrix. Once we find those smallest values, we determine which observations they belong to, and look at how those observations were classified. We assign whichever value of the classification that was most common among the k nearest neighbors as our guess (predicted value) for the current observation, and then move on to the next row of the distance matrix. Once we've looked at every row of the distance matrix, we'll have classified every observation, and can compare the predicted classification with the actual classification. To see how well we've done, various error rates can be examined. If the observations are classified as TRUE / FALSE, for example disease or no disease, then we can look at two types of error rates. The first type of error rate, known as Type I error, occurs when we say that an observation should be classified as TRUE when it really should have been FALSE. The other type of error (Type II) occurs when we say that an observation should be classified as FALSE when it should have been TRUE. When the classification is something other than TRUE/FALSE, we can report an overall error rate, that is, the fraction of observations for which our prediction was not correct. In either case, the error rates can be calculated in $R$ by using the table function. As a simple example, suppose we have two vectors: actualvalues, which contains
the actual values of a classification variable, and predvalues, the value that our classification predicted:

```
> actualvalues = c(TRUE,TRUE,TRUE,FALSE,FALSE,TRUE,FALSE,TRUE,FALSE,FALSE)
> predvalues = c(TRUE,TRUE,TRUE,TRUE,FALSE,FALSE,FALSE,TRUE,FALSE,TRUE)
> tt = table(actualvalues,predvalues)
> tt
            predvalues
actualvalues FALSE TRUE
    FALSE 3 2
    TRUE 1 4
```

The observations that contribute to Type I error (the actual value is false but we predicted true) can be found in the first row and second column; those that contribute to Type II error can be found in the second row and first column. Since the table function returns a matrix, we can calculate the rows as follows:

```
> tot = sum(tt)
> type1 = tt['FALSE','TRUE'] / tot
> type2 = tt['TRUE','FALSE'] / tot
> type1
[1] 0.2
> type2
[1] 0.1
```


### 9.3 Cross Validation

There's one problem with the above scheme. We used the data that we're making predictions about in the process of making those predictions. In other words, the data that we're making predictions for is not independent of the data that we're using to make the predictions. As might be expected, it's been shown in practice that calculating error rates this way will almost always make our classification method look better than it should be. If the data can be naturally (or even artificially) divided into two groups, then one can be used as a training set, and the other can be used as a test set - we'd calculate our error rates only from the classification of the test set using the training set to make our predictions. Many statisticians don't like the idea of having to "hold back" some of their data when building models, so an alternative way to bring some independence to our predictions known as vfold cross validation has been devised. The idea is to first divide the entire data set into v groups. To classify objects in the first group, we don't use any of the first group to make our predictions; in the case of k-th nearest neighbor classification, that would mean that when we're looking for the smallest distances in order to classify an observation, we don't consider any of the distances corresponding to other members of the same group that the current one belongs to. The basic idea is that we want to make the prediction for an observation as
independent from that observation as we can. We continue through each of the v groups, classifying observations in each group using only observations from the other groups. When we're done we'll have a prediction for each observation, and can compare them to the actual values as in the previous example.

Another example of cross-validation is leave-out-one cross-validation. With this method, we predict the classification of an observation without using the observation itself. In other words, for each observation, we perform the analysis without using that observation, and then predict where that observation would be classified using that analysis.

### 9.4 Linear Discriminant Analysis

One of the oldest forms of classification is known as linear discriminant analysis. The idea is to form linear combinations of predictor variables (similar to a linear regression model) in such a way that the average value of these linear combinations will be as different as possible for the different levels of the classification variable. Based on the values of the linear combinations, linear discriminant analysis reports a set of posterior probabilities for every level of the classification, for each observation, along with the level of the classification variable that the analysis predicted. Suppose we have a classification variable that can take one of three values: after a linear discriminant analysis, we will have three probabilities (adding up to one) for each variable that tell how likely it is that the observation be categorized into each of the three categories; the predicted classificiation is the one that had the highest probability, and we can get insight into the quality of the classification by looking at the values of the probabilities.

To study the different classification methods, we'll use a data set about different wines. This data set contains various measures regarding chemical and other properties of the wines, along with a variable identifying the Cultivar (the particular variety of the grape from which the wine was produced). We'll try to classify the observations based on the Cultivar, using the other variables. The data is available at http://www.stat.berkeley.edu/classes/s133/data/wine.data; information about the variables is at http://www.stat.berkeley.edu/classes/s133/data/wine.names

First, we'll read in the wine dataset:

```
wine = read.csv('http://www.stat.berkeley.edu/classes/s133/data/wine.data',header=FALSE)
names(wine) = c("Cultivar", "Alcohol", "Malic.acid", "Ash", "Alkalinity.ash",
    "Magnesium", "Phenols", "Flavanoids", "NF.phenols", "Proanthocyanins",
    "Color.intensity","Hue", "OD.Ratio", "Proline")
wine$Cultivar = factor(wine$Cultivar)
```

Notice that I set wine\$Cultivar to be a factor. Factors are very important and useful in modeling functions because categorical variables almost always have to be treated differently than numeric variables, and turning a categorical variable into a factor will insure that they are always used properly in modeling functions. Not surprisingly, the dependent variable for lda must be a factor.

The class library of R provides two functions for nearest neighbor classification. The first, knn, takes the approach of using a training set and a test set, so it would require holding back some of the data. The other function, knn.cv uses leave-out-one cross-validation, so it's more suitable to use on an entire data set.

Let's use knn.cv on the wine data set. Since, like cluster analysis, this technique is based on distances, the same considerations regarding standardization as we saw with cluster analysis apply. Let's examine a summary for the data frame:

| Cultivar Alcohol Malic.acid Ash Alkalinity.ash |  |  |  |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| 1:59 | Min. | :11.03 | Min. | :0.740 | Min. | :1.360 | Min. | 10.60 |
| 2:71 | 1st Qu. | : 12.36 | 1st Qu. | :1.603 | 1st Qu | :2.210 | 1st Qu | : 17.20 |
| 3:48 | Median | :13.05 | Median | :1.865 | Median | :2.360 | Median | :19.50 |
|  | Mean | :13.00 | Mean | :2.336 | Mean | :2.367 | Mean | :19.49 |
|  | 3rd Qu. | :13.68 | 3rd Qu. | 3.083 | 3rd Qu | :2.558 | 3rd Qu | :21.50 |
|  | Max. | : 14.83 | Max. | :5.800 | Max. | :3.230 | Max. | :30.00 |
| Magnesium |  | Phenols |  | Flavanoids |  | NF.phenols |  |  |
| Min. | 70.00 | Min. | :0.980 | Min. | :0.340 | Min. | :0.1300 |  |
| 1st Qu.: | 88.00 | 1st Qu | :1.742 | 1 st Qu | :1.205 | 1st Qu. | :0.2700 |  |
| Median : | 98.00 | Median | :2.355 | Median | :2.135 | Median | $: 0.3400$ |  |
| Mean : | 99.74 | Mean | :2.295 | Mean | :2.029 | Mean | :0.3619 |  |
| 3rd Qu.:1 | 107.00 | 3rd Qu | :2.800 | 3rd Qu | :2.875 | 3rd Qu | :0.4375 |  |
| Max. :1 | 162.00 | Max. | :3.880 | Max. | :5.080 | Max. | :0.6600 |  |
| Proanthoc | cyanins | Color.in | ntensity | Hue |  | OD.Ratio |  |  |
| Min. :0 | 0.410 | Min. | 1.280 | Min. | :0.4800 | Min. | :1.270 |  |

```
1st Qu.:1.250 1st Qu.: 3.220 1st Qu.:0.7825 1st Qu.:1.938
Median :1.555 Median : 4.690 Median :0.9650 Median :2.780
Mean :1.591 Mean : 5.058 Mean :0.9574 Mean :2.612
3rd Qu.:1.950 3rd Qu.: 6.200 3rd Qu.:1.1200 3rd Qu.:3.170
Max. :3.580 Max. :13.000 Max. :1.7100 Max. :4.000
    Proline
Min. : 278.0
1st Qu.: 500.5
Median : 673.5
Mean : 746.9
3rd Qu.: 985.0
Max. :1680.0
```

Since the scale of the variables differ widely, standardization is probably a good idea. We'll divide each variable by its standard deviation to try to give each variable more equal weight in determining the distances:

```
> wine.use = scale(wine[,-1],scale=apply(wine[,-1],2,sd))
> library(class)
> res = knn.cv(wine.use,wine$Cultivar,k=3)
> names(res)
NULL
> length(res)
[1] }17
```

Since there are no names, and the length of res is the same as the number of observations, knn.cv is simply returning the classifications that the method predicted for each observation using leave-out-one cross validation. This means we can compare the predicted values to the true values using table:

```
> table(res,wine$Cultivar)
res 1 2 3
    159 4 0
    2 0 63 0
    3 0 4 48
```

To calculate the proportion of incorrect classifications, we can use the row and col functions. These unusual functions don't seem to do anything very useful when we simply call them:

```
> tt = table(res,wine$Cultivar)
> row(tt)
\begin{tabular}{lrrr}
{\([, 1]\)} & {\([, 2]\)} & {\([, 3]\)} \\
{\([1]\),} & 1 & 1 & 1
\end{tabular}
```

| $[2]$, | 2 | 2 | 2 |
| :--- | ---: | ---: | ---: |
| $[3]$, | 3 | 3 | 3 |
| $>\operatorname{col}(t t)$ |  |  |  |
|  | $[, 1]$ | $[, 2]$ | $[, 3]$ |
| $[1]$, | 1 | 2 | 3 |
| $[2]$, | 1 | 2 | 3 |
| $[3]$, | 1 | 2 | 3 |

However, if you recall that the misclassified observations are those that are off the diagonal, we can find those observations as follows:

```
> tt[row(tt) != col(tt)]
[1] 0 0 4 4 0 0
```

and the proportion of misclassified observations can be calculated as:

```
> sum(tt[row(tt) != col(tt)]) / sum(tt)
[1] 0.04494382
```

or a missclassification rate of about 4.5
Could we have done better if we used 5 nearest neighbors instead of 3 ?

```
> res = knn.cv(wine.use,wine$Cultivar,k=5)
> tt = table(res,wine$Cultivar)
> sum(tt[row(tt) != col(tt)]) / sum(tt)
[1] 0.02808989
```

How about using just the single nearest neighbor?

```
> res = knn.cv(wine.use,wine$Cultivar,k=1)
> tt = table(res,wine$Cultivar)
> sum(tt[row(tt) != col(tt)]) / sum(tt)
[1] 0.04494382
```

For this data set, using $\mathrm{k}=5$ did slightly better than 1 or 3 .
In R, linear discriminant analysis is provided by the lda function from the MASS library, which is part of the base R distribution.

Like many modeling and analysis functions in R, lda takes a formula as its first argument. A formula in R is a way of describing a set of relationships that are being studied. The dependent variable, or the variable to be predicted, is put on the left hand side of a tilda $\left(^{\sim}\right)$ and the variables that will be used to model or predict it are placed on the right hand side of the tilda, joined together by plus signs (+). To save typing, you an provide the name of a data frame through the data= argument, and use the name of the variables in the data frame in your formula without retyping the data frame name or using the with function.

A convenience offered by the modeling functions is that a period (.) on the right-hand side of the tilda in a formula is interpreted as meaning "all the other variables in the data
frame, except the dependent variable". So a very popular method of specifying a formula is to use the period, and then use subscripting to limit the data= argument to just the variables you want to fit. In this example, we don't need to do that, because we really do want to use all the variables in the data set.

```
> wine.lda = lda(Cultivar ~ .,data=wine)
```

We'll see that most of the modeling functions in R share many things in common. For example, to predict values based on a model, we pass the model object to the predict function along with a data frame containing the observations for which we want predictions:

```
> pred = predict(wine.lda,wine)
```

To see what's available from the call to predict, we can look at the names of the pred object:

```
> names(pred)
[1] "class" "posterior" "x"
```

The predicted classification is stored in the class component of the object returned by predict Now that we've got the predicted classes, we can see how well the classification went by making a cross-tabulation of the real Cultivar with our prediction, using the table function:

```
> table(wine$Cultivar,pred$class)
    predclass
        1 2 3
    159 0 0
    2 071 0
    3 0}004
```

Before we get too excited about these results, remember the caution about predicting values based on models that were built using those values. The error rate we see in the table (0) is probably an overestimate of how good the classification rule is. We can use v-fold cross validation on the data, by using the lda command repeatedly to classify groups of observations (folds) using the rest of the data to build the model. We could write this out "by hand", but it would be useful to have a function that could do this for us. Here's such a function:

```
vlda = function(v,formula,data,cl){
    require(MASS)
    grps = cut(1:nrow(data),v,labels=FALSE)[sample(1:nrow(data))]
    pred = lapply(1:v,function(i,formula,data){
        omit = which(grps == i)
        z = lda(formula,data=data[-omit,])
        predict(z,data[omit,])
        },formula,data)
```

```
    wh = unlist(lapply(pred,function(pp)pp$class))
    table(wh,cl[order(grps)])
}
```

This function accepts four arguments: v, the number of folds in the cross classification, formula which is the formula used in the linear discriminant analysis, data which is the data frame to use, and cl, the classification variable (wine\$Cultivar in this case).

By using the sample function, we make sure that the groups that are used for crossvalidation aren't influenced by the ordering of the data - notice how the classification variable (cl) is indexed by order (grps) to make sure that the predicted and actual values line up properly.

Applying this function to the wine data will give us a better idea of the actual error rate of the classifier:

```
> vlda(5,Cultivar~.,wine,wine$Cultivar)
wh 1 2 3
    159 1 0
    2 0 69 1
    3 0
```

While the error rate is still very good, it's not quite perfect:

```
> error = sum(tt[row(tt) != col(tt)]) / sum(tt)
> error
```

[1] 0.01685393

Note that because of the way we randomly divide the observations, you'll see a slightly different table every time you run the vlda function.

We could use a similar method to apply v-fold cross-validation to the kth nearest neighbor classification. Since the knn function accepts a training set and a test set, we can make each fold a test set, using the remainder of the data as a training set. Here's a function to apply this idea:

```
vknn = function(v,data,cl,k){
    grps = cut(1:nrow(data),v,labels=FALSE)[sample(1:nrow(data))]
    pred = lapply(1:v,function(i,data,cl,k){
        omit = which(grps == i)
        pcl = knn(data[-omit,],data[omit,],cl[-omit],k=k)
        },data,cl,k)
    wh = unlist(pred)
    table(wh,cl[order(grps)])
}
```

Let's apply the function to the standardized wine data:

```
> tt = vknn(5,wine.use,wine$Cultivar,5)
> tt
wh 1 2 3
    159 2 0
    2 0 66 0
    3 0 3 48
> sum(tt[row(tt) != col(tt)]) / sum(tt)
[1] 0.02808989
```

Note that this is the same misclassification rate as acheived by the "leave-out-one" cross validation provided by knn.cv.

Both the nearest neighbor and linear discriminant methods make it possible to classify new observations, but they don't give much insight into what variables are important in the classification. The scaling element of the object returned by lda shows the linear combinations of the original variables that were created to distinguish between the groups:

```
> wine.lda$scaling
```

|  | LD1 | LD2 |
| :--- | ---: | ---: |
| Alcohol | -0.403399781 | 0.8717930699 |
| Malic.acid | 0.165254596 | 0.3053797325 |
| Ash | -0.369075256 | 2.3458497486 |
| Alkalinity.ash | 0.154797889 | -0.1463807654 |
| Magnesium | -0.002163496 | -0.0004627565 |
| Phenols | 0.618052068 | -0.0322128171 |
| Flavanoids | -1.661191235 | -0.4919980543 |
| NF.phenols | -1.495818440 | -1.6309537953 |
| Proanthocyanins | 0.134092628 | -0.3070875776 |
| Color.intensity | 0.355055710 | 0.2532306865 |
| Hue | -0.818036073 | -1.5156344987 |
| OD.Ratio | -1.157559376 | 0.0511839665 |
| Proline | -0.002691206 | 0.0028529846 |

It's really not that easy to interpret them, but variables with large absolute values in the scalings are more likely to influence the process. For this data, Flavanoids, NF.phenols, Ash, and Hue seem to be among the important variables.

A different way to get some insight into this would be to examine the means of each of the variables broken down by the classification variable. Variables which show a large difference among the groups would most likely be the ones that are useful in predicting which group an observation belongs in. One graphical way of displaying this information is with a barplot. To make sure we can see differences for all the variables, we'll use the standardized version of the data:

```
> mns = aggregate(wine.use,wine['Cultivar'],mean)
```

```
> rownames(mns) = mns$Cultivar
> mns$Cultivar = NULL
> barplot(as.matrix(mns),beside=TRUE,cex.names=.8,las=2)
```

The las parameter rotates the labels on the x -axis so that we can see them all. Here's the plot:


It seems like the big differences are found in Flavanoids, Hue and OD. Ratio
Now let's take a look at a method that makes it very clear which variables are useful in distinguishing among the groups.

### 9.5 Recursive Partitioning

An alternative classification method, developed in the 1980s, has attracted a lot of attention in a variety of different fields. The technique, known as recursive partitioning or CART (Classification and Regression Trees), can be use for either classification or regression - here we'll concentrate on its use for classification. The basic idea is to examine, for each of the variables that we're using in our classification model, the results of splitting the data set
based on one of the values of that variable, and then examining how that split helps us distinguish between the different classes of interest. For example, suppose we're using just one variable to help distinguish between two classes:

```
> mydata = data.frame(x=c(7,12,8,3,4,9,2,19),grp=c(1,2,1,1,1,2,2,2))
> mydata
    x grp
1 7 1
2 12 2
3
4 3 1
5 4 1
6 9 2
7 2 2
819 2
```

We'd consider each value of x in the data, and split the data into two groups: one where x was less than or equal to the value and the other where x is greater than the value. We then look at how our classification variable (grp in this example) breaks down when the data is split this way. For this example, we can look at all the possible cross-tabulations:

```
> tbls = sapply(mydata$x,function(val)table(mydata$x <= val,mydata$grp))
> names(tbls) = mydata$x
> tbls
> tbls
$"7"
    12
    FALSE 1 3
    TRUE 3 1
$"12"
    12
    FALSE 0 1
    TRUE 4 3
$"8"
    12
    FALSE 0 3
    TRUE 4 1
```

```
$"3"
```

12
FALSE 33
TRUE 11
\$"4"

12
FALSE 23
TRUE 21
\$"9"

12
FALSE 02
TRUE 42
\$"2"
12
FALSE 43
TRUE 01
\$"19"

12
TRUE 44

If you look at each of these tables, you can see that when we split with the rule x <= 8, we get the best separation; all three of the cases where x is greater than 8 are classified as 2 , and four out of five of the cases where $x$ is less than 8 are classified as 1 . For this phase of a recursive partitioning, the rule $\mathrm{x}<=8$ would be chosen to split the data.

In real life situations, where there will always be more than one variable, the process would be repeated for each of the variables, and the chosen split would the one from among all the variables that resulted in the best separation or node purity as it is sometimes known. Now that we've found the single best split, our data is divided into two groups based on that split. Here's where the recursive part comes in: we keep doing the same thing to each side of the split data, searching through all values of all variables until we find the one that gives us the best separation, splitting the data by that value and then continuing. As implemented in R through the rpart function in the rpart library, cross validation is used internally to
determine when we should stop splitting the data, and present a final tree as the output. There are also options to the rpart function specifying the minimum number of observations allowed in a split, the minimum number of observations allowed in one of the final nodes and the maximum number of splits allowed, which can be set through the control= argument to rpart. See the help page for rpart. control for more information.

To show how information from recursive partitioning is displayed, we'll use the same data that we used with lda. Here are the commands to run the analysis:

```
> library(rpart)
> wine.rpart = rpart(Cultivar~.,data=wine)
> wine.rpart
n= 178
node), split, n, loss, yval, (yprob)
    * denotes terminal node
1) root 178 107 2 (0.33146067 0.39887640 0.26966292)
    2) Proline>=755 67 10 1 (0.85074627 0.05970149 0.08955224)
    4) Flavanoids>=2.165 59 2 1 (0.96610169 0.03389831 0.00000000) *
    5) Flavanoids< 2.165 8 2 3 (0.00000000 0.25000000 0.75000000) *
    3) Proline< 755 111 44 2 (0.01801802 0.60360360 0.37837838)
    6) OD.Ratio>=2.115 65 4 2 (0.03076923 0.93846154 0.03076923) *
    7) OD.Ratio< 2.115 46 6 3 (0.00000000 0.13043478 0.86956522)
        14) Hue>=0.97 2 2 (0.00000000 0.71428571 0.28571429) *
        15) Hue< 0.9 39 1 3 (0.00000000 0.02564103 0.97435897) *
```

The display always starts at the root (all of the data), and reports the splits in the order they occured. So after examining all possible values of all the variables, rpart found that the Proline variable did the best job of dividing up the observations into the different cultivars; in particular of the 67 observations for which Proline was greater than 755 , the fraction that had Cultivar $==1$ was .8507 . Since there's no asterisk after that line, it indicates that rpart could do a better job by considering other variables. In particular if Proline was $i=755$, and Flavanoids was $i=2.165$, the fraction of Cultivar 1 increases to .9666 ; the asterisk at the end of a line indicates that this is a terminal node, and, when classifying an observation if Proline was $i=755$ and Flavanoids was $i=2.165$, rpart would immediately assign it to Cultivar 1 without having to consider any other variables. The rest of the output can be determined in a similar fashion.

An alternative way of viewing the output from rpart is a tree diagram, available through the plot function. In order to identify the parts of the diagram, the text function also needs to be called.

```
> plot(wine.rpart)
> text(wine.rpart,use.n=TRUE,xpd=TRUE)
```

The xpd=TRUE is a graphics parameter that is useful when a plot gets truncated, as sometimes happens with rpart plots. There are other options to plot and text which will change the appearance of the output; you can find out more by looking at the help pages for plot.rpart and text.rpart. The graph appears below.


In order to calculate the error rate for an rpart analysis, we once again use the predict function:

```
> pred.rpart = predict(wine.rpart,wine)
```

As usual we can check for names to see how to access the predicted values:

```
> names(pred.rpart)
NULL
```

Since there are no names, we'll examine the object directly:

```
> head(pred.rpart)
    1 2 3
10.96610169 0.03389831 0.00000000
2 0.96610169 0.03389831 0.00000000
3 0.96610169 0.03389831 0.00000000
40.96610169 0.03389831 0.00000000
50.03076923 0.93846154 0.03076923
60.96610169 0.03389831 0.00000000
```

All that predict returns in this case is a matrix with estimated probabilities for each cultivar for each observation; we'll need to find which one is highest for each observation. Doing it for one row is easy:

```
> which.max(rped.rpart[1,])
1
1
```

To repeat this for each row, we can pass which.max to apply, with a second argument of 1 to indicate we want to apply the function to each row:

```
> table(apply(pred.rpart,1,which.max),wine$Cultivar)
```

|  | 1 | 2 | 3 |
| ---: | ---: | ---: | ---: |
| 1 | 57 | 2 | 0 |
| 2 | 2 | 66 | 4 |
| 3 | 0 | 3 | 44 |

To compare this to other methods, we can again use the row and col functions:
> sum(tt[row(tt) != col(tt)]) / sum(tt)
[1] 0.06179775
Since rpart uses cross validation internally to build its decision rules, we can probably trust the error rates implied by the table.

## Chapter 10

## Simulations

### 10.1 Hypothesis Testing

Much of classical statistics is concerned with the idea of hypothesis testing. This is a formal framework that we can use to pose questions about a variety of topics in a consistent form that lets us apply statistical techniques to make statements about how results that we've gathered relate to questions that we're interested in. If we carefully follow the rules of hypothesis testing, then we can confidently talk about the probability of events that we've observed under a variety of hypotheses, and put our faith in those hypotheses that seem the most reasonable. Central to the idea of hypothesis testing is the notion of null and alternative hypotheses. We want to present our question in the form of a statement that assumes that nothing has happened (the null hypothesis) versus a statement that describes a specific relation or condition that might better explain our data.

For example, suppose we've got a coin, and we want to find out if it's true, that is, if, when we flip the coin, are we as likely to see heads as we are to see tails. A null hypothesis for this situation could be
$H_{0}$ : We're just as likely to get heads as tails when we flip the coin.
A suitable alternative hypothesis might be:
$H_{a}$ : We're more likely to see either heads or tails when we flip the coin.
An alternative hypothesis such as this is called two-sided, since we'll reject the null hypothesis if heads are more likely or if tails are more likely. We could use a one-sided alternative hypothesis like "We're more likely to see tails than heads," but unless you've got a good reason to believe that it's absolutely impossible to see more heads than tails, we usually stick to two-sided alternative hypotheses.

Now we need to perform an experiment in order to help test our hypothesis. Obviously, tossing the coin once or twice and counting up the results won't help very much. Suppose I say that in order to test the null hypothesis that heads are just as likely as tails, I'm going to toss the coin 100 times and record the results. Carrying out this experiment, I find that I saw 55 heads and 45 tails. Can I safely say that the coin is true? Without some further guidelines, it would be very hard to say if this deviation from $50 / 50$ really provides much evidence one way or the other. To proceed any further, we have to have some notion of what we'd expect to see in the long run if the null hypothesis was true. Then, we can come up with some rule to use in deciding if the coin is true or not, depending on how willing we are to make a mistake. Sadly, we can't make statements with complete certainty, because there's always a chance that, even if the coin was true, we'd happen to see more heads than tails, or, conversely, if the coin was weighted, we might just happen to see nearly equal numbers of heads and tails when we tossed the coin many times. The way we come up with our rule is by stating some assumptions about what we'd expect to see if the null hypothesis was true, and then making a decision rule based on those assumptions. For tossing a fair coin (which is what the null hypothesis states), most statisticians agree that the number of heads (or tails) that we would expect follows what is called a binomial distribution. This distribution takes
two parameters: the theoretical probability of the event in question (let's say the event of getting a head when we toss the coin), and the number of times we toss the coin. Under the null hypothesis, the probability is .5 . In R , we can see the expected probability of getting any particular number of heads if we tossed a coin 100 times by plotting the density function for the binomial distribution with parameters 100 and .5 .
> barplot(dbinom(1:100,100,.5), names.arg=1:100)


As you'd probably expect, the most common value we'd see would be 50 , but there are lots of reasonable values that aren't exactly 50 that would also occur pretty often. So to make a decision rule for when we will reject the null hypothesis, we would first decide how often we're willing to reject the null hypothesis when it was actually true. For example, looking at the graph, there's a tiny probability that we'd see as few as 30 heads or as many as 70 heads when we tossed a true coin 100 times. But if we tossed a coin 100 times and only saw 30 heads, we'd be wise if we said the coin wasn't true because 30 heads out of 100 is such a rare event. On the other hand, we can see on the graph that the probability of getting, say 45 heads is still pretty high, and we might very well want to accept the null hypothesis in this case. Without any compelling reason to choose otherwise, people usually will accept an error of $5 \%$ when performing a hypothesis test, although you might want to alter that value in situations when making such an error is more or less of a problem than usual. With a two-sided hypothesis like this one, to come up with a decision rule that would be wrong only $5 \%$ of the time, we'd need to find the number of heads for which we'd see fewer heads $2.5 \%$ of the time, and the number of heads for which we'd see more heads $2.5 \%$ of the time. To find quantities like this for the binomial distribution, we can use the qbinom function. The lower limit we want is the result of calling qbinom with an argument of 0.025 , and the upper limit is the result of calling qbinom with an argument of 0.975 :

```
> qbinom(.025,100,.5)
[1] 40
> qbinom(.975,100,.5)
[1] 60
```

So in this experiment, if the number of heads we saw was between 40 and 60 (out of 100 tosses), we would tentatively accept the null hypothesis; formally we would say that there's not enough evidence to reject the null hypothesis. If we saw fewer than 40 or more than 60 tosses, we would say we had enough evidence to reject the null hypothesis, knowing that we would be wrong only $5 \%$ of the time. When we reject the null hypothesis when it was actually true, it's said to be a Type I error. So in this example, we're setting the Type I error rate to $5 \%$.

To summarize, the steps for performing a hypothesis test are:

1. Describe a null hypothesis and an alternative hypothesis.
2. Specify a significance or alpha level for the hypothesis test. This is the percent of the time that you're willing to be wrong when you reject the null hypothesis.
3. Formulate some assumptions about the distribution of the statistic that's involved in the hypothesis test. In this example we made the assumption that a fair coin follows a binomial distribution with $\mathrm{p}=0.50$.
4. Using the assumptions you made and the alpha level you decided on, construct the rejection region for the test, that is, the values of the statistic for which you'll be willing to reject the null hypothesis. In this example, the rejection region is broken up into two sections: less than 40 heads and more than 60 heads.

Although it's not always presented in this way, one useful way to think about hypothesis testing is that if you follow the above steps, and your test statistic is in the rejection region then either the null hypothesis is not reasonable or your assumptions are wrong. By following this framework, we can test a wide variety of hypotheses, and it's always clear exactly what we're assuming about the data.

Most of hypothesis testing is focused on the null hypothesis, and on possibly rejecting it. There are two main reasons for this. First, there is only one null hypothesis, so we don't have to consider a variety of possibilities. Second, as we've seen, it's very easy to control the error rate when rejecting the null hypothesis. The other side of the coin has to do with the case where the null hypothesis is not true. This case is much more complicated because there are many different ways to reject the null hypothesis, and it would be naive to believe that they'd all behave the same way. When the null hypothesis is not true, we might mistakenly accept the null hypothesis anyway. Just as we might see an unusually high number of heads for a true coin, we might coincidentally see nearly equal numbers of heads and tails with a coin that was actually weighted. The case where the null hypothesis is not true, but we fail to reject it results in a Type II error. Type II error is usually expressed as power, which is 1 minus the probability of making an error. Power is the proportion of the time that you
correctly reject the null hypothesis when it isn't true. Notice that the power of a hypothesis test changes depending on what the alternative is. In other words, it makes sense that if we had a coin that was so heavily weighted that it usually had a probability of 0.8 of getting heads, we'd have more power in detecting the discrepancy from the null distribution than if our coin was only weighted to give a 0.55 probability of heads. Also, unlike Type I error, we can't set a Type II error rate before we start the analysis - the only way to change the Type II error rate is to get more samples or redesign the experiment.

### 10.2 Determining Power

For many years, the only way to answer questions about power required complex mathematical computations, and power was often ignored because sometimes it was too difficult or even impossible to calculate. Even if it was easy to calculate, the fact that power varies depending on the alternative hypothesis would make considering power a much more difficult task than thinking about Type I error. But more recently, statisticians have come to realize that it's often a good idea to estimate power for alternative hypotheses of interest.

Using computers, we can calculate the power of any alternative hypothesis we please by doing the following:

1. Follow the general hypothesis testing procedure outlined above.
2. Repeatedly generate simulated data which corresponds to an alternative hypothesis that you're interested in. For each set of data that you simulate (sometimes refered to as a trial), calculate the statistic, and decide whether to reject the null hypothesis or not.
3. When you're done with all the trials, count how often you (correctly) rejected the null hypothesis, and divide by the total number of trials to obtain the power of the experiment for that specific alternative distribution.

To generate random values from the binomial distribution, to simulate a coin toss, we can use the rbinom function. You pass this function the number of samples you'd like, the size of the sample, and the probability. Before diving into the power computation, let's verify that, when the null hypothesis is true, using the rejection region we developed previously will actually result in a Type I error rate of $5 \%$. First, let's simulate a single set of 100 tosses a few times to see if it makes sense

```
> rbinom(1,100,.5)
[1] 45
> rbinom(1,100,.5)
[1] 52
> rbinom(1,100,.5)
[1] 52
> rbinom(1,100,.5)
[1] 46
```

That seems reasonable. Now let's generate 1000 such samples, and count how many of them had less than 40 heads or more than 60 heads:

```
> rr = rbinom(1000,100,.5);sum(rr<40|rr>60)/1000
[1] 0.042
> rr = rbinom(1000,100,.5);sum(rr<40|rr>60)/1000
[1] 0.03
> rr = rbinom(1000, 100,.5);sum(rr<40|rr>60)/1000
[1] 0.043
> rr = rbinom(1000,100,.5);sum(rr<40|rr>60)/1000
[1] 0.029
```

The values are a little low, but it's because we've got a discrete distribution and we had to choose the nearest integer value of heads. To see the exact probabilities that the values 40 and 60 represent, we can use the pbinom function:

```
> pbinom(40,100,.5)
[1] 0.02844397
> pbinom(60,100,.5)
[1] 0.9823999
```

If we make the rejection region larger, then the probability will become too high:

```
> rr = rbinom(1000, 100,.5);sum(rr<41|rr>59)/1000
[1] 0.054
> rr = rbinom(1000,100,.5);sum(rr<41|rr>59)/1000
[1] 0.064
> rr = rbinom(1000,100,.5);sum(rr<41|rr>59)/1000
[1] 0.056
> rr = rbinom(1000, 100,.5);sum(rr<41|rr>59)/1000
[1] 0.068
> rr = rbinom(1000,100,.5);sum(rr<41|rr>59)/1000
[1] 0.064
```

So it seems that the idea of using less than 40 or greater than 60 as a rejection region will give us a Type I error as close to $5 \%$ as is possible.

### 10.3 Determining Power

Now let's ask a much more interesting question. If I had a coin that really had a $55 \%$ chance of heads instead of a $50 \%$ chance, and I tossed the coin 100 times, how often would I correctly reject the null hypothesis? In other words, what is the power of the test against an alternative that the actual chances of getting heads is $55 \%$ ? I can do exactly the same thing:

```
> rr = rbinom(1000,100,.55);sum(rr<40|rr>60)/1000
[1] 0.139
> rr = rbinom(1000,100,.55);sum(rr<40|rr>60)/1000
[1] 0.112
> rr = rbinom(1000,100,.55);sum(rr<40|rr>60)/1000
[1] 0.134
> rr = rbinom(1000,100,.55);sum(rr<40|rr>60)/1000
[1] 0.133
```

We'd only correctly identify the coin as being untrue in about $13 \%$ of the cases. It's better than the $5 \%$ we'd expect when the coin was true, but not very impressive. Maybe tossing more coins would help. Let's see what happens to the power when we do 500 tosses instead of just 100. First we need to find the correct rejection region:

```
> qbinom(.975, 500,.5)
[1] 272
> qbinom(.025,500,.5)
[1] 228
```

Now we can try the simulation:

```
> rr = rbinom(1000,500,.55);sum(rr<228|rr>272)/1000
[1] 0.595
> rr = rbinom(1000,500,.55);sum(rr<228|rr>272)/1000
[1] 0.587
> rr = rbinom(1000,500,.55);sum(rr<228|rr>272)/1000
[1] 0.577
> rr = rbinom(1000,500,.55);sum(rr<228|rr>272)/1000
[1] 0.61
> rr = rbinom(1000,500,.55);sum(rr<228|rr>272)/1000
[1] 0.611
```

That's quite a bit better. But suppose we wanted to find out how big of a sample size we'd need to be able to detect the $55 \%$ coin $95 \%$ of the time. Probably the easiest way is to try a bunch of different numbers in the simulation. It's getting complicated enough that we should probably write a function:

```
> coin.power = function(ntoss=100,nsim=1000,prob=.5){
+ lower = qbinom(.025,ntoss,.5)
+ upper = qbinom(.975,ntoss,.5)
+ rr = rbinom(nsim,ntoss,prob)
+ sum(rr < lower | rr > upper) / nsim
+ }
```

We can use sapply to call the coin. power function for a variety of number of tosses:

```
> ntosses = c(10,100,200,500,600,800,1000,1500,2000,2500)
> res = sapply(ntosses,coin.power,prob=.55)
> names(res) = ntosses
> res
    10
0.040 0.135 0.289 0.583 0.697 0.773 0.884 0.967 0.989 0.999
```

Intuitively, if the coin was more dishonest, we'd expect our test to have better power. Let's try the same thing with a coin that's weighted to give $70 \%$ heads:

```
> res = sapply(ntosses,coin.power,prob=.70)
> names(res) = ntosses
> res
    10
0.153 0.986 1.000 1.000 1.000 1.000 1.000 1.000 1.000 1.000
```

With just 100 tosses, we're pretty much guaranteed to be able to recognize the coin as weighted. What if the coin was just barely weighted, say $51 \%$ instead of $50 \%$ :

```
> res = sapply(ntosses,coin.power,prob=.51)
> names(res) = ntosses
> res
    10
0.019 0.035 0.051 0.067 0.071 0.087 0.084 0.129 0.125 0.158
```

Even after 2500 tosses, we'd only have about a $16 \%$ chance of detecting the weighted coin.

### 10.4 Probability Distributions

The naming conventions that were used for the binomial probability functions in the previous section are used consistently with all of the different distributions that are supported by R . To summarize:

1. To get an overall idea of how values are distributed, we can examine (usually graphically), the probability density function for a distribution. For example, the familiar bell curve is the density function for a normal distribution. In R, density functions begin with the letter " d ".

| beta | Beta | binom | Binomial |
| :--- | :--- | :--- | :--- |
| cauchy | Cauchy | chisq | Chi-squared |
| exp | Exponential | exp | Exponential |
| f | F | gamma | Gamma |
| geom | Geometric | hyper | Hypergeometric |
| lnorm | Lognormal | logis | Logistic |
| nbinom | Negative Binomial | norm | Normal |
| pois | Poisson | signrank | Signed Rank |
| t | Student's t | unif | Uniform |
| weibull | Weibull | wilcox | Wilcoxon's Rank Sum |

2. To find out what value corresponds to a particular probability (like 0.025 and 0.975 in the previous example), we can call the quantile function for the distribution. These functions accept an argument between 0 and 1 (i.e. a probability) and return the value for that distribution where the probability that an observation would be smaller than that value is equal to the probability passed to the function. When you perform a statistical test, choose a significance level, and look up the statistic's value in a table, you're actually using the quantile function. Quantile functions in $R$ begin with the letter "q".
3. If you've got a value for an observation that comes from a particular distribution, and you want to know the probability that observations from the distribution would be less than that value, you can pass the value to a probability function (like pbinom) and it will return the probability. In R, these functions begin with the letter " p ".
4. When you want to generate random numbers from a distribution, you can call the appropriate random number generator. Random number generators in $R$ begin with the letter "r".

The following table shows the distributions for which these four types of functions are available in R. In each case, precede the name in the table with a $d, q$, $p$, or $r$ to get the function you want.

### 10.5 A Note about Random Numbers in R

Some people like to make a distinction between truly random numbers (like those formed from physically tossing dice or counting the number of clicks of a Geiger counter in a given time interval) and the kinds of random numbers that are generated on a computer. (If you think the second example is impractical, take a look at http://www.fourmilab.ch/hotbits/. Another source of truly random numbers can be found at http://www.lavarnd.org.)

Some chip manufacturers are developing chips which allow noise in the circuitry (which is truly random) to be measured and used as a source of random numbers. But the programs in $R$ that generate random numbers produce them by applying a reproducible set of rules
(a computer program), so they are not really random, and some people refer to them as psuedo-random numbers for that reason. In general, we won't make any such distinction between truly random numbers and the ones we get from the computer.

In R and most other computer programs, all of the random number generators are based on the uniform distribution. By developing programs that are guaranteed to give random numbers with the right distribution if they are provided by a uniform random number generator, only one distribution (the uniform) needs to be studied to insure that it's truly random. The uniform random number generator in $R$ has been extensively tested, so you can have confidence that all the random number generators in R are reliable.

While it's obviously a useful feature that R's default behaviour is to give you a different set of random numbers each time that you call any of the random number generators, sometimes it creates problems or misunderstandings. Because of this, $R$ provides a simple way to set the random number generators to a reproducible state, so that the exact same sequence of random numbers will be generated every time a program is run. By passing an integer to the set.seed function, you can insure that the sequence of random numbers that are generated will be the same everytime you run an identical program.

## 10.6 t-tests

One of the most common tests in statistics is the t-test, used to determine whether the means of two groups are equal to each other. The assumption for the test is that both groups are sampled from normal distributions with equal variances. The null hypothesis is that the two means are equal, and the alternative is that they are not. It is known that under the null hypothesis, we can calculate a t-statistic that will follow a t-distribution with $\mathrm{n} 1+\mathrm{n} 2-2$ degrees of freedom. There is also a widely used modification of the t-test, known as Welch's t-test that adjusts the number of degrees of freedom when the variances are thought not to be equal to each other. Before we can explore the test much further, we need to find an easy way to calculate the t-statistic.

The function t .test is available in R for performing t -tests. Let's test it out on a simple example, using data simulated from a normal distribution.

```
> x = rnorm(10)
> y = rnorm(10)
> t.test(x,y)
    Welch Two Sample t-test
data: x and y
t = 1.4896, df = 15.481, p-value = 0.1564
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
    -0.3221869 1.8310421
sample estimates:
    mean of }x\mathrm{ mean of }
    0.1944866 -0.5599410
```

Before we can use this function in a simulation, we need to find out how to extract the $t$-statistic (or some other quantity of interest) from the output of the $t$. test function. For this function, the R help page has a detailed list of what the object returned by the function contains. A general method for a situation like this is to use the class and names functions to find where the quantity of interest is. In addition, for some hypothesis tests, you may need to pass the object from the hypothesis test to the summary function and examine its contents. For t.test it's easy to figure out what we want:

```
> ttest = t.test(x,y)
> names(ttest)
[1] "statistic" "parameter" "p.value" "conf.int" "estimate"
[6] "null.value" "alternative" "method" "data.name"
```

The value we want is named "statistic". To extract it, we can use the dollar sign notation, or double square brackets:

```
> ttest$statistic
    t
1.489560
> ttest[['statistic']]
    t
1.489560
```

Of course, just one value doesn't let us do very much - we need to generate many such statistics before we can look at their properties. In R, the replicate function makes this very simple. The first argument to replicate is the number of samples you want, and the second argument is an expression (not a function name or definition!) that will generate one of the samples you want. To generate 1000 t-statistics from testing two groups of 10 standard random normal numbers, we can use:

```
> ts = replicate(1000,t.test(rnorm(10),rnorm(10))$statistic)
```

Under the assumptions of normality and equal variance, we're assuming that the statistic will have a t-distribution with $10+10-2=18$ degrees of freedom. (Each observation contributes a degree of freedom, but we lose two because we have to estimate the mean of each group.) How can we test if that is true?

One way is to plot the theoretical density of the t-statistic we should be seeing, and superimposing the density of our sample on top of it. To get an idea of what range of $x$ values we should use for the theoretical density, we can view the range of our simulated data:

```
> range(ts)
> range(ts)
[1] -4.564359 4.111245
```

Since the distribution is supposed to be symmetric, we'll use a range from -4.5 to 4.5 . We can generate equally spaced $x$-values in this range with seq:

```
> pts = seq(-4.5,4.5,length=100)
> plot(pts,dt(pts,df=18),col='red',type='l')
```

Now we can add a line to the plot showing the density for our simulated sample:

```
> lines(density(ts))
```

The plot appears below.


Another way to compare two densities is with a quantile-quantile plot. In this type of plot, the quantiles of two samples are calculated at a variety of points in the range of 0 to 1 , and then are plotted against each other. If the two samples came from the same distribution with the same parameters, we'd see a straight line through the origin with a slope of 1 ; in other words, we're testing to see if various quantiles of the data are identical in the two samples. If the two samples came from similar distributions, but their parameters were different, we'd still see a straight line, but not through the origin. For this reason, it's very common to draw a straight line through the origin with a slope of 1 on plots like this. We can produce a quantile-quantile plot (or QQ plot as they are commonly known), using the qqplot function. To use qqplot, pass it two vectors that contain the samples that you want to compare. When comparing to a theoretical distribution, you can pass a random sample from that distribution. Here's a QQ plot for the simulated t-test data:

```
> qqplot(ts,rt(1000,df=18))
> abline(0,1)
```



We can see that the central points of the graph seems to agree fairly well, but there are some discrepancies near the tails (the extreme values on either end of the distribution). The tails of a distribution are the most difficult part to accurately measure, which is unfortunate, since those are often the values that interest us most, that is, the ones which will provide us with enough evidence to reject a null hypothesis. Because the tails of a distribution are so important, another way to test to see if a distribution of a sample follows some hypothesized distribution is to calculate the quantiles of some tail probabilities (using the quantile function) and compare them to the theoretical probabilities from the distribution (obtained from the function for that distribution whose first letter is "q"). Here's such a comparison for our simulated data:

```
> probs = c(.9, .95,.99)
> quantile(ts,probs)
    90% 95% 99%
1.427233 1.704769 2.513755
> qt(probs,df=18)
[1] 1.330391 1.734064 2.552380
```

The quantiles agree fairly well, especially at the .95 and .99 quantiles. Performing more simulations, or using a large sample size for the two groups would probably result in values even closer to what we have theoretically predicted.

One final method for comparing distributions is worth mentioning. We noted previously that one of the assumptions for the t-test is that the variances of the two samples are equal. However, a modification of the t-test known as Welch's test is said to correct for this problem by estimating the variances, and adjusting the degrees of freedom to use in the test.

This correction is performed by default, but can be shut off by using the var.equal=TRUE argument. Let's see how it works:

```
> t.test(x,y)
    Welch Two Sample t-test
data: x and y
t = -0.8103, df = 17.277, p-value = 0.4288
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
    -1.0012220 0.4450895
sample estimates:
mean of x mean of y
0.2216045 0.4996707
> t.test(x,y,var.equal=TRUE)
    Two Sample t-test
data: x and y
t = -0.8103, df = 18, p-value = 0.4284
alternative hypothesis: true difference in means is not equal to 0
95 percent confidence interval:
    -0.9990520 0.4429196
sample estimates:
mean of x mean of y
0.2216045 0.4996707
```

Since the statistic is the same in both cases, it doesn't matter whether we use the correction or not; either way we'll see identical results when we compare the two methods using the techniques we've already described. Since the degree of freedom correction changes depending on the data, we can't simply perform the simulation and compare it to a different number of degrees of freedom. The other thing that changes when we apply the correction is the p-value that we would use to decide if there's enough evidence to reject the null hypothesis. What is the behaviour of the p-values? While not necessarily immediately obvious, under the null hypothesis, the p-values for any statistical test should form a uniform distribution between 0 and 1 ; that is, any value in the interval 0 to 1 is just as likely to occur as any other value. For a uniform distribution, the quantile function is just the identity function. A value of .5 is greater than $50 \%$ of the data; a value of .95 is greater than $95 \%$ of the data. As a quick check of this notion, let's look at the density of probability values when the null hypothesis is true:

```
> tps = replicate(1000,t.test(rnorm(10),rnorm(10))$p.value)
```

```
> plot(density(tps))
```

The graph appears below.


Another way to check to see if the probabilities follow a uniform distribution is with a QQ plot:
> qqplot(tps,runif(1000))
> abline ( 0,1 )

The graph appears below.


The idea that the probabilities follow a uniform distribution seems reasonable.
Now, let's look at some of the quantiles of the p-values when we force the $t$. test function to use var. equal=TRUE:

```
> tps = replicate(1000,t.test(rnorm(10),rnorm(10),var.equal=TRUE)$p.value)
> probs = c(.5,.7,.9,.95,.99)
> quantile(tps,probs)
    50% 70% 90% 95% 99%
0.4873799 0.7094591 0.9043601 0.9501658 0.9927435
```

The agreement actually looks very good. What about when we let $t . t e s t$ decide whether to make the correction or not?

```
> tps = replicate(1000,t.test(rnorm(10),rnorm(10))$p.value)
> quantile(tps,probs)
    50% 70% 90% 95% 99%
0.4932319 0.7084562 0.9036533 0.9518775 0.9889234
```

There's not that much of a difference, but, of course, the variances in this example were equal. How does the correction work when the variances are not equal?

```
> tps = replicate(1000,t.test(rnorm(10),rnorm(10,sd=5),var.equal=TRUE)$p.value)
> quantile(tps,probs)
    50% 70% 90% 95% 99%
0.5221698 0.6926466 0.8859266 0.9490947 0.9935562
> tps = replicate(1000,t.test(rnorm(10),rnorm(10,sd=5))$p.value)
> quantile(tps,probs)
```

```
    50% 70% 90% 95% 99%
0.4880855 0.7049834 0.8973062 0.9494358 0.9907219
```

There is an improvement, but not so dramatic.

### 10.7 Power of the t-test

Of course, all of this is concerned with the null hypothesis. Now let's start to investigate the power of the t-test. With a sample size of 10 , we obviously aren't going to expect truly great performance, so let's consider a case that's not too subtle. When we don't specify a standard deviation for rnorm it uses a standard deviation of 1 . That means about $68 \%$ of the data will fall in the range of -1 to 1 . Suppose we have a difference in means equal to just one standard deviation, and we want to calculate the power for detecting that difference. We can follow the same procedure as the coin tossing experiment: specify an alpha level, calculate the rejection region, simulate data under the alternative hypothesis, and see how many times we'd reject the null hypothesis. As in the coin toss example, a function will make things much easier:

```
t.power = function(nsamp=c(10,10),nsim=1000,means=c(0,0),sds=c(1,1)){
    lower = qt(.025,df=sum(nsamp) - 2)
    upper = qt(.975,df=sum(nsamp) - 2)
    ts = replicate(nsim,
        t.test(rnorm(nsamp[1],mean=means[1],sd=sds[1]),
            rnorm(nsamp [2],mean=means[2],sd=sds[2]))$statistic)
    sum(ts < lower | ts > upper) / nsim
}
```

Let's try it with our simple example:

```
> t.power(means=c(0,1))
```

[1] 0.555

Not bad for a sample size of 10 !
Of course, if the differences in means are smaller, it's going to be harder to reject the null hypothesis:

```
> t.power(means=c(0,.3))
[1] 0.104
```

How large a sample size would we need to detect that difference of .3 with $95 \%$ power?

```
> samps = c(100,200,300,400,500)
> res = sapply(samps,function(n)t.power(means=c(0,.3),nsamp=c(n,n)))
> names(res) = samps
> res
    100 200 300 400 500
0.567 0.841 0.947 0.992 0.999
```

It would take over 300 samples in each group to be able to detect such a difference.
Now we can return to the issue of unequal variances. We saw that Welch's adjustment to the degrees of freedom helped a little bit under the null hypothesis. Now let's see if the power of the test is improved using Welch's test when the variances are unequal. To do this, we'll need to modify our $t$. power function a little:

```
t.power1 = function(nsamp=c(10,10),nsim=1000,means=c(0,0),sds=c(1, 1),var.equal=TRUE){
    tps = replicate(nsim,
        t.test(rnorm(nsamp[1],mean=means[1],sd=sds[1]),
            rnorm(nsamp [2],mean=means[2],sd=sds[2]))$p.value)
    sum(tps < . 025 | tps > .975) / nsim
}
```

Since I set var . equal=TRUE by default, Welch's adjustment will not be used unless we specify var.equal=FALSE. Let's see what the power is for a sample of size 10, assuming the mean of one of the groups is 1 , and its standard deviation is 2 , while the other group is left at the default of mean $=0$ and $\mathrm{sd}=1$ :

```
> t.power1(nsim=10000,sds=c(1,2),mean=c(1,2))
[1] 0.1767
> t.power1(nsim=10000,sds=c (1,2),mean=c (1,2),var.equal=FALSE)
[1] 0.1833
```

There does seem to be an improvement, but not so dramatic.
We can look at the same thing for a variety of sample sizes:

```
> res1 = sapply(sizes,function(n)t.power1(nsim=10000,sds=c(1,2),
+ mean=c(1,2),nsamp=c(n,n)))
> names(res1) = sizes
> res1
    10 20 50 100
0.1792 0.3723 0.8044 0.9830
> res2 = sapply(sizes,function(n)t.power1(nsim=10000,sds=c(1,2),
+ mean=c(1,2),nsamp=c(n,n),var.equal=FALSE))
> names(res2) = sizes
> res2
    10 20 50 100
0.1853 0.3741 0.8188 0.9868
```


## Chapter 11

## Graphical User Interfaces (GUIs)

### 11.1 Graphical User Interfaces

While using R through the command line provides a great deal of flexibility, there are times when a simpler interface would be useful. For example, you may develop an $R$ program that performs a complex analysis, and you'd like others to be able to run the program by, say just specifying a file to be read, and choosing a couple of options through checkboxes or a drop down list. There may be a set of operations that your routinely do when first studying a data set, and you'd like to be presented with a list of available data, and just click on the one that you want.

There are several different options available in R to produce graphical user interfaces (GUIs); we are going to focus on a simple, portable one based on the $\mathrm{Tcl} / \mathrm{Tk}$ library originally developed by John Ousterhout when he was in the Computer Science department here at Berkeley. Tcl is a scripting language (like perl or python), and Tk is a graphical toolkit designed to work with that language. Since the Tk toolkit is portable, easy-to-use, and provides most of the basic elements needed to create GUIs, interfaces to it are available in many languages, so if you understand the basics of Tk GUIs, you may see the same techniques used later on in your career by some other program. To use the $\mathrm{Tcl} / \mathrm{Tk}$ library in $R$, you must load the library with the library (tcltk) command. This library is part of the base R distribution, so you don't have to download anything in order to use it (although you may choose to download some optional components later on.)

If you look at the help pages for the functions in the tcltk library, you'll probably be surprised to see how little information or guidance there is. However, once you work with the library for a while, you'll get accustomed to the way Tk functions are mapped to R functions, and you'll be able to use any documentation about Tk that you can find on the web or elsewhere to get more information. There are a wide variety of sample programs at http://www.sciviews.org/_rgui/tcltk/, but they use a different geometry method and some require external packages. I'll try to provide examples here to help you get started, but don't hesitate to look around the web for more examples and ideas.

The process of creating a GUI can be broken down into two parts: choosing the elements (often refered to as widgets) that will make up the GUI, and arranging for the elements to be placed in the appropriate positions and displayed. This second step is sometimes known as geometry management. Tk actually offers several different geometry management methods; we are going to focus on one known as packing. In the packing geometry model, the GUI is considered a collection of separate frames, each containing some of the widgets that make up the final GUI. The widgets are loaded into the frames in a carefully chosen order, and they "spread out" to fill the frame. When you pack a widget into a frame, you can specify the side to which to pack it, choosing among left, right, top or bottom. With a little practice and experimentation, you can usually get the widgets to line up the way you want them to.

Most of the widgets that are available through the Tk toolbox should look familiar, as common applications like email clients and web browser use these same elements in their GUIs. Some examples of available widgets are:

- text entry fields
- drop down menus
- check buttons
- radio buttons
- file selection browsers
- sliding scales

Since the Tk toolbox is not integrated entirely into $R$, it's necessary to use special techniques to get information out of the $\mathrm{Tcl} / \mathrm{Tk}$ environment and into R . Many of the widgets, for example a text entry widget, will need a Tcl variable associated with them to hold necessary information. All of the variables that will be captured by the GUI will be character variables. The tclVar function can be used to create an empty tcl variable which can then be used in call to functions in the tcltk library as follows:

```
myvar = tclVar('')
```

Later, when you need to get the information that was put into the Tk variable back into the $R$ environment, you can use the tclvalue function:

```
rmyvar = tclvalue(myvar)
```

Another aspect of GUI programming that is different from regular programs has to do with associating actions with certain GUI elements. An obvious example is a button, which when pressed needs to do something. Widgets like this will have an argument, usually called command= which will accept the name of a function that will be called when the button (or other action) is recognized. Such functions, often called callbacks, should be written using the ... notation for their argument lists, and should not have any returned values. It sometimes becomes necessary to "remember" things over the course of a GUI's execution. For example, you may want to count the number of times a button is pressed, or display a different message based on the value of a previous response. Since all of the actions which the GUI will initiate are carried out in functions, any modifications to variables that are made in those functions will be lost when the function returns. While not usually a good practice, you can use the special assignment operator <<- inside a function to modify global variables, which will retain their values after the function exits.

To make some of these concepts clearer, let's consider the construction of a GUI to accept input to the coin. power program that we developed earlier. Recall that the program accepts the number of simulations, number of coin tosses, probability of getting heads for the coin, and returns the power. We want to make a GUI with three entries, one for each of the parameters, a place to display the answer, and buttons to run the simulation or close the window. The first step in creating a GUI with the tcltk library in $R$ is loading the library and calling the tktoplevel function, which creates an initial window into which we will pack the frames containing the widgets. Since we can control the order of packing into individual frames, each set of related elements can be put into a separate frame. For this
example, we'll create a separate frame for each entry and its associated label, as well as a frame to hold those entries and another frame for the two buttons; the area for the answer can be packed into the toplevel frame.

In the code that follows, you'll notice that usually widgets are packed directly into their enclosing frames, but the label widget that will hold the answer is assigned to a variable before being packed. If you'll need to communicate with the widget at some point in the running of the program, it's vital to store the widget in a variable. In this example, we'll create a blank label, and use the tkconfigure function when we have an answer to change what the label displays. Here's the code to create the GUI:

```
require(tcltk)
coin.power = function(ntoss=100,nsim=1000,prob=.5){
        lower = qbinom(.025,ntoss,.5)
        upper = qbinom(.975,ntoss,.5)
        rr = rbinom(nsim,ntoss,prob)
        sum(rr < lower | rr > upper) / nsim
}
destroy = function(...)tkdestroy(base)
tst = function(...){
    nsim = as.numeric(tclvalue(nsim_))
    ntoss = as.numeric(tclvalue(ntoss_))
    prob = as.numeric(tclvalue(prob_))
    res = coin.power(ntoss=as.numeric(ntoss),nsim=as.numeric(nsim),prob=as.numeric(prob))
    tkconfigure(ans,text=paste(res))
}
base = tktoplevel()
tkwm.title(base,'Coin Toss')
# create a frame to hold the three entries
nfrm = tkframe(base)
# create tcl variables to associate with the
# entry fields -- to include starting values
# replace the '' with the desired value
nsim_ = tclVar('')
ntoss_ = tclVar('')
prob_ = tclVar('')
f1 = tkframe(nfrm)
tkpack(tklabel(f1,text='Nsim',width=8),side='left')
```

```
tkpack(tkentry(f1,width=10,textvariable=nsim_),side='left')
f2 = tkframe(nfrm)
tkpack(tklabel(f2,text='Ntoss',width=8), side='left')
tkpack(tkentry(f2,width=10,textvariable=ntoss_),side='left')
f3 = tkframe(nfrm)
tkpack(tklabel(f3,text='Prob',width=8),side='left')
tkpack(tkentry(f3,width=10,textvariable=prob_),side='left')
# the widgets were packed in the frames, but the frames have
# not yet been packed. Remember that nothing can actually be
# displayed unless it's been packed.
tkpack(f1,side='top')
tkpack(f2,side='top')
tkpack(f3,side='top')
tkpack(nfrm)
# now we can repeat the process for the label to hold the
# answer, and the frame containing the buttons
ans = tklabel(base,text=' ')
tkpack(ans,side='top')
bfrm = tkframe(base)
tkpack(tkbutton(bfrm,text='Run',command=tst),side='left')
tkpack(tkbutton(bfrm,text='Quit',command=destroy),side='right')
tkpack(bfrm,side='bottom')
```

When we run the program (for example by using the source command inside of R), we see the left hand image; after making some entries and hitting the Run button, we see the image on the right.


### 11.2 Appearance of Widgets

The previous example was a very minimalistic approach, with no concern with the actual appearance of the final product. One simple way to improve the appearance is to add a little space around the widgets when we pack them. The tkpack function accepts two arguments, padx $=$ and pady $=$ to control the amount of space around the widgets when they are packed. Each of these arguments takes a scalar or a vector of length 2 . When a scalar is given, that much space (in pixels) is added on either side of the widget in the specified dimension. When a list is given the first number is the amount of space to the left (padx) or the top (pady), and the second number is the amount of space to the right (padx) or the bottom (pady). Like most aspects of GUI design, experimentation is often necessary to find the best solution. The following code produces a version of the coin power GUI with additional padding:

```
base = tktoplevel()
tkwm.title(base,'Coin Toss')
nfrm = tkframe(base)
nsim_ = tclVar('')
ntoss_ = tclVar('')
prob_ = tclVar('')
f1 = tkframe(nfrm)
tkpack(tklabel(f1,text='Nsim',width=8), side='left',pady=c(5,10))
tkpack(tkentry(f1,width=10,textvariable=nsim_), side='left', padx=c(0, 20),pady=c(5,10))
f2 = tkframe(nfrm)
tkpack(tklabel(f2,text='Ntoss',width=8), side='left', pady=c(5,10))
tkpack(tkentry(f2,width=10,textvariable=ntoss_), side='left',padx=c(0, 20),pady=c(5,10))
f3 = tkframe(nfrm)
tkpack(tklabel(f3,text='Prob', width=8), side='left', pady=c(5,10))
tkpack(tkentry(f3,width=10,textvariable=prob_),side='left',padx=c(0, 20),pady=c(5,10))
tkpack(f1,side='top')
tkpack(f2,side='top')
tkpack(f3,side='top')
tkpack(nfrm)
ans = tklabel(base,text=' ')
tkpack(ans,side='top')
```

```
bfrm = tkframe(base)
tkpack(tkbutton(bfrm,text='Run', command=tst), side='left')
tkpack(tkbutton(bfrm,text='Quit',command=destroy),side='right')
```

tkpack(bfrm, side='bottom', pady=c $(0,10)$ )

Here are side-by-side pictures showing the difference between the two versions:


Another way to modify a GUI's appearance is through three-dimensional effects. These are controlled by an argument called relief=, which can take values of "flat", "groove", "raised", "ridge", "solid", or "sunken". The following code produces a (non-functioning) GUI showing the different relief styles applied to labels and buttons:

```
require(tcltk)
types = c('flat','groove','raised','ridge','solid','sunken')
base = tktoplevel()
tkwm.title(base,'Relief Styles')
frms = list()
mkframe = function(type){
    fr = tkframe(base)
    tkpack(tklabel(fr,text=type,relief=type),side='left',padx=5)
```

```
    tkpack(tkbutton(fr,text=type,relief=type),side='left',padx=5)
    tkpack(fr,side='top',pady=10)
    fr
}
sapply(types,mkframe)
```

Here's a picture of how it looks:


### 11.3 Fonts and Colors

Several arguments can be used to modify color. The background= argument controls the overall color, while the foreground= argument controls the color of text appearing in the widget. (Remember that things like this can be changed while the GUI is running using the tkconfigure command. Each of these arguments accepts colors spelled out (like "lightblue", "red", or "green") as well as web-style hexadecimal values (like "\#add8e6", "\#ff0000" or "\#00ff00").

To change from the default font (bold Helvetica), you must first create a Tk font, using the tkfont.create function. This function takes a number of arguments, but only the font family is required. The available font families will vary from platform to platform; the as.character (tkfont.families()) command will display a list of the available fonts. Some of the other possible arguments to tkfont. create include:

1. size=, the size of the font in points.
2. weight=, either "normal" or "bold"
3. slant=, either "roman" or "italic"
4. underline=, either TRUE or FALSE
5. overstrike=, either TRUE or FALSE

As mentioned earlier, colors can be specified as either names or web-style hexadecimal values. Generally, the argument to change the color of a widget is background=; the argument to change the color of any text appearing in the widget is foreground=. If these choices don't do what you expect, you may need to check the widget-specific documentation.

Here's a simple program that chooses some randomly selected colors and fonts, and displays them as labels.

```
require(tcltk)
allfonts = as.character(tkfont.families())
somefonts = sample(allfonts,9)
somecolors = c('red','blue','green','yellow','lightblue','tan',
'darkred','lightgreen','white')
txt = 'ABCDEFGHIJKLMNOPQRSTUVWXYZabcdefghijklmnopqrstuvwxyz'
base = tktoplevel()
tkwm.title(base,'Fonts')
mkfonts = function(font,color){
    thefont = tkfont.create(family=font,size=14)
```

```
    tkpack(tklabel(base,text=paste(font,':',txt),
    font=thefont,background=color),
    side='top')
}
mapply(mkfonts,somefonts,somecolors)
```

Here's how it looks:

| X-w Fonts |  |
| :---: | :---: |
|  | MAEKED FASL : ABPDEFSHIUKL ANAPARE |
|  | varee : ABCDEFGHIJKLMNOPQRSTU |
|  | SWiff : ABCDEFGHIJKLMNOPQRSTUV |
|  | times new roman : ABCDEFGHHJKLMNOP <br>  |
|  | sawasdee : ABCDEFGHIJKLMNOPQR: |
|  | Ne: $\triangle B C D E F G H-L K L M N O P O R S$ |
|  |  |

## loma : ABCDEFGHIJKLMNOPQRST

Note that only the specific widget for which background= was set changes - if you want to change the background for the entire GUI, you'll probably have to pass the background= argument to every widget you use.

### 11.4 Plotting

When developing a TK-based GUI for plotting, there are two possibilities available. The first, which is the only choice if you need to interact with the graph using locator or identify, is to create a GUI with the controls for the plot, and to let R open a normal plotting window. The second option utilizes the tkrplot library, available from CRAN, to create a label widget with an image of the plot; this label can be placed anywhere that any other widget can be placed.

To illustrate the use of a GUI with plotting, consider the problem of mixtures of normal distributions. Many times a sample will actually contain two separate distributions, even though it will be treated as a single distribution. Obviously data like this will create problems when we try to analyze it, so it's important to be able to recognize such data, using, say a density plot. To get an idea of how the density of mixtures of distributions would look,
we can create a GUI using a scale or slider widget that will allow us to control the fraction of each of two distributions that will be combined. Many times the first step in making a GUI is writing the function that the GUI will eventually call to actually do the work. This helps to identify the parameters that need to be supplied to the function so that the GUI can be designed in such a way to get all the necessary information. For this case, we'll want to specify the mean and standard deviation of the first distribution, the mean and standard deviation of the second distribution, and the fraction of the second distribution to use. (The fraction for the first distribution will just be 1 minus the fraction for the first distribution.) Here's such a function:

```
genplot = function(m1,s1,m2,s2,frac,n=100){
    dat = c(rnorm((1-frac)*n,m1,s1),rnorm(frac*n,m2,s2))
    plot(density(dat),type='l',main='Density of Mixtures')
}
```

Now we can create the interface. We'll make three frames: the first will accept the mean and standard deviation for the first distribution, the second will have the mean and standard deviation for the second distribution, and the third will have the slider to determine the fraction of each distribution to use. Recall that we need to create tcl variables, and then convert them into R variables before we can call our function, so I'll use an intermediate function which will do the translations and then call genplot as a callback. Although there is a fair amount of code, most of it is very similar.

```
require(tcltk)
doplot = function(...){
    m1 = as.numeric(tclvalue(mean1))
    m2 = as.numeric(tclvalue(mean2))
    s1 = as.numeric(tclvalue(sd1))
    s2 = as.numeric(tclvalue(sd2))
    fr = as.numeric(tclvalue(frac))
    genplot(m1,s1,m2,s2,fr,n=100)
}
base = tktoplevel()
tkwm.title(base,'Mixtures')
mainfrm = tkframe(base)
mean1 = tclVar(10)
mean2 = tclVar(10)
sd1 = tclVar(1)
sd2 = tclVar(1)
frac = tclVar(.5)
```

```
m1 = tkframe(mainfrm)
tkpack(tklabel(m1,text='Mean1, SD1',width=10), side='left')
tkpack(tkentry(m1,width=5,textvariable=mean1),side='left')
tkpack(tkentry(m1,width=5,textvariable=sd1),side='left')
tkpack(m1,side='top')
m2 = tkframe(mainfrm)
tkpack(tklabel(m2,text='Mean2, SD2',width=10),side='left')
tkpack(tkentry(m2,width=5,textvariable=mean2),side='left')
tkpack(tkentry(m2,width=5,textvariable=sd2),side='left')
tkpack(m2,side='top')
m3 = tkframe(mainfrm)
tkpack(tkscale(m3, command=doplot,from=0,to=1, showvalue=TRUE,
    variable=frac,resolution=.01,orient='horiz'))
tkpack(m3,side='top')
tkpack(mainfrm)
```

Here's how the interface looks:


To produce the same sort of GUI, but with the plot in the same frame as the slider, we can use the tkrplot library. To place the plot in the same frame as the slider, we must first create a tkrplot widget, using the tkrplot function. After loading the tkrplot library, we call this function with two arguments; the frame in which the plot is to be displayed, and a callback function (using . . . as the only argument) that will draw the desired plot. In this example, we can use the same function (doplot) as in the standalone version:

```
img = tkrplot(mainfrm,doplot)
```

Since the tkrplot widget works by displaying an image of the plot, the only way to change the plot is to change this image, which is exactly what the tkrreplot function does. The only argument to tkrreplot is the tkrplot widget that will need to be redrawn. Thus, the slider can be constructed with the following statements:

```
scalefunc = function(...)tkrreplot(img)
s = tkscale(mainfrm,command=scalefunc,from=0,to=1,showvalue=TRUE,
    variable='frac',resolution=.01,orient='horiz')
```

By packing the tkrplot object first, followed by the frames for the mean and standard deviations, and packing the slider widget last, we can produce the GUI shown below:


The complete code for this GUI is as follows:

```
require(tcltk)
require(tkrplot)
genplot = function(m1,s1,m2,s2,frac,n=100){
    dat = c(rnorm((1-frac)*n,m1,s1),rnorm(frac*n,m2,s2))
            plot(density(dat),type='l',main='Density of Mixtures')
    }
doplot = function(...){
    m1 = as.numeric(tclvalue(mean1))
    m2 = as.numeric(tclvalue(mean2))
```

```
    s1 = as.numeric(tclvalue(sd1))
    s2 = as.numeric(tclvalue(sd2))
    fr = as.numeric(tclvalue(frac))
    genplot(m1,s1,m2,s2,fr,n=100)
}
base = tktoplevel()
tkwm.title(base,'Mixtures')
mainfrm = tkframe(base)
mean1 = tclVar(10)
mean2 = tclVar(10)
sd1 = tclVar(1)
sd2 = tclVar(1)
frac = tclVar(.5)
img = tkrplot(mainfrm,doplot)
scalefunc = function(...)tkrreplot(img)
s = tkscale(mainfrm,command=scalefunc,from=0,to=1,showvalue=TRUE,
    variable=frac,resolution=.01,orient='horiz')
tkpack(img)
m1 = tkframe(mainfrm)
tkpack(tklabel(m1,text='Mean1, SD1',width=10), side='left')
tkpack(tkentry(m1,width=5,textvariable=mean1),side='left')
tkpack(tkentry(m1,width=5,textvariable=sd1),side='left')
tkpack(m1,side='top')
m2 = tkframe(mainfrm)
tkpack(tklabel(m2,text='Mean2, SD2',width=10),side='left')
tkpack(tkentry(m2,width=5,textvariable=mean2),side='left')
tkpack(tkentry(m2,width=5,textvariable=sd2),side='left')
tkpack(m2,side='top')
tkpack(s)
tkpack(mainfrm)
```


### 11.5 Binding

For those widgets that naturally have an action or variable associated with them, the Tk interface provides arguments like textvariable=, or command= to make it easy to get these

| <Return> | <FocusIn> |
| :--- | :--- |
| <Key-x> | <FocusOut> |
| <Alt-x> | <Button-1>, <Button-2>, etc. |
| <Control-x> | <ButtonRelease-1>, <ButtonRelease-2>, etc. |
| <Destroy> | <Double-Button-1>, <Double-Button-2>, etc. |

widgets working as they should. But we're not limited to associating actions with only those widgets that provide such arguments. By using the tkbind command, we can associate a function (similar to those accepted by functions that use a command= argument) to any of a large number of possible events. To indicate an event, a character string with the event's name surrounded by angle brackets is used. The following table shows some of the actions that can have commands associated with them. In the table, a lower case x is used to represent any key on the keyboard.

As an example, suppose we wish to create a GUI that will allow the user to type in the name of a data frame, and when the user hits return in the entry field, a set of radio buttons, one for each variable in the data frame, will open up below the entry field. Finally, a button will allow for the creation of a histogram from the selected variable.

```
require(tcltk)
makehist = function(...){
    df = get(tclvalue(dfname))
    thevar = tclvalue(varname)
    var = as.numeric(df[[thevar]])
    hist(var,main=paste("Histogram of",thevar),xlab=thevar)
}
showb = function(...){
    df = get(tclvalue(dfname))
    vars = names(df)
    frms = list()
    k = 1
    mkframe = function(var){
        fr = tkframe(base)
        tkpack(tklabel(fr,width=15,text=var),side='left')
        tkpack(tkradiobutton(fr,variable=varname,value=var),side='left')
        tkpack(fr,side='top')
        fr
    }
    frms = sapply(vars,mkframe)
```

```
    tkpack(tkbutton(base,text='Run',command=makehist),side='top')
}
base = tktoplevel()
tkwm.title(base,'Chooser')
dfname = tclVar()
varname = tclVar()
efrm = tkframe(base)
tkpack(tklabel(efrm,text='Dataframe: '),side='left')
dfentry = tkentry(efrm,textvariable=dfname,width=20)
tkbind(dfentry,'<Return>',showb)
tkpack(dfentry,side='left')
tkpack(efrm)
```

Here's a picture of the widget in both the "closed" and "open" views:


### 11.6 Checkbuttons

When we created radiobuttons, it was fairly simple, because we only needed to create one tcl variable, which would contain the value of the single chosen radiobutton. With checkbuttons, the user can choose as many selections as they want, so each button must have a separate tcl variable associated with it. While it's possible to do this by hand for each choice provided, the following example shows how to use the sapply function to do this in a more general way. Notice that special care must be taken when creating a list of tcl variables to insure
that they are properly stored. In this simple example, we print the choices, by using sapply to convert the list of tcl variables to R variables. Remember that all the toplevel variables that you create in an R GUI are available in the console while the GUI is running, so you examine them in order to see how their information is stored.

```
require(tcltk)
tt <- tktoplevel()
choices = c('Red','Blue','Green')
bvars = lapply(choices,function(i)tclVar('0'))
# or bvars = rep(list(tclVar('0')),length(bvars))
names(bvars) = choices
mkframe = function(x){
    nn = tkframe(tt)
    tkpack(tklabel(nn,text=x,width=10),side='left')
    tkpack(tkcheckbutton(nn,variable=bvars[[x]]),side='right')
    tkpack(nn,side='top')
}
sapply(choices,mkframe)
showans = function(...){
    res = sapply(bvars,tclvalue)
    res = names(res)[which(res == '1')]
    tkconfigure(result,text = paste(res,collapse=' '))
}
result = tklabel(tt,text='')
tkpack(result,side='top')
bfrm = tkframe(tt)
tkpack(tkbutton(bfrm, command=showans,text='Select'),side='top')
tkpack(bfrm,side='top')
```

The figure below shows what the GUI looks like after two choices have been made, and the button is pressed.


### 11.7 Opening Files and Displaying Text

While it would be very simple (and not necessarily a bad idea) to use an entry field to specify a file name, the Tk toolkit provides a file browser which will return the name of a file which a user has chosen, and will usually be a better choice if you need to open a file.

Another issue that arises has to do with displaying output. If the output is a plot, it's simple to just open a graph window; if the output is text, you can just print it in the normal way, and it will display in the same place as you typed the R command to display the GUI. While this is useful while debugging your program, if there are printed results they should usually be displayed in a separate window. For this purpose, Tk provides the tktext object. To display output in this way, we can use the capture. output function, which takes the output of any R command and, instead of displaying it to the screen, stores the output in a vector of character values. Alternatively, the output could be written to a file, then read back into a character vector.

The following example program invokes tkgetOpenFile to get the name of a file to be opened; it then opens the file, reads it as a CSV file and displays the results in a text window with scrollbars. The wrap='none' argument tells the text window not to wrap the lines; this is appropriate when you have a scrollbar in the x-dimension. Finally, to give an idea of how the text window can be modified, a button is added to change the text window's display from the listing of the data frame to a data frame summary.

```
require(tcltk)
summ = function(...){
    thestring = capture.output(summary(myobj))
    thestring = paste(thestring,collapse='\n')
    tkdelete(txt,'@0,0','end')
    tkinsert(txt,'@0,0',thestring)
}
```

```
fileName<-tclvalue(tkgetOpenFile())
myobj = read.csv(fileName)
base = tktoplevel()
tkwm.title(base,'File Open')
yscr <- tkscrollbar(base,
        command=function(...)tkyview(txt,...))
xscr <- tkscrollbar(base,
                            command=function(...)tkxview(txt,...),orient='horiz')
txt <- tktext(base,bg="white",font="courier",
    yscrollcommand=function(...)tkset(yscr,...),
    xscrollcommand=function(...)tkset(xscr,...),
    wrap='none',
        font=tkfont.create(family='lucidatypewriter',size=14))
tkpack(yscr,side='right',fill='y')
tkpack(xscr,side='bottom',fill='x')
tkpack(txt,fill='both',expand=1)
tkpack(tkbutton(base,command=summ,text='Summary'),side='bottom')
thestring = capture.output(print(myobj))
thestring = paste(thestring,collapse='\n')
tkinsert(txt,"end",thestring)
tkfocus(txt)
```

The first picture shows the file chooser (as displayed on a Linux system); the second picture shows the diabetes data set displayed in a text window, and the third picture shows the result of pressing the summary button.

| Open |  | - $\square$ |
| :---: | :---: | :---: |
| Directory: | faccounts/staff/spector/stat133/data | - |
|  |  |  |
| F |  |  |
| Fle name: | pima-indians-diabetes.data | Open |
| Files of type: |  | Cancel |

File Open



### 11.8 Using Images with the tcltk package

The current version of tcl that ships with R allows you to display images in your GUIs, but only if they are in GIF format. Fortunately, it's very easy to change the format of images if they are, for example JPEG or PNG files. On any SCF machine, the command:
mogrify -format gif *.jpg
will convert all the files ending in .jpg to files with the same name, but in the GIF format. You can then use the .gif files that are created to display in your GUI.

To use images with the tcltk library, first create a Tcl variable representing the image with code like:

```
myimage = tclVar()
tcl("image","create","photo",myimage,file="picture.gif")
```

Next, create a tklabel using the image= argument pointing to the tcl variable that holds the image:

```
img = tklabel(frame,image=myimage)
```

Like any other widget, you can change the image during the execution of your program using the tkconfigure function. Suppose we have another tcl variable called otherimage that has an image associated with it. To change the img widget to display that image, use

```
tkconfigure(img,image=otherimage)
```

If you have many pictures, it will be more convenient to store the tcl image variables in a list. Suppose the R list pics contains the full pathname of several GIF files. (It's usually simplest to use setwd to change to the directory where you're storing the GIF files, so that you only need to type their names, not their full paths. The command

```
setwd(file.choose())
```

allows you to navigate to the directory with the GIF files.)
The following example displays pictures of three fruits, chosen from a list of five. When the button is pressed, it uses tkconfigure to change each picture many times, to give the illusion of a slot machine. Note the use of sapply to create a list of images, regardless of the number of images used.

```
require(tcltk)
pics = list.files('fruits',pattern='\\.gif$')
pics = paste('fruits/',pics,sep='')
n = length(pics)
theimages = sapply(pics,function(pic)
                                    tcl("image","create","photo",tclVar(),file=pic))
spinner = function(...){
    for(i in 1:50){
        r = sample(1:n,size=3,replace=TRUE)
        tkconfigure(img1,image=theimages[[r[1]]])
        tkconfigure(img2,image=theimages[[r[2]]])
```

tkconfigure (img3,image=theimages[[r[3]]])

```
tcl('update')
```

Sys.sleep(.07)
\}
\}
top $=$ tktoplevel()
f1 = tkframe(top)
f2 = tkframe(top)
r = sample(1:n, size=3, replace=TRUE)
img1 = tklabel(f1,image=theimages[[r[1]]])
img2 $=$ tklabel (f1,image=theimages[[r[2]]])
img3 $=$ tklabel (f1,image=theimages[[r[3]]])
tkpack(img1,side='left')
tkpack(img2,side='left')
tkpack(img3,side='left')
tkpack(tkbutton(f2,text='Spin', command=spinner), side='bottom')
tkpack(f1,side='top')
tkpack(f2,side='bottom')

A picture of the GUI before spinning is shown below


## Chapter 12

## CGI Programming

### 12.1 Web Servers

We're all familiar with the use of a webserver - we type an address or click on a link, and then the page we want appears in our browser. But what actually happens when we type in a web address? Web servers are simply programs that listen for requests on a particular port (port 80 by default), and then send out information to the connection that requested it. Such a two-way connection is known as a socket. To see what really happens when a request is sent to a webserver, we can write an R program that creates a socket on an unused port, and then try to access that port through a web browser. Then we can have our program simply send back whatever it received in order to see what's really going on. The program is surprisingly simple:

```
webecho = function(){
    xx = make.socket('localhost',port=1888,server=TRUE)
    on.exit(close.socket(xx))
    stuff = read.socket(xx,maxlen=1024)
    write.socket(xx,stuff)
}
```

The function opens a socket to port 1888, reads whatever gets sent to it, and then sends it right back to the same place as the request came from, so it can be displayed in a browser. The call to on.exit makes sure that the socket is closed after the communication takes place. To run the program so that it will be able to respond to requests, we place it in a loop:

```
> while(1)webecho()
```

(If you run the program on a UNIX system, you'll have to quit your R session (with control$\backslash$ ) to stop it; on a Windows system you may be prompted to quit your R session when you try to exit.)

Now let's type the following address into a browser:
http://localhost:1888/something
Here's what appears in the browser:
GET /something HTTP/1.1
Host: localhost:1888
User-Agent: Mozilla/5.0 (X11; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20051010 Galeon/1
Accept: text/xml, application/xml, application/xhtml+xml, text/html;q=0.9,text/plain;q=0.8,
Accept-Language: en
Accept-Encoding: gzip,deflate
Accept-Charset: ISO-8859-1,utf-8;q=0.7,*;q=0.7
Keep-Alive: 300
Connection: keep-alive

The output consists of the actual request (the line with the GET), and a series of headers. This is all the information that is transmitted from the browser to the webserver when a request is made for a particular page. Once a webserver receives a request like this, it returns the page that the user requested (as specified in the GET directive). If that page contains images, documents or additional programs, they would be sent to the browser through the same mechanism.

This is fine for ordinary, static pages, but what about the case where we accept input from the user? This would be the case when data is entered into a field, or checkboxes are checked on a page, and then a button is clicked to send the information from the browser to the web server. Web pages that accept information are known as forms. There are two mechanisms that can be used to send information from a web browser to a webserver; GET (which is the default, if you don't explicitly state a method) and POST. (We'll look at their differences shortly.) For example, the HTML that would be used on a web page to accept a text field and use the GET method to send the information would look like this:

```
<form action='http://localhost:1888' method=GET>
<input type=text name=myvar><br>
<input type=submit value='GET'>
</form>
</html>
```

Notice the action= specification in the form tag; this specifies the program which will be executed once the information is sent from the browser to the web server. The name= specification, which must always be present in an HTML that will accept information from a user, defines the name of a CGI variable. CGI stands for "Common Gateway Interface", and is a catch-all term for any program which is executed by a web server in response to a request from a browser.

Here's how this html would display in a browser:

File Edit View Go Bookmarks Tools Help


## GET

## Done

What happens if we enter something in the field, and click on the button? Let's put the words "hello, world" in the field and see:


First, notice that the address has changed, reflecting the address given in the action= specification. Additionally, some text has been added to the end of the displayed URL, and
we can see that this same text was sent to the web server as part of the GET specification.
The extra text that's in the URL and the GET specification is said to be urlencoded; non-alphanumeric characters (like the comma) are replaced with a percent sign followed by the two-digit hexadecimal representation of the character, and spaces are replaced with plus signs. (A complete list of the encodings can be found at http://www.w3schools.com/tags/ref_urlencode.asp)

This method of transfering information has its limitations. First of all, it's obvious that it won't work for things like files, because there's just not enough room in a URL to accomodate files of arbitrary length. Secondly, it may not be prudent to display the information that you're transfering in the URL where it can easily be seen. An alternative to GET is known as POST. Let's see how it differs from GET by creating a form identical to the first one, but with the method specified as POST. The html looks like this:

```
<form action='http://localhost:1888' method=post>
<input type=text name=myvar><br>
<input type=submit value='POST'>
</form>
```

Here's how it displays in the browser:


## Done

Once again, we'll enter "hello, world", and click on the button:

## POST / HTTP/l.1

Host: localhost:1888

```
User-Agent: Mozilla/5.0 (Xll; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20
```

Accept: text/xml,application/xml,application/xhtml+xml,text/html;q=0.9,te
Accept-Language: en-us,en; $q=0.5$
Accept-Encoding: gzip,deflate
Accept-Charset: IS0-8859-1, utf-8; $q=0.7$, *; $q=0.7$
Keep-Alive: 300
Connection: keep-alive
Content-Type: application/x-www-form-urlencoded
Content-Length: 20
myvar=hello\%2C+world
1
Done

Notice that the URL no longer has any information about the CGI variables; the urlencoded string with the values now appears after the header information that the web browser sent. (Remember that for protocols like HTTP, a single completely blank line indicates the end of the headers.) Since the information in the form is not placed in the URL, this should allow us to upload local files to a CGI program. Here's the HTML code for a form that will upload a file:

```
<form action='http://localhost:1888' method=post enctype="multipart/form-data">
<input type=file name='myfile'>
<input type=submit value='POST'>
</form>
```

Here it is displayed in a browser:

File Edit View Go Bookmarks Tools Help



## Done

The Browse... button is generated automatically when type=file is specified for an input element. For file uploading, the method must be set to post; using get just won't work. Now I'll fill out the form with the name of the file that holds the source for the webecho function that we've been using to see how it gets transfered.

```
POST / HTTP/l.l
```

POST / HTTP/l.l
Host: localhost:1888
Host: localhost:1888
User-Agent: Mozilla/5.0 (Xll; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20
User-Agent: Mozilla/5.0 (Xll; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20
Accept: text/xml,application/xml,application/xhtml+xml,text/html;q=0.9,te
Accept: text/xml,application/xml,application/xhtml+xml,text/html;q=0.9,te
Accept-Language: en-us,en;q=0.5
Accept-Language: en-us,en;q=0.5
Accept-Encoding: gzip,deflate
Accept-Encoding: gzip,deflate
Accept-Charset: IS0-8859-1,utf-8;q=0.7,*;q=0.7
Accept-Charset: IS0-8859-1,utf-8;q=0.7,*;q=0.7
Keep-Alive: 300
Keep-Alive: 300
Connection: keep-alive
Connection: keep-alive
Content-Type: multipart/form-data; boundary=-----------------------------
Content-Type: multipart/form-data; boundary=-----------------------------
Content-Length: 409
Content-Length: 409
-----------------------------770005061899741590183404268
-----------------------------770005061899741590183404268
Content-Disposition: form-data; name="myfile"; filename="webecho.r"
Content-Disposition: form-data; name="myfile"; filename="webecho.r"
Content-Type: application/octet-stream
Content-Type: application/octet-stream
webecho = function(){
webecho = function(){
xx = make.socket('localhost',port=1888,server=TRUE)
xx = make.socket('localhost',port=1888,server=TRUE)
on.exit(close.socket(xx))
on.exit(close.socket(xx))
stuff = read.socket(xx,maxlen=1024)
stuff = read.socket(xx,maxlen=1024)
write.socket(xx,stuff)
write.socket(xx,stuff)
}
}
770005061899741590183404268-
770005061899741590183404268-
4

```
4
```

Done

The file is sent (after the headers) in a form very similar to an email attachment. One big difference is that, if the file to be transmitted is a non-text file (like an image or document), no encoding needs to be done - the HTTP protocol utilizes all 8 bits of each byte. You may have noticed the enctype="multipart/form-data" specification in the previous form. This is what causes the web browser to send it's data in the "attachment" style, and is required
when you're uploading a file. If you specify it in a normal form, it will send the CGI variable information in a similar fashion. With a form like this:

```
<form action='http://localhost:1888' method=post enctype="multipart/form-data">
<input type=text name=myvar><br>
<input type=submit value='POST'>
</form>
```

entering "hello, world" results in the following:
POST / HTTP/1.1
Host: localhost:1888
User-Agent: Mozilla/5.0 (X11; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20051010 Firefox/
Accept: text/xml,application/xml,application/xhtml+xml,text/html;q=0.9,text/plain;q=0.8,
Accept-Language: en-us,en;q=0.5
Accept-Encoding: gzip,deflate
Accept-Charset: ISO-8859-1,utf-8; q=0.7,*; q=0.7
Keep-Alive: 300
Connection: keep-alive
Content-Type: multipart/form-data; boundary=-----------------------------14394547745218385
Content-Length: 178
----------------------------14394547745218385925125258
Content-Disposition: form-data; name="myvar"
hello, world
----------------------------14394547745218385925125258--
Note that in this case, there was no urlencoding of the variable's value.

### 12.2 CGI Scripting

Before continuing, it's worth making note of some very practical details that you'll have to consider before beginning a project that uses CGI scripting. The programs which a web server will execute in response to a request need to be in specially designated directories, or the web server will treat them as ordinary documents, not programs. In general, access to such directories will be limited, both for financial and security reasons. In addition, a program which requires large amounts of computer resources may make it difficult for others who use the server to get anything done.

When you are writing CGI programs, it's very important to avoid allowing users manipulate any input which might find its way outside of the web server's slightly protected environment. What this means is that programs that call operating system programs, (for example calls to system in R), should generally be avoided.

Now that we've seen what's going on behind the scenes, we can start to look at the facilities in R that will allow us to write CGI scripts. The CGIwithR library provides a "wrapper" script that sets up an environment in which R can run. The most important function of the CGIwithR library is to gather all the information that the web browser has sent to the web server (regardless of how it was sent to the browser) and to make it easily available inside of R. The CGIwithR library takes all of the CGI variables (defined in the forms that a user has responded to), and places them in a list called formData, which can be manipulated like any other list in R. Note that the library resolves all issues regarding which method (get or post) was used in the form that generated the variables, and that the formData list is the only object you need to look at to get the values of the CGI variables defined in the form.

Once your program has received the information from a user's web browser, any printing statements that you make in your program will be directed back to the browser. This means that you need to follow the rules of HTML when you are displaying results, not the ordinary rules that would apply for an regular $R$ session. The cat function is very useful in this regard, because it displays exactly what you tell it to, without any element numbering or formatting. If you know the basics of HTML, you may prefer to simply use cat to generate most or all of the HTML your CGI script creates. (There is a library called R2HTML that automates the "HTML-ization" of R objects, and you may want to study it on your own, but we won't be using it here.) Here are some ideas for generating appropriate output in CGI programs written with R .

- The CGIwithR library provides a few helper functions that make generating useful HTML much easier:
- HTMLheader - This function, called with no arguments, prints the appropriate information at the beginning of your output so that all browsers will realize that they're receiving HTML. It's recommended that you call this function before you produce any output in an CGI script.
- tag and untag - These functions accept unquoted arguments and produce either the opening or closing tag required for most HTML constructs. For example, a large title line can be specified in HTML by beginning with <h1> and ending with </h1>. You could generate a title using tag and untag as follows:
$\operatorname{tag}(\mathrm{h} 1)$
cat('Here's my title')
untag (h1)
- br - To indicate a line break in HTML, the <br> tag must be used; HTML pays no attention to newline characters. The br function will print such a tag, so it can be inserted into your CGI program wherever you want to insert line breaks. An optional argument (defaulting to 1) tells br how many lines you want inserted.
- The HTML <pre> tag specifies that you don't want the browser that displays the output to perform any formatting. Suppose you want your CGI program to display
the results of the summary function for a variable x in a browser window just as it would appear in a command-line R session. You could use the following:

```
tag(pre)
print(summary(x))
untag(pre)
```

- The $\langle\mathrm{p}\rangle$ tag is an alternative way of placing line breaks into your output.


### 12.3 A First CGI program with R

As a simple way of getting started with CGI programming, let's take the output from the first simple form that we created and see how the information gets translated from the CGI environment into the R environment. I'm assuming that your SCF account is s133xx and that you've followed the instructions at/http://www.stat.berkeley.edu/classes/s133/projects/tech/Cgiprogs.htm to prepare your account to use CGI scripting. Typically, you would put the page containing the html in your public_html directory. Suppose the following is placed in a file called form1.html in your publichtml directory:

```
<html>
<form action='cgi-bin/R.cgi/test1.cgi' method=get>
<input type=text name=myvar><br>
<input type=submit value='GET'>
</form>
</html>
```

Since file names in HTML are interpreted relative to the directory that the HTML resides in, we can refer to the CGI program relative to the cgi-bin directory. Notice that this will allow you to use the same form whether you're running on the SCF network or through a tunnel. In addition to the formData list that holds the values of the CGI variables, information is also passed to your CGI program through environmental variables. These variables can be accessed with the Sys.getenv function, but for our purposes here, we can use the showEnvironmentVariables function that's part of the CGIwithR package. Here's a simple program that will just print out some information about the formData list and the environmental variables that are transfered into the environment:

Here's the test1.cgi program:

```
HTMLheader()
cat('Class of formData=',class(formData),' Mode of formData=',mode(formData),'<br>')
cat('Names of formData=',names(formData),'<br>')
tag(pre)
```

```
print(formData)
untag(pre)
showEnvironmentVariables()
cat('</body></html>')
```

If we run the program (by pointing a browser at http://springer/ s133xx/form1.html, entering "hello, world" and pressing the button), here's what the output looks like:
Class of formData= list Mode of formData= list
Names of formData= myvar
\$myvar
[1] "hello, world"
SERVER_SIGNATURE
R_INCLUDE_DIR
HTTP_KEEP_ALIVE
HTTP_USER_AGENT
SERVER_PORT
HTTP_HOST
LD_LIBRARY_PATH
DOCUMENT_ROOT
HTTP_ACCEPT_CHARSET
SCRIPT_FILENAME
REQUEST_URI
SCRIPT_NAME
R_GSCMD
HTTP_CONNECTION
PATH_INFO
REMOTE_PORT
PATH
R_LIBS
PWD
SERVER_ADMIN
R_SHARE_DIR
LANG
HTTP_ACCEPT_LANGUAGE
PATH_TRANSLATED
HTTP_REFERER
HTTP_ACCEPT
REMOTE_ADDR
SHLVL

```
Apache/2.0.54 (Ubuntu) Server at springer Port }8
/usr/local/linux/R-2.2.1/include
300
Mozilla/5.0 (X11; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20051
80
springer
/usr/local/linux/R-2.2.1/lib:/usr/local/lib64:/usr/lib/gcc/x86_6
/mirror/data/pub/html/classes/s133
ISO-8859-1,utf-8;q=0.7,*;q=0.7
/class/u/s133/s133xx/public_html/cgi-bin/R.cgi
/~s133xx/cgi-bin/R.cgi/test1.cgi?myvar=hello%2C+world
/~s133xx/cgi-bin/R.cgi
/usr/bin/gs
keep-alive
/test1.cgi
4 8 2 4 2
/usr/local/bin:/usr/bin:/bin
/class/u/s133/s133xx/public_html/cgi-bin
webmaster@localhost
/usr/local/linux/R-2.2.1/share
en
/class/u/s133/s133xx/public_html/cgi-bin/test1.cgi
http://springer/~}s133xx/form1.html
text/xml,application/xml,application/xhtml+xml,text/html;q=0.9,t
128.32.135.22
1
```

| SERVER_NAME | springer |
| :--- | :--- |
| FORM_DATA | myvar=hello\%2C+world |
| SERVER_SOFTWARE | Apache/2.0.54 (Ubuntu) |
| QUERY_STRING | myvar=hello\%2C+world |
| SERVER_ADDR | 128.32 .135 .22 |
| GATEWAY_INTERFACE | CGI/1.1 |
| R_HOME | /usr/local/linux/R-2.2.1 |
| SERVER_PROTOCOL | HTTP/1.1 |
| HTTP_ACCEPT_ENCODING | gzip, deflate |
| R_DOC_DIR | /usr/local/linux/R-2.2.1/doc |
| REQUEST_METHOD | GET |
| R_SESSION_TMPDIR | /tmp/RtmpPPrmxy |
| R_PLATFORM | x86_64-unknown-linux-gnu |
| R_PAPERSIZE | letter |
| R_PRINTCMD | lpr |
| R_LATEXCMD | /usr/bin/latex |
| R_DVIPSCMD | /usr/bin/dvips |
| R_MAKEINDEXCMD | /usr/bin/makeindex |
| R_RD4DVI | ae |
| R_RD4PDF | times,hyper |
| R_UNZIPCMD | /usr/bin/unzip |
| R_ZIPCMD | /usr/bin/zip |
| R_BROWSER | /usr/bin/firefox |
| EDITOR | vi |
| PAGER | /usr/bin/less |
| R_PDFVIEWER | /usr/local/linux/bin/acroread |
| AWK | gawk |
| EGREP | grep |
| MAKE | make |
| PERL | /usr/bin/perl |
| TAR | tar |
| LN_S | ln -s |
| R_USE_AQUA_SUBDIRS | no |
|  |  |

You may have noticed that the URL we used for the action= specification makes it look like R.cgi is a directory, not a file. What happens is that the R.cgi program gets invoked by the web server, and it examines the PATH_INFO variable to find the name of your script (test1.cgi in this case.) It then loads up the formData list and calls your program.

If you examine the information that our simple web echoing program displayed, you'll see that each of the headers that were passed to the program have been transfered to environmental variables with a prefix of HTTP_. Although you most likely won't need them, you can examine the list of environmental variables to find information that you might want to use in your CGI programs and then access the information by using Sys.getenv.

The most important thing to notice is that the myvar CGI variable, defined in the input field of the HTML form, is available inside your R program, in unencoded form, in the element with the name myvar. This is the mechanism by which all the CGI variables are transfered into the R environment.

### 12.4 A First CGI program with R

As a simple way of getting started with CGI programming, let's take the output from the first simple form that we created and see how the information gets translated from the CGI environment into the R environment. I'm assuming that your SCF account is s133xx and that you've followed the instructions at http://www.stat.berkeley.edu/classes/s133/projects/tech/Cgiprogs.htm to prepare your account to use CGI scripting. Typically, you would put the page containing the html in your public_html directory. Suppose the following is placed in a file called form1.html in your public_html directory:

```
<html>
<form action='cgi-bin/R.cgi/test1.cgi' method=get>
<input type=text name=myvar><br>
<input type=submit value='GET'>
</form>
</html>
```

Since file names in HTML are interpreted relative to the directory that the HTML resides in, we can refer to the CGI program relative to the cgi-bin directory. Notice that this will allow you to use the same form whether you're running on the SCF network or through a tunnel. In addition to the formData list that holds the values of the CGI variables, information is also passed to your CGI program through environmental variables. These variables can be accessed with the Sys.getenv function, but for our purposes here, we can use the showEnvironmentVariables function that's part of the CGIwithR package. Here's a simple program that will just print out some information about the formData list and the environmental variables that are transfered into the environment:

Here's the test1.cgi program:

```
HTMLheader()
```

cat('Class of formData=', class(formData),' Mode of formData=', mode(formData),' <br>')
cat('Names of formData=', names(formData),'<br>')
tag (pre)
print(formData)
untag(pre)
showEnvironmentVariables()
cat('</body></html>')

If we run the program (by pointing a browser at http://springer/~s133xx/form1.html, entering "hello, world" and pressing the button), here's what the output looks like:

Class of formData= list Mode of formData= list

Names of formData= myvar

## \$myvar

[1] "hello, world"
SERVER_SIGNATURE
R_INCLUDE_DIR
HTTP_KEEP_ALIVE
HTTP_USER_AGENT
SERVER_PORT
HTTP_HOST
LD_LIBRARY_PATH
DOCUMENT_ROOT
HTTP_ACCEPT_CHARSET
SCRIPT_FILENAME
REQUEST_URI
SCRIPT_NAME
R_GSCMD
HTTP_CONNECTION
PATH_INFO
REMOTE_PORT
PATH
R_LIBS
PWD
SERVER_ADMIN
R_SHARE_DIR
LANG
HTTP_ACCEPT_LANGUAGE
PATH_TRANSLATED
HTTP_REFERER
HTTP_ACCEPT
REMOTE_ADDR
SHLVL
SERVER_NAME
FORM_DATA
SERVER_SOFTWARE
QUERY_STRING
SERVER_ADDR
GATEWAY_INTERFACE
R_HOME
SERVER_PROTOCOL
HTTP_ACCEPT_ENCODING

Apache/2.0.54 (Ubuntu) Server at springer Port 80 /usr/local/linux/R-2.2.1/include
300
Mozilla/5.0 (X11; U; Linux x86_64; en-US; rv:1.7.12) Gecko/20051 80
springer
/usr/local/linux/R-2.2.1/lib:/usr/local/lib64:/usr/lib/gcc/x86_6
/mirror/data/pub/html/classes/s133
ISO-8859-1,utf-8;q=0.7,*; q=0.7
/class/u/s133/s133xx/public_html/cgi-bin/R.cgi
/~s133xx/cgi-bin/R.cgi/test1.cgi?myvar=hello\%2C+world
/~s133xx/cgi-bin/R.cgi
/usr/bin/gs
keep-alive
/test1.cgi
48242
/usr/local/bin:/usr/bin:/bin
/class/u/s133/s133xx/public_html/cgi-bin
webmaster@localhost
/usr/local/linux/R-2.2.1/share
en
/class/u/s133/s133xx/public_html/cgi-bin/test1.cgi
http://springer/~s133xx/form1.html
text/xml, application/xml, application/xhtml+xml, text/html;q=0.9,t
128.32.135.22

1
springer
myvar=hello\%2C+world
Apache/2.0.54 (Ubuntu)
myvar=hello\%2C+world
128.32.135.22

CGI/1.1
/usr/local/linux/R-2.2.1
HTTP/1.1
gzip,deflate

| R_DOC_DIR | /usr/local/linux/R-2.2.1/doc |
| :--- | :--- |
| REQUEST_METHOD | GET |
| R_SESSION_TMPDIR | /tmp/RtmpPPrmxy |
| R_PLATFORM | x86_64-unknown-linux-gnu |
| R_PAPERSIZE | letter |
| R_PRINTCMD | lpr |
| R_LATEXCMD | /usr/bin/latex |
| R_DVIPSCMD | /usr/bin/dvips |
| R_MAKEINDEXCMD | /usr/bin/makeindex |
| R_RD4DVI | ae |
| R_RD4PDF | times,hyper |
| R_UNZIPCMD | /usr/bin/unzip |
| R_ZIPCMD | /usr/bin/zip |
| R_BROWSER | /usr/bin/firefox |
| EDITOR | vi |
| PAGER | /usr/bin/less |
| R_PDFVIEWER | /usr/local/linux/bin/acroread |
| AWK | gawk |
| EGREP | grep -E |
| MAKE | make |
| PERL | /usr/bin/perl |
| TAR | tar |
| LN_S | ln -s |
| R_USE_AQUA_SUBDIRS | no |

You may have noticed that the URL we used for the action= specification makes it look like R.cgi is a directory, not a file. What happens is that the R.cgi program gets invoked by the web server, and it examines the PATH_INFO variable to find the name of your script (test1.cgi in this case.) It then loads up the formData list and calls your program.

If you examine the information that our simple web echoing program displayed, you'll see that each of the headers that were passed to the program have been transfered to environmental variables with a prefix of HTTP_. Although you most likely won't need them, you can examine the list of environmental variables to find information that you might want to use in your CGI programs and then access the information by using Sys.getenv.

The most important thing to notice is that the myvar CGI variable, defined in the input field of the HTML form, is available inside your R program, in unencoded form, in the element with the name myvar. This is the mechanism by which all the CGI variables are transfered into the R environment.

### 12.5 Data

The R.cgi script calls your R program in such a way that it doesn't automatically load any data into the R environment. So if you want to have data available to your CGI program,
you'll need to explicitly get the data into R's environment. For reasons of efficiency, your program should always use the load function to load a previously saved binary version of the data you need. The most convenient place to store these objects is right in the cgi-bin directory from which your program will execute.

Suppose we wish to create a CGI program that will accept the name of one of the variables from the wine data frame, and then display a summary of the data. Before you plan to run the script, the wine data should be saved in a simple R session that's started after you've changed your working directory to be your cgi-bin directory. The command to do this is

```
save(wine,file='wine.rda')
```

Next, we can create a form, which would be saved in the public_html directory. Here's a simple example, which we'll save in the file wine.html:

```
<html><body>
<h1>Summary for Wine Variables</h1>
<form action='cgi-bin/R.cgi/dowine.cgi'>
Enter the name of the variable:
<input type=text name=winevar><br>
<center>
<input type=submit value='Run'>
</center>
</form>
</body></html>
```

The dowine.cgi program would look like this:

```
load('wine.rda')
HTMLheader()
winevar = formData$winevar
tag(h1)
cat('Summary for wine$',winevar,sep='')
untag(h1)
tag(h2)
tag(pre)
print(summary(wine[[winevar]]))
untag(pre)
untag(h2)
cat('</body></html>')
```

Here's the form:

File Edit View Go Bookmarks Tools Help $\measuredangle \rightarrow \square$ • $\triangle$ http://springer/~sl33ar/wine.html

## Summary for Wine Variables

Enter the name of the variable: Alcohol

Here's the result of submitting the form:

File Edit View Go Bookmarks Tools Help

## Summary for wine\$Alcohol



Mean 3rd Qu. $13.00 \quad 13.68$

## Done

### 12.6 Combo Forms

Of course, having the user remember the name of the variable they're interested in isn't a very user-friendly strategy, but the thought of manually preparing a form that lists all the variables isn't very appealing either. The problem can be solved by having the CGI program generate the form the first time it's called, and then processing the form when it's submitted back to the web server. If we call the CGI program directly (not through a form submission), the formData list will be empty, and we can use that condition to tell whether we need to generate the form or respond to it. Since R will be generating the form, it's very easy to have it provide a choice for each variable. For this example, let's use a drop down menu that will display the names of each variable. Here's a program that will both generate the form and respond to it:

```
if(length(formData) == 0){
    HTMLheader()
    tag(h1)
    cat('Summary for Wine Variables')
    untag(h1)
    cat("<form action='dowine1.cgi'>")
    cat("Choose the variable:")
```

```
        cat("<select name='winevar'>")
        load("wine.rda")
        sapply(names(wine),function(x)cat("<option value='", x,"'>", x,"<br>\n",sep=''))
        cat("</select>")
        cat('<input type="submit" value="Run">')
        cat("</form></body></html>")
} else {
    load('wine.rda')
    HTMLheader()
    winevar = formData$winevar
    tag(h1)
    cat('Summary for wine$',winevar,sep='')
    untag(h1)
    tag(h2)
    tag(pre)
    print(summary(wine[[winevar]]))
    untag(pre)
    untag(h2)
    untag(h2)
    cat('</body></html>')
}
```

One very important thing to notice if you use this approach - the action= argument should specify only the name of the program, without the usual R.cgi/; since R is already calling your program, it thinks it's in the R.cgi "directory".

Here's the result of calling the program directly:

File Edit View Go Bookmarks Tools Help
$\checkmark \backsim \backsim \square$ http://springer/~sl33ar/cgi-bin/R.cgi/dowinel

## Summary for Wine Variables

Choose the variable: Magnesium $\quad \boxed{ }$
and here's the result after making a choice:

## Summary for wine\$Magnesi

## Done

### 12.7 Graphs

Certainly one of the most useful functions of CGI scripting with R is to display graphics generated by $R$, based on a user's choices as specified on a web form. This would provide a simple way to allow people unfamiliar with R to produce attractive graphs; if a means is provided for data input, and enough options are provided through checkboxes, drop-down menus, radiobuttons, etc, a complete web-based graphing solution could be developed.

To properly create and display graphics with a CGI program, it's necessary to understand the difference between the internal paths (which your R program will see) and the external paths (which are the addresses typed into the browser's address field.) For example, the way the class webserver is configured, the directory into which you would put HTML pages is (once again assuming your SCF id is s133xx):
/class/u/s133/s133xx/public_html/
This directory provides a convenient place to place graphics generated by your scripts. To the outside world, this directory would be indicated as:
http://springer/~s133xx/
or
http://localhost:8080/~s133xx/
So as far as the webserver is concerned (i.e. the way the outside world would find your files through a URL), the directory is known as

```
/~s133xx/
```

To create graphics from your CGI script, you first create a variable called graphDir and set it equal to the full internal name of the directory into which you'll write your graphs. In our example it would be /class/u/s133/s133xx/public_html/. Then use the webPNG function, specifying the name (without any leading directories) that you want to use for your graph. In order to generate the appropriate HTML so that your image will be displayed, you can use the img function of the CGIwithR library. This function takes two arguments. The first is the name of the graphic you produced via webPNG, and the second is called graphURLroot, and should be set to the "outside" view of your public_html directory, namely / ~s133xx/. (Note the trailing slashes in both the graphDir and graphURLroot; they are required.)

To illustrate, let's create a simple CGI program that will generate some random data and create a conditioning plot containing histograms.

```
library(lattice)
x = data.frame(z = rnorm(1000), g = factor(sample(1:5,size=1000,replace=TRUE)))
graphDir='/class/u/s133/s133xx/public_html/'
cat("Now I'm going to plot some histograms:<br>")
webPNG(file='hist.png')
histogram(~z|g,data=x)
invisible(dev.off())
img(src='hist.png',graphURLroot='/~ s133xx/')
cat("</body></html>")
```

The size of the plot can be controlled by passing width= and height= arguments to webPNG; the units for these arguments are pixels.

If you are using lattice graphics and your plot does not appear, try passing the call to the lattice function to the print function.

Notice the call to dev.off; without it, your graph may not be properly terminated, and only some (or possibly none) of the graph will be displayed.

### 12.8 Hidden Variables

Suppose we have a web page that displays a choice of data frames for possible further analysis. Once a data frame is chosen, another page could display the variables that are available from that data frame, and a choice of plots could be provided. Remember that each time our CGI program is called, a new R process begins. So how can we "remember" the data set name in between invocations of our program? The answer is to use hidden variables. Any time
you create an HTML form, you can create as many hidden variables as you need to store information that needs to be available in the next step of processing. These hidden variables are exactly like any other CGI variable, but there is no visible sign of the variable on the form that is displayed in the user's browser. To create a hidden variable, use code like the following:

```
<input type="hidden" name="varname" value="the value">
```

Here's an implementation of a program that looks in the current directory for any files with an extension of .rda, provides a drop down menu of data set names, then allows a choice of variables, and finally produces the requested plot:

HTMLheader ()
if(length (formData) == 0) \{
datasources = list.files('.', pattern='<br>.rda\$')
datasources $=$ sub('<br>.rda\$',', ,datasources)
cat('<form action="doplot.cgi">')
cat ('<select name=dataset>\n')
sapply(datasources,function(x)cat('<option value="', \(x\), '">', $x, '</ o p t i o n>\backslash n '))$
cat ('</select>\n')
cat('<center><button type="submit">Run</button></center></form>')
\} else if('dataset' \%in\% names (formData)) \{
dataset $=$ formData\$dataset
dataset = gsub(' ',', ,dataset)
load(paste (dataset, '.rda', sep=''))
cat('<form action="doplot.cgi">\n')
cat('<p>X-variable:<br>\n')
sapply (names (get (dataset)), function(i)cat('<input type="radio" name="xvar" value="',
cat ('<p>Y-variable:<br>\n')
sapply (names (get (dataset)), function(i)cat('<input type="radio" name="yvar" value="',
cat('<input type="hidden" name="set" value="', dataset, '">\n')
cat('<center><button type="submit">Run</button></center></form>')
cat ('</form>')
\} else\{
dataset $=\operatorname{gsub}(, \quad,, '$, formData\$set)
load(paste(dataset,'.rda', sep=' '))
xvar=gsub(' , ,', formData\$xvar)
yvar=gsub(', ,', formData\$yvar)
graphDir = '/home/spector/public_html/'
webPNG(file='theplot.png',graphDir=graphDir)
thedata $=$ get (dataset)
plot(thedata[[xvar]], thedata[[yvar]], xlab=xvar, ylab=yvar)
img(src='theplot.png',graphURLroot='/~spector/')
invisible(dev.off())

```
    }
cat('</body></html>')
```

This program has three sections: the first displays the initial form showing the data frame names (invoked when no formData is available); the second displays the variable choices (invoked when a dataframe variable is specified), and the third, which is invoked when formData is available, but the dataset variable is not defined.

### 12.9 Outgoing HTTP Headers

We've already seen that when a web browser makes a request to a web server, it sends a series of headers before the actual content (if any). The web server also sends headers to the browser, but up until now we've let the R.cgi wrapper script take care of that detail for us. In most cases, the only header that needs to be sent to a browser is one that informs the browser that we're sending it HTML (as opposed to, say an image or other binary file). That header looks like this:

Content-type: text/html
and it would be followed by a completely blank line to signal the end of the headers. The R.cgi script examines what you're about to send to the web browser, and, if it doesn't find the "Content-type" line, it inserts it before it sends your output to the browser. Thus, if you do insert that line, you are taking responsibility for the outgoing headers, and, if desired, you can add additional ones.

Just about the only header line that you might consider adding is one that specifies the value of a cookie to the browser. Cookies are small pieces of text, associated with a particular website, that are stored by a browser, and sent to web servers if they match the domain and possibly the path of the URL that initially set them. There are two types of cookies: session cookies, which expire when a particular browser session is ended and the browser is shut down, and persistent cookies, that are stored in a text file on the computer on which the browser is running, and will expire at a date specified in the header that defined the cookie. For this example, we'll create a session cookie, and then access it through a different script. If every web transaction had a form associated with it, we could use hidden CGI variables to do much of the work that cookies do, but, since they're stored on the user's computer, they are more reliable, and don't require any special programming. Here's an example of a script that sets a cookie:

```
if(length(formData) == 0){
    HTMLheader()
    cat("What is your name?")
    cat('<form action="setcookie.cgi">\n')
    cat('<input type="entry" name="name"><br>\n')
    cat('<button type="submit">Run</button>\n')
```

```
} else if('name' %in% names(formData)){
    name = formData$name
    cat("Content-type: text/html\nSet-Cookie: thename=",name,"; path=/~ s133xx/\n\n",sep=
    cat("Hello there, ",name)
}
cat('</body></html>')
```

Since everyone in class is sharing the same webserver, I've added a path= specification to the cookie header. For this class, it probably is a good idea to prevent people from getting cookies set by other programs. Note the two newlines at the end of the header line - these are essentially to make sure that the browser understands that the headers are done and the content is following. If you want to create persistent headers, you need to add an expires= specification to the Set-cookie header. The format of the expiration time must be followed precisely; in particular, the parts of the date much be separated by dashes, and the only allowable time zone is GMT. Here's an example of a header containing a variable, path and expiration date:

Set-Cookie: thename=Somebody; path=/~s133xx/; expires=Monday, 09-May-10 00:00:00 GMT
Now let's look at a program that will retrieve an already set cookie. When a browser recognizes a domain/path/time combination for which it has an active cookie, it sends it back to the webserver in a Cookie: header, not as a CGI variable. The format of the cookie is name=value, similar to the format in which CGI variables are transmitted. This means that we'll need to use Sys.getenv to access the environmental variable called HTTP_COOKIE.

```
HTMLheader()
cookie = Sys.getenv('HTTP_COOKIE')
name = gsub('^ *thename=(.*)$','\\1',cookie)
cat('Welcome back, ',name)
cat('</body></html>')
```

Notice that you can only access the cookies in a CGI program, not in ordinary HTML, but you don't need any form elements to get the cookie.

### 12.10 Creating Pretty Output

Since the output created by CGI programs is interpreted by the browser as HTML, we can use any HTML commands by simply having our program generate the necessary HTML statements. One simple way of organizing output in HTML is the HTML table. A table begins with the string <table>, and ends with </table>. Each row of the table begins with <tr>, and ends with </tr>; each element within a row begins with <td> and ends with </td>. To specify headings, the th tag can be used in place of td. This suggests the following function to produce one row of an HTML table:

```
makerow = function(x,tag='td'){
    st = paste('<',tag,'>',sep='')
    end= paste('</',tag,'>',sep='')
    cat(paste(paste('<tr>',st,sep=''),
        paste(x,collapse=paste(end,st,sep='')),
            paste(end,'</tr>',sep='')),"\n")
}
```

To print an entire data frame, we can first print the names as a header line, then use apply to print the body of the data frame:

```
dftable = function(df){
    cat('<table border=1>')
    makerow(names(df),tag='th')
    apply(df,1,makerow)
    cat('</table>')
}
```

An example of using these functions will be presented in the next section.

### 12.11 File Upload

We've already seen that that an input element with type=file will create an entry field and browse button to allow a user to specify a file for upload. In the following program, we'll create such a field to allow a user to specify a local comma-separated file which will then be read into R, and displayed as a table. File upload using the CGIwithR library simply places the content of the uploaded file into a character string in the formData list corresponding to the name of the CGI variable specified in the HTML form. To treat this character string as a file, we can use the textConnection function.

The following program will upload a comma-separated file, which will then be read by read.csv, and displayed using the dftable function from the previous section:

```
HTMLheader()
if(length(formData) == 0){
    cat('<form action="readcsv.cgi" method=post enctype="multipart/form-data">\n')
    cat('<input type=file name=thefile><br>')
    cat('<input type=submit value="Upload">')
    cat('</form>')
} else{
    makerow = function(x,tag='td'){
        st = paste('<',tag,'>',sep='')
        end= paste('</',tag,'>',sep='')
        cat(paste(paste('<tr>',st,sep=''),
            paste(x,collapse=paste(end,st,sep='')),
```

```
        paste(end,'</tr>', sep='')),"\n")
    }
    dftable = function(df){
        cat('<table border=1>')
        makerow(names(df),tag='th')
        apply(df,1,makerow)
            cat('</table>')
        }
    txtcon = textConnection(formData$thefile)
    df = read.csv(txtcon)
    dftable(df)
}
cat('</body></html>')
```


### 12.12 Debugging CGI Programs

The first step in debugging an $R$ program is to make sure that there are no obvious syntax errors. This can be done easily by changing directories to the location of your CGI programs, running R and using the source command to execute your program. If you see any syntax errors, they should be corrected before attempting to run your program through the web server. You can simulate input from a form by creating a list called formData and loading appropriate elements into named values in that list.

When a program is run as a CGI program through a webserver, the program's standard error, which contains error messages, is normally routed to the webserver's error logs. Unless you are the owner of the webserver, these logs are usually not readable. To redirect error messages to your browser (which represents the standard output stream of a CGI program), you can use the following command inside your CGI program:
sink(file=stdout(), type='message')
Remember that the error messages will not be displayed using HTML, so they may be difficult to read.

If simulating your web data through an artificially constructed formData list is not sufficient to resolve problems in getting your program to run properly through the webserver, you can have a form generate the formData list, and save it to a file; then when you are testing the program offline, you can load that copy of formData, giving you an interactive session with the same data as would be generated by the web page.

## Chapter 13

## Smoothers

### 13.1 Smoothers

In many of the graphs we've looked at, we added a straight line representing the best linear regression line that went through the data we were plotting. Such lines can be very helpful when there are lots of points, or when outliers might detract from our seeing a relationship among the points. But plotting the best linear regression line has some limitations. For one thing, the regression has to fit all the data, so finding a good regression fit is often a compromise between being true to the data in any given range, and trying to come up with a single line that does reasonably well throughout the entire range. For some data, this may be appropriate. For example, if we know that two variables really follow a linear relationship, then we'd have to assume that deviations from that relationship are just noise, and the best straight line would be a meaningful way to display their relationship on a graph. However, situations like that are not that common. To come up with a way of visualizing relationships between two variables without resorting to a regression lines, statisticians and mathematicians have developed techniques for smoothing curves. Essentially this means drawing lines through the points based only on other points from the surrounding neighborhood, not from the entire set of points. There are many different types of smoothers available, and most of them offer an option that controls how much smoothing they will do as well as options to control the basic methods that they use, so it's usually possible to find a smoother that will work well for a particular set of data.

### 13.2 Kernel Smoothers

Kernel smoothers work by forming a weighted average of all the $y$-values corresponding to points whose x -values are close to the x -value of a point being plotted. The function that defines the weights is known as a kernel, and the number of points involved in the weighted average is based on a parameter known as the bandwidth. The default kernel is a box function; in other words, it simply averages together $y$-values which are within the specified bandwidth of a given x -value, and uses that average as the y -value for the x -value in question. With a very tiny bandwidth, this corresponds to a "connect-the-dots" type of drawing. With a very large bandwidth, it will basically estimate every y-value as the mean of all the $y$-values. However, even when the bandwidth is carefully chosen, using the box kernel rarely will result in a truly smooth graph. For example, consider a plot of OD.Ratio versus Proanthocyanins from the wine data set that we've used in previous examples. The following code produces a plot of the variables, and superimposes a line representing a box kernel smooth with the default bandwidth:

```
> plot(wine$Proanthocyanins,wine$OD.Ratio)
> lines(ksmooth(wine$Proanthocyanins,wine$OD.Ratio))
```

Here's the graph:


Notice how choppy the line is, especially where there isn't much data. That's because the box kernel is too extreme - it either adds in a point or not. So using the box kernel is like stacking up a bunch of square boxes around each point, and we don't really get a smooth result.

More commonly, kernels will have a maximum at distances that are very small, and will decrease gradually as the (absolute value) of the distance from the center of the kernel increases. This means that nearby points will have lots of influence on the weighted estimate that will be plotted, but as we move away from a particular point, the neighboring points will have less and less influence. We can modify how many points are considered through the bandwidth - including more points tends to give smoother curves that don't respond as well to local variation, while decreasing the bandwidth tends to make the curve look "choppier". One of the most common kernels used in smoothing is the Gaussian or normal kernel. This kernel is the familiar "bell curve" - largest in the middle (corresponding in this cases to distances of zero from a particular point), and gradually decreasing over it's supported range. The width of that range is determined by the bandwith when using a kernel smoother. Here's the Proanthocyanins vs. OD.Ratio plot, smoothed with a normal kernel using the default bandwidth:


Notice the change in the line when switching to the normal kernel; the line is now smooth, and we can see that a linear relationship that holds up until around a Proanthocyanin concentration of about 2 .

The argument that controls the size of the neighborhood that's used by ksmooth to estimate the smoothed value at each point is called bandwidth. We can examine the effect of changing the bandwidth as follows;

```
kplotfn = function(bw){
    plot(wine$Proanthocyanins,wine$OD.Ratio,main=bw)
    lines(ksmooth(wine$Proanthocyanins,wine$OD.Ratio,bandwidth=bw),col='green')
}
bws = seq(.1,1,by=.1)
par(mfrow=c(5,2),mar=c (2,4,2,1)+.1)
sapply(bws,kplotfn)
```



After adjusting the margins, the plot we got looks something like a lattice plot. But how could we produce an actual lattice plot with this data? We would need a data frame with x and y values for each bandwidth. What does ksmooth return?

```
> result = ksmooth(wine$Proanthocyanins,wine$OD.Ratio)
> class(result)
[1] "list"
> names(result)
[1] "x" "y"
```

Since the lengths of x and y must be equal, we can convert the output to a data frame directly. Let's write a function which will generate a data frame with $\mathrm{x}, \mathrm{y}$ and bandwidth values for a single bandwidth:

```
kfun = function(bw)
    data.frame(bw=bw, as.data.frame(ksmooth(wine$Proanthocyanins,wine$OD.Ratio, bandwidth=b
```

Notice that R realized it had to repeat the single bw value to make it compatible with x and y. As always, we should test the function:

```
> result = kfun(.5)
> head(result)
    bw x y
10.5 0.4100000 1.881429
2 0.5 0.4279096 1.881429
3 0.5 0.4458192 1.812500
40.5 0.4637288 1.812500
5 0.5 0.4816384 1.879000
6 0.5 0.4995480 1.879000
```

Now we can create a list of data frames, one for each bandwidth:

```
> frames = lapply(seq(.1,1,by=.1),kfun)
> allbws = do.call(rbind,frames)
> dim(allbws)
[1] 1780 3
```

Notice the use of the do.call function, which is used here to call rbind with the data frames for all of the different bandwidths.

To get both points and lines on each panel, we can create a custom panel function:

```
mypanel = function(x,y,...){
    panel.xyplot(wine$Proanthocyanins,wine$OD.Ratio);
    panel.xyplot(x,y,type='l',col='red')
}
xyplot(y~}\mp@subsup{|}{|}{\prime}|\textrm{factor(bw),data=allbws,type='l',as.table=TRUE,layout=c(2,5),panel=mypanel)
```



The resulting plot appears below:

### 13.3 Locally Weighted Regression Smoothers

Another approach that is often used to smooth curves is locally weighted regression. Instead of taking a weighted average of $y$-values near the $x$-values we want to plot, the nearby points are used in a (usually quadratic) weighted regression, and predicted values from these local regressions are used as the y-values that are plotted. The lowess function in R implements this technique by using the reciprocal of the residuals of successive fits as the weights, downgrading those points that don't contribute to a smooth fit. In the lowess function, the argument $f=$ specifies the fraction of the data to be used in the local regressions. Specifying a larger value results in a smoother curve.

To illustrate, consider a plot of literacy versus phys, the number of physicians per 100000 people, from the world data set that we've used in previous examples. The following code produces a plot of the data with a lowess smoothed curve superimposed:

```
> plot(world$literacy,world$phys)
> lines(lowess(world$literacy,world$phys))
```

The graph appears below:


The argument to lowess that controls the level of smoothing is $f$, the fraction of the data which will be used in the local regressions. Let's compare the results of smoothing the literacy/physician curve using different values of $f$

```
lplotfn = function(f){
    plot(world$literacy,world$phys,main=f)
    lines(lowess(world$literacy,world$phys,f=f),col='orange')
}
fs = seq(.1,1,by=.1)
par(mfrow=c(5,2),mar=c (2,4,2,1)+.1)
sapply(fs,lplotfn)
```

For this particular data set, there's not much difference in the appearance of the smoothed curve, although there is a bit of noise when using the lowest value of $f$


### 13.4 Supersmoother

While most smoothers require specification of a bandwidth, fraction of data, or level of smoothing, supersmoother is different in that it figures these things out for itself. Thus, it's an excellent choice for situations where smoothing needs to be done without any user intervention. Supersmoother works by performing lots of simple local regression smooths, and, at each x -value it uses those smooths to decide the best y -value to use. In R, supersmoother is made available through the supsmu function.

To illustrate, consider the car data which we used earlier when we were studying cluster analysis. The following lines produce a plot of weight versus MPG, and superimposes a supersmoother line.

```
> plot(cars$Weight,cars$MPG)
> lines(supsmu(cars$Weight,cars$MPG))
```

The plot appears below:


As another example, we can revisit the wheat data that we used earlier with spline smoothing:

```
> plot(wheat$year,wheat$production)
> lines(supsmu(wheat$year,wheat$production))
```

Here's the plot:


### 13.5 Smoothers with Lattice Plots

When working with lattice graphics, we've already seen the use of panel.lmline, which displays the best regression line in each panel of a lattice plot. A similar function, panel.loess, is available to superimpose a locally weighted regression smoother in each panel of a plot. As a simple illustration, consider the built-in Orange data set, which has information about the age and circumference of several orange trees. First, let's look at a plot with the best regression line smoother superimposed on the plot of age versus circumference for each Tree:

```
> library(lattice)
> xyplot(circumference~age|Tree,data=Orange,
+ panel=function(x,y,...){panel.xyplot(x,y,\ldots.);panel.lmline(x,y,...)})
```

Here's the plot:


To create the same plot, but using the panel.loess function, we can use the following:

```
> xyplot(circumference~ age|Tree,data=Orange,
+ panel=function(x,y,\ldots.){panel.xyplot(x,y,\ldots);panel.loess(x,y,\ldots.)})
```

Here's how the plot looks:


If a panel. function doesn't exist for a smoother you'd like to use, you can use the panel.lines function to plot it directly:
> xyplot(circumference~age|Tree, data=Orange,
$+\quad$ panel=function( $x, y, \ldots$ )\{panel.xyplot ( $x, y, \ldots$ );z=supsmu( $x, y$ );panel.lines $(z \$ x, z \$ y$
In this case supersmoother came closer to a straight line than lowess.


## Chapter 14

## Linear Regression

### 14.1 Linear Regression

Linear regression is a very popular procedure for modeling the value of one variable on the value(s) of one or more other variables. The variable that we're trying to model or predict is known as the dependent variable, and the variables that we use to make predictions are known as independent variables, or covariates. Linear regression makes the assumption that the changes in the dependent variable can be modeled as a monotonic linear function of the independent variables; that is, we assume that a change of a certain amount in the independent variables will result in a change in the dependent variable, and the amount of change in the dependent variable is constant across the range of the independent variables. As a simple example, suppose we're interested in the relationship between the horsepower of a car (the independent variable) and the miles per gallon of gas (MPG) of the car. When we fit a linear regression model, we're saying that a change of one horsepower will have the same effect on the MPG regardless of the value of horsepower that we're changing. In other words, a linear regression model would assume that if we had a car with 100 horsepower, and compared it to a car with 101 horsepower, we'd see the same difference in MPG as if we had a car with 300 horsepower and compared it to a car with 301 horsepower. Relationships like this often hold for a limited range of independent variable values, but the linear regression model assumes that it applies for the entire range of the independent variables.

Even with these limitations, linear regression has proven itself to be a very valuable tool for modeling, and it's widely used in many branches of research. There are also a variety of diagnostic measures, both numerical and graphical, that can help us to determine whether the regression is doing a good job, so it's not unreasonable that many people use linear regression as their first tool when trying to model a variable of interest.

### 14.2 The lm command

The lm command uses the model-based formula interface that we've already seen in the context of lattice graphics. The dependent variable is placed on the left-hand side of the tilde ( $\sim$ ), and the independent variables are placed on the right-hand side, joined together with plus signs $(+)$. When you want to use all the variables in a data frame (except for the dependent variable) as independent variables, you can use a period (.) for the right-hand side of the equation.

These models correspond to a mathematical model that looks like this:

$$
\begin{equation*}
y_{i}=\beta_{0}+\beta_{1} x_{1}+\beta_{2} x_{2}+\cdots+\beta_{p} x_{p}+e_{i} \quad \text { for } i=1, \ldots, n \tag{14.1}
\end{equation*}
$$

The $\beta \mathrm{s}$ represent coefficients that measure how much the dependent variable changes for each unit of change in the independent variable, and are often refered to as the slopes. The term $\beta_{0}$ is often known as the intercept. (To omit the intercept in a formula in R , insert the term -1.) The e's represent the part of the observed dependent variable that can't be explained by the regression model, and in order to do hypothesis testing, we assume that these errors follow a normal distribution. For each term in the model, we test the hypothesis
that the $\beta$ corresponding to that term is equal to 0 , against the alternative that the $\beta$ is different from 0 .

To illustrate the use of the $\operatorname{lm}$ command, we'll construct a regression model to predict the level of Alcohol in the wine data set, using several of the other variables as independent variables. First, we'll run lm to create an lm object containing all the information about the regression:

To see a very brief overview of the results, we can simply view the lm object:
> wine.lm

Call:
lm(formula $=$ Alcohol ~ Malic.acid + Alkalinity.ash + Proanthocyanins + Color.intensi
Coefficients:
(Intercept) Malic.acid Alkalinity.ash Proanthocyanins
$11.333283 \quad 0.114313 \quad-0.032440 \quad-0.129636$
Color.intensity OD.Ratio Proline
$0.158520 \quad 0.225453 \quad 0.001136$
To get more information about the model, the summary function can be called:
> summary(wine.lm)
Call:
lm(formula = Alcohol ~ Malic.acid + Alkalinity.ash + Proanthocyanins + Color.intensity + OD.Ratio + Proline, data = wine[-1])

## Residuals:

| Min | 1Q | Median | 3Q | Max |
| ---: | ---: | ---: | ---: | ---: |
| -1.502326 | -0.342254 | 0.001165 | 0.330049 | 1.693639 |

Coefficients:

| Estimate Std. Error t value $\operatorname{Pr}(>\|t\|)$ |  |  |  |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| (Intercept) | 11.3332831 | 0.3943623 | 28.738 | < 2e-16 | *** |
| Malic.acid | 0.1143127 | 0.0397878 | 2.873 | 0.00458 | ** |
| Alkalinity.ash | -0.0324405 | 0.0137533 | -2.359 | 0.01947 | * |
| Proanthocyanins | -0.1296362 | 0.0846088 | -1.532 | 0.12732 |  |
| Color.intensity | 0.1585201 | 0.0231627 | 6.844 | 1.32e-10 | * |
| OD.Ratio | 0.2254528 | 0.0834109 | 2.703 | 0.00757 | ** |
| Proline | 0.0011358 | 0.0001708 | 6.651 | $3.76 \mathrm{e}-10$ | *** |
|  |  |  |  |  |  |
| Signif. codes: | $0^{\prime * * * '} 0.001{ }^{\prime * *} 0.01{ }^{\prime}{ }^{\prime} 0.05{ }^{\prime} .{ }^{\prime} 0.1$ ' |  |  |  |  |

```
Residual standard error: 0.5295 on 171 degrees of freedom
```

Multiple R-Squared: 0.5889, Adjusted R-squared: 0.5745
F-statistic: 40.83 on 6 and 171 DF, p-value: < $2.2 \mathrm{e}-16$

The probability levels in the last column of the bottom table are for testing the null hypotheses that the slopes for those variables are equal to 0 ; that is, we're testing the null hypothesis that changes in the independent variable will not result in a linear change in the dependent variable. We can see that most of the variables in the model do seem to have an effect on the dependent variable.

One useful measure of the efficacy of a regression model is the multiple R-Squared statistic. This essentially measures the squared correlation of the dependent variable values with the values that the model would predict. The usual interpretation of this statistic is that it measures the fraction of variability in the data that is explained by the model, so values approaching 1 mean that the model is very effective. Since adding more variables to a model will always inflate the R-Squared value, many people prefer using the adjusted R-Squared value, which has been adjusted to account for the number of variables included in the model.

When you pass a model object to the plot function, it will display one or more plots that the author of the model fitting function felt were appropriate for studying the effectiveness of the model. For the lm object, four plots are created by default:

1. A plot of residuals versus fitted (predicted) values - The residuals are the part of the dependent variable that the model couldn't explain, and they are our best available estimate of the error term from the regression model. They're calculated by subtracting the predicted value from the actual value of the dependent variable. Under the usual assumptions for the linear regression model, we don't expect the variability of the residuals to change over the range of the dependent variable, so there shouldn't be any discernable pattern to this plot. Note that outliers in the plot will be labeled by their observation number making it easy to track them down.
2. A normal quantile-quantile plot of the standardized residuals - For the probabilities we saw in the summary table to be accurate, we have assumed that the errors of the model follow a normal distribution. Thus, we'd expect a normal quantile-quantile plot of the residuals to follow a straight line. Deviations from a straight line could mean that the errors don't follow a normal distribution.
3. A scale-location plot - This plot is similar to the residuals versus fitted values plot, but it uses the square root of the standardized residuals. Like the first plot, there should be no discernable pattern to the plot.
4. A Cook's distance plot - Cook's distance is a statistic that tries to identify points which have more influence than other points. Generally these are points that are distant from other points in the data, either for the dependent variable or one or more independent variables. Each observation is represented as a line whose height is
indicative of the value of Cook's distance for that observation. There are no hard and fast rules for interpreting Cook's distance, but large values (which will be labeled with their observation numbers) represent points which might require further investigation.

Here are the four plots for the wine.lm object:


### 14.3 Using the model object

The design of the R modeling functions makes it very easy to do common tasks, regardless of the method that was used to model the data. We'll use lm as an example, but most of these techniques will work for other modeling functions in R. We've already seen that the plot function will produce useful plots after a model is fit. Here are some of the other functions that are available to work with modeling objects. In each case, the modeling object is passed to the function as its first argument.

1. Coefficients - The coef function will return a vector containing the coefficients that the model estimated, in this case, the intercept and the slopes for each of the variables:
```
> coef(wine.lm)
    (Intercept) Malic.acid Alkalinity.ash Proanthocyanins Color.intensity
    11.333283116
            OD.Ratio
    0.225452840
        0.114312670 -0.032440473 -0.129636226 0.158520051
        Proline
        0.001135776
```

2. Predicted Values - The predict function, called with no additional arguments, will return a vector of predicted values for the observations that were used in the modeling process. To get predicted values for observations not used in building the model, a data frame containing the values of the observations can be passed to predict through the
newdata $=$ argument. The variables in the data frame passed to predict must have the same names as the variables used to build the model. For example, to get a predicted value of Alcohol for a mythical wine, we could use a statement like this:
```
> predict(wine.lm,newdata=data.frame(Malic.acid=2.3,Alkalinity.ash=19,
+ Proanthocyanins=1.6,Color.intensity=5.1,0D.Ratio=2,6,Proline=746.9))
[1] 12.88008
```

3. Residuals - The residuals function will return a vector of the residuals from a model.

In addition, the summary function, which is usually used to display a printed summary of a model, often contains useful information. We can see what it contains by using the names function:

```
> names(summary(wine.lm))
\begin{tabular}{llll} 
[1] "call" & "terms" & "residuals" & "coefficients" \\
[5] "aliased" & "sigma" & "df" & "r.squared" \\
[9] "adj.r.squared" "fstatistic" & "cov.unscaled" &
\end{tabular}
```


### 14.4 Regression Diagnostics

The four plots produced by the plot command are a good start towards examining the quality of a regression, but it is still possible that there may be problems that those plots don't point out. One of the biggest problems with linear regression is that points that are distant from the bulk of the observations (sometimes refered to as outliers), may have undue influence on the results of the regression. Such points are said to have high influence, or high leverage. To illustrate the problem consider this trivial data set, which exhibits a high leverage point in the extreme:

```
> baddata = data.frame(x=c(.1,.2,.3,.5,.7,5),y=c(.9,.7,.5,.3,.1,2.5))
> plot(baddata$x, baddata$y)
> abline(lm(y~x,data=baddata)
```

Here's the plot:


Notice how the single distant point completely outweighs all the other points and drives the regression line in a direction opposite to the bulk of the data. The extreme point in the data set was unusual in both the $x$ - and $y$-values What about the case where the data is extreme in only the $x$-values? We can see what happens by replacing the $y$-value for the outlier with a more reasonable one.
$>$ baddata1 = data.frame $(\mathrm{x}=\mathrm{c}(.1, .2, .3, .5, .7,5), \mathrm{y}=\mathrm{c}(.9, .7, .5, .3, .1, .5))$
> plot(baddata1\$x, baddata1\$y)
> abline(lm(y~x,data=baddata1))
Here's the plot:


In this case, it appears that there's no relationship between the x - and y - values, when there's a strong relationship except for the single outlier. Naturally, problems like this are obvious in a small data set with just two variables, but they will be more difficult to discover in larger data sets with many variables.

Before going further, it should be mentioned that the discovery of an influential observation in a regression provides no justification for removing that point from the model; it simply helps to identify observations which may deserve further study; in fact, the influential points are often perfectly valid observations that simply do a good job of representing the relationships that occur in the data. So when an influential point is identified, it simply means
that it should be examined more closely to see whether or not it is a potential problem.

Two statistics which have proven to be useful in identifying influential observations are Cook's distance and a statistic known as the hat statistic. Cook's distance is calculated for each observation by comparing the results of the regression with that observation included to the results when that particular observation is removed. Thus, it can find observations which are outliers with regard to both the dependent variables and the independent variables. In $R$, the cooks.distance function calculates the statistics given an lm model object. The hat statistic is based entirely on the independent variables of the model, so it focuses on observations which are distant from the others with regard to the independent variables in the model. In R, the lm.influence function will return a list, including a component named hat, which contains the hat statistic. For simple regressions, with just one independent variable, influential observations are usually at the far reaches of the range of either the dependent or independent variables. For example, for the wine.lm model, Proline was one of the independent variables which seemed effective in predicting alcohol. Let's perform a simple regression using this variable, and then plot the results, highlighting those points that had unusually high Cook's distances or hat statistic values:

```
> simple.lm = lm(Alcohol~Proline,data=wine)
> cooks = cooks.distance(simple.lm)
> hat = lm.influence(simple.lm)$hat
> par(mfrow=c(2,1))
> plot(wine$Proline,wine$Alcohol,col=ifelse(cooks > quantile(cooks,.90),'red','black'))
> plot(wine$Proline,wine$Alcohol,col=ifelse(hat > quantile(hat,.90),'blue','black'))
```

The plots are displayed below:


In the top graph, the points displayed in red represent the observations with large Cook's distances; in the bottom graph, the blue points are those with high hat statistic values. Of course, with more variables in the model, things are not so simple. Let's look at a plot of predicted values versus actual values for the full regression model for this data, using the same coloring conventions:

```
> cooks = cooks.distance(wine.lm)
> hat = lm.influence(wine.lm)$hat
> par(mfrow=c(2,1))
> plot(wine$Alcohol,predict(wine.lm),col=ifelse(cooks > quantile(cooks,.9),'red','black'
```

```
> plot(wine$Alcohol,predict(wine.lm),col=ifelse(hat > quantile(hat,.9),'blue','black'))
```

Here are the plots:



The extreme Cook's distance points seem to congregate at the outer edges of the predicted values, but the extreme hat statistics points don't follow a simple pattern. In practice, many statisticians use the rule of thumb that Cook's distances bigger than the 10th percentile of an F distribution with p and n -p degrees of freedom represent potential problems, where n is the number of observations, and $p$ is the number of parameters estimated. For the wine data, that cutoff point can be calculated as follows:

```
> qf(.1,7,178-7)
[1] 0.4022056
```

In fact, for this data set none of the Cook's distances are greater than this value.
For the hat statistic, a cutoff of $2 * p / n$ has been proposed; for the wine data this corresponds to a value of 0.079 . With the wine example, there are ten such points. Plotting each independent variable against the dependent variable, and highlighting the extreme points in orange helps to show where these points are:

```
> par(mfrow=c (3,2))
> sapply(names(coef(wine.lm)[-1]),
+ function(x)plot(wine[[x]],wine$Alcohol,
+ col=ifelse(hat >.0786 ,'orange','black'),xlab=x))
```

Here are the plots:


### 14.5 Collinearity

Another problem which might occur when using linear regression is known as collinearity. This problem occurs when the independent variables are so highly correlated that they contain redundant information, which confuses the regression process. When data is collinear, the standard errors of the parameter estimates get very large, and removing one or two variables may make the coefficients change dramatically. In addition, collinearity can mask important relationships in the data. The classic data set to illustrate collinearity is known as the Longley data set, available in $R$ under the name longley. This data set contains a variety of measurements about the population of the US in an attempt to predict employment. Let's take a look at the result of regressing Employed against the other variables in the Longley data set:

```
> lreg = lm(Employed ~ .,data=longley)
> summary(lreg)
Call:
lm(formula = Employed ~ ., data = longley)
Residuals:
    Min 1Q Median 3Q Max
-0.41011-0.15767-0.02816 0.10155 0.45539
```

Coefficients:

|  | Estimate |  |  |  | Std. Error |
| :--- | ---: | :--- | ---: | :--- | :--- |
|  | t value $\operatorname{Pr}(>\|t\|)$ |  |  |  |  |
| (Intercept) | $-3.482 \mathrm{e}+03$ | $8.904 \mathrm{e}+02$ | -3.911 | 0.003560 |  |$* *$

Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.11

Residual standard error: 0.3049 on 9 degrees of freedom Multiple R-squared: 0.9955,Adjusted R-squared: 0.9925
F-statistic: 330.3 on 6 and 9 DF, p-value: $4.984 \mathrm{e}-10$

On the surface, nothing seems wrong - in fact, with an adjusted R-squared of .9925 , it seems great. We can see the problem with the data by looking at the pairwise scatterplots, using the pairs function:

```
> pairs(longley)
```

Here's the plot:


Many of the variables seem to be correlated with each other, so it's difficult to see which is causing the problem. A statistic known as VIF (Variance Inflation Factor) can be very useful in situations like this. In R, the vif function in the car package will provide this statistic. Before using vif on the Longley data, let's look at the wine data we used previously:

```
> wine.lm = lm(Alcohol~.,data=subset(wine,select=-Cultivar))
> library(car)
> vif(wine.lm)
    Malic.acid
\begin{tabular}{rrrr} 
Ash & Alkalinity.ash & Magnesium & Phenols \\
2.180108 & 2.179282 & 1.417855 & 4.330552
\end{tabular}
    Flavanoids
        NF.phenols Proanthocyanins Color.intensity
    2.493007
                                    Hue
            7.029040
            1.793883
                        Proline
            OD.Ratio
            3.736818
                        2.441810
```

None of the inflation factors is bigger than 10, which indicates collinearity is not a problem



There does seem to be a linear relationship between Flavanoids and Phenols - not surprisingly those two variables have the highest VIFs.

Now let's return to the Longley data.

```
> vif(lreg)
```

| GNP.deflator | GNP | Unemployed | Armed.Forces | Population | Year |
| ---: | ---: | ---: | ---: | ---: | ---: |
| 135.53244 | 1788.51348 | 33.61889 | 3.58893 | 399.15102 | 758.98060 |

The two largest VIFs are for GNP and Year. Let's eliminate them from the model, and see how the VIFs change:

```
> lreg1 = lm(Employed ~ .,data=subset(longley,select=-c(GNP,Year)))
> summary(lreg1)
Call:
lm(formula = Employed ~ ., data = subset(longley, select = -c(GNP,
    Year)))
Residuals:
\begin{tabular}{rrrrr} 
Min & 1Q & Median & 3Q & Max \\
-0.6561730 & -0.2576601 & -0.0008123 & 0.1213544 & 1.2225443
\end{tabular}
```

Coefficients:

|  | Estimate | Std. Error | t value $\operatorname{Pr}(>\|\mathrm{t}\|)$ |  |  |
| :--- | ---: | ---: | ---: | ---: | :--- | :--- |
| (Intercept) | 13.781314 | 6.886470 | 2.001 | 0.070657 | . |
| GNP.deflator | 0.207046 | 0.081376 | 2.544 | 0.027270 | $*$ |
| Unemployed | -0.012412 | 0.002780 | -4.465 | $0.000955^{* *}$ |  |
| Armed.Forces | -0.005968 | 0.003325 | -1.795 | 0.100170 |  |
| Population | 0.306601 | 0.123795 | 2.477 | 0.030755 * |  |

Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.11
Residual standard error: 0.5671 on 11 degrees of freedom
Multiple R-squared: 0.9809,Adjusted R-squared: 0.9739
F-statistic: 141.1 on 4 and 11 DF, p-value: 2.26e-09

```
> vif(lreg1)
GNP.deflator Unemployed Armed.Forces Population
    35.970754 3.147600 2.497795 34.588299
```

The reduced model is probably more realistic than the full model, but GNP.deflator and Population are still highly correlated

```
> with(longley,cor(GNP.deflator,Population))
```

[1] 0.9791634

Removing GNP.deflator results in a model that seems to make sense:

```
> lreg2 = lm(Employed ~ .,data=subset(longley,select=-c(GNP,Year,GNP.deflator)))
> summary(lreg2)
Call:
lm(formula = Employed ~ ., data = subset(longley, select = -c(GNP,
    Year, GNP.deflator)))
Residuals:
    Min 1Q Median 3Q Max
-1.3835-0.2868-0.1353 0.3596 1.3382
Coefficients:
\begin{tabular}{|c|c|c|c|c|}
\hline & Estimate & Std. Error & t value & \(\operatorname{Pr}(>|t|)\) \\
\hline (Intercept) & -1.323091 & 4.211566 & -0.314 & 0.75880 \\
\hline Unemployed & -0.012292 & 0.003354 & -3.665 & 0.00324 \\
\hline Armed.Forces & -0.001893 & 0.003516 & -0.538 & 0.60019 \\
\hline Population & 0.605146 & 0.047617 & 12.7 & \(2.55 \mathrm{e}-0\) \\
\hline
\end{tabular}
---
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
Residual standard error: 0.6843 on 12 degrees of freedom
Multiple R-squared: 0.9696,Adjusted R-squared: 0.962
F-statistic: 127.7 on 3 and 12 DF, p-value: 2.272e-09
> vif(lreg2)
    Unemployed Armed.Forces Population
        3.146686 1.918225 3.514335
```

Now let's look at some alternatives to ordinary linear regression.

### 14.6 Generalized Additive Models (gam)

One of the most useful alternative methods to regression is known as a generalized additive model. Instead of fitting a single linear parameter to try to explain the relationship between independent variables and dependent variables, GAM models perform spline smooths on selected variables, and use these smoothed versions of the independent variables to try to explain the values of the dependent variables. To try to make the information from the analysis similar to the familiar lm output, an estimated number of degrees of freedom is calculated for each variable, based on how different the fitted spline smooth for that variable is from the strictly linear relationship that 1 m uses for prediction, and an F-statistic is produced for each independent variable to test whether the smoothed version of the variable
made a significant contribution to the predicted value of the dependent variable. In R, the gam function is provided by the mgcv library. This library also provides the s function, which is used by gam to identify the variables that should be smoothed before they are used to predict the dependent variable. Without prior knowledge, it's not unreasonable to try smoothing on all the variables. We can fit a gam model by using the same formula as we used with lm, passing each variable in the model to the s function:

```
> library(mgcv)
> wine.gam = gam(Alcohol~s(Malic.acid)+s(Alkalinity.ash)+
+ s(Proanthocyanins)+s(Color.intensity)+
+ s(OD.Ratio)+s(Proline),data=wine[-1])
> wine.gam
```

Family: gaussian
Link function: identity

Formula:

```
Alcohol ~ s(Malic.acid) + s(Alkalinity.ash) + s(Proanthocyanins) +
```

    \(s(\) Color.intensity) \(+s(O D . R a t i o)+s(P r o l i n e)\)
    Estimated degrees of freedom:
17.9207173 .4928264 .02218913 .567478 total $=22.00321$
GCV score: 0.2314599

Like the lm function, gam provides a more familiar table when the summary method is invoked:

```
> summary(wine.gam)
```

Family: gaussian
Link function: identity
Formula:
Alcohol ~ s(Malic.acid) + s(Alkalinity.ash) + s(Proanthocyanins) +
$s($ Color.intensity) $+s(O D . R a t i o)+s(P r o l i n e)$
Parametric coefficients:
Estimate Std. Error $t$ value $\operatorname{Pr}(>|t|)$
(Intercept) $13.00062 \quad 0.03376385 .1<2 e-16 * * *$
---
Signif. codes: $0{ }^{\prime} * * * ' 0.001^{\prime} * * ' 0.01^{\prime} * ' 0.05$ ', 0.1 , 1
Approximate significance of smooth terms:


The relative importance of the variables has changed somewhat from the linear regression results. Notice that the adjusted R-squared value is 0.692 , as compared to 0.575 for linear regression, showing an improvement in prediction by using the smoothed versions of the independent variable.

Applying the plot function to a gam model is often the most useful part of the analysis. The plots produced show how the independent variable was smoothed before fitting, so a straight (or nearly straight) line for a particular variable means a truly linear relationship was found, while deviations from linearity describe the nature of non-linear relationships that exist. Here's the results of using plot on our gam model. For convenience, I've put all the plots in a single graphic; in practice, you might want to examine each plot separately. I've used the par function to adjust the margins so that the individual plots will be a little larger:

```
> par(mfrow=c(3,2),mar=c}(2,4,1,2)+.1,oma=c(0,0,4,0),xpd=FALSE
> plot(wine.gam)
```

Here's the plot:


For the variables Malic.acid and OD.ratio, the relationships do seem to be linear; this is supported by the fact that gam only used a single degree of freedom to fit these terms. For some of the other variables, it's clear that linear relationships hold only over a limited range of the data. The Alkalinity. ash plot is particularly interesting, but it may indicate oversmoothing.

### 14.7 Recursive Partitioning

We've already seen how recursive partitioning can be used for classification, but it can also be used for regression if the dependent variable passed to rpart is not a factor. When used for regression, rpart follows a similar strategy as for classification; each variable is tested for all possible splits, looking for large separation between the dependent variable values for one side of the split as opposed to the other. As is the case for classification, rpart presents its results as a tree, with terminal nodes representing the best prediction the model can provide. Here are the results of using recursive partitioning on the wine data frame to predict Alcohol. I'm using a period on the right hand side of the model to indicate that rpart should consider all of the variables in the data frame (except Cultivar):

```
> library(rpart)
> wine.rpart = rpart(Alcohol ~ . ,data=wine[-1])
> wine.rpart
n= 178
node), split, n, deviance, yval
    * denotes terminal node
```

1) root 178116.65400013 .00062
2) Color.intensity< $3.32550 \quad 9.16149812 .13980$
4) $\mathrm{Ash}>=2.41131 .26936911 .86846$ *
5) Ash< 2.41376 .59872412 .23514 *
3) Color.intensity>=3.325 $128 \quad 55.969350 \quad 13.33687$
6) Proline< 9007928.97490013 .05013
12) Color.intensity< $8.31561 \quad 21.58676012 .93197$
24) Proline< 722.54314 .29171012 .80209
48) Malic.acid< $3.127 \quad 8.14206712 .62889$
96) NF.phenols>=0.33 142.38849312 .30929 *
97) NF.phenols< 0.33132 .78347712 .97308 *
49) Malic.acid>=3.1 163.97279413 .09437 *
25) Proline $>=722.5184 .83711113 .24222$ *
13) Color.intensity $>=8.315183 .65029413 .45056$ *
7) Proline>=900 $49 \quad 10.025970 \quad 13.79918$
14) Color.intensity< $4.4410 \quad 0.78741013 .27700$ *
15) Color.intensity>=4.44 395.812631 13.93308 *

Since rpart doesn't actually estimate any coefficients, we can't produce a table of hypothesis tests as we did for lm or gam, but we can get a sort of multiple R -squared value by squaring the correlation between the true value of the dependent variable and the value that rpart predicts:

```
> cor(wine$Alcohol,predict(wine.rpart))^2
```

This unadjusted R -squared value is a little higher than the adjusted R -squared value from the gam model.

### 14.8 Comparison of the 3 Methods

A very simple way to get an idea of how the three methods compare with each other is to make a plot of predicted versus actual values for the three methods, using a different color for each:

```
> plot(predict(wine.lm),wine$Alcohol,col='red',xlab='Predicted',ylab='Actual')
> points(predict(wine.gam),wine$Alcohol,col='blue')
> points(predict(wine.rpart),wine$Alcohol,col='green')
> legend('topleft',legend=c('lm','gam','rpart'),col=c('red','blue','green'),pch=1,cex=.8
```

Here's the plot:


## Chapter 15

Analysis of Variance

### 15.1 Analysis of Variance

In its simplest form, analysis of variance (often abbreviated as ANOVA), can be thought of as a generalization of the t-test, because it allows us to test the hypothesis that the means of a dependent variable are the same for several groups, not just two as would be the case when using a t-test. This type of ANOVA is known as a one-way ANOVA.

In cases where there are multiple classification variables, more complex ANOVAs are possible. For example, suppose we have data on test scores for students from four schools, where three different teaching methods were used. This would describe a two-way ANOVA. In addition to asking whether the means for the different schools were different from each other, and whether the means for the different teaching methods were different from each other, we could also investigate whether the differences in teaching methods were different depending on which school we looked at. This last comparison is known as an interaction, and testing for interactions is one of the most important uses of analysis of variance.

Before getting to the specifics of ANOVA, it may be useful to ask why we perform an analysis of variance if our interest lies in the differences between means. If we were to concentrate on the differences between the means, we would have many different comparisons to make, and the number of comparisons would increase as we increased the number of groups we considered. Thus, we'd need different tests depending on how many groups we were looking at. The reasoning behind using variance to test for differences in means is based on the following idea: Suppose we have several groups of data, and we calculate their variance in two different ways. First, we put together all the data, and simply calculate its variance disregarding the groups from which the data arose. In other words, we evaluate the deviations of the data relative to overall mean of the entire data set. Next, we calculate the variance by adding up the deviations around the mean of each of the groups. The idea of analysis of variance is that if the two variance calculations give us very similar results, then each of the group means must have been about the same, because using the group means to measure variation didn't result in a big change than from using the overall mean. But if the overall variance is bigger than the variance calculated using the group means, then at least one of the group means must have been different from the overall mean, so it's unlikely that the means of all the groups were the same. Using this approach, we only need to compare two values (the overall variance, and the variance calculated using each of the group means) to test if any of the means are different, regardless of how many groups we have.

To illustrate how looking at variances can tell us about differences in means, consider a data set with three groups, where the mean of the first group is 3 , and the mean for the other groups is 1 . We can generate a sample as follows:
$>\operatorname{mydf}=$ data.frame (group=rep $(1: 3, r e p(10,3)), x=\operatorname{rnorm}(30, \operatorname{mean}=c(r e p(3,10), r e p(1,20))))$
Under the null hypothesis of no differences among the means, we can center each set of data by the appropriate group mean, and then compare the data to the same data centered by the overall mean. In R, the ave function will return a vector the same length as its' input, containing summary statistics calculated by grouping variables. Since ave accepts an unlimited number of grouping variables, we must identify the function that calculates the
statistic as the FUN= argument. Let's look at two histograms of the data, first centered by the overall mean, and then by the group means. Recall that under the null hypothesis, there should be no difference.

```
> ovall = mydf$x - mean(mydf$x)
> group = mydf$x - ave(mydf$x,mydf$group,FUN=mean)
> par(mfrow=c(2,1))
> hist(ovall,xlim=c(-2,2.5))
> hist(group,xlim=c(-2,2.5))
```




Notice how much more spread out the data is when we centered by the overall mean. To show that this isn't a trick, let's generate some data for which the means are all equal:

```
> mydf1 = data.frame(group=rep(1:3,rep (10,3)),x=rnorm(30))
> ovall = mydf1$x - mean(mydf1$x)
> group = mydf1$x - ave(mydf1$x,mydf1$group,FUN=mean)
> par(mfrow=c(2,1))
> hist(ovall,xlim=c(-2.5,3.2))
> hist(group,xlim=c(-2.5,3.2))
```



Notice how the two histograms are very similar.

To formalize the idea of a one-way ANOVA, we have a data set with a dependent variable and a grouping variable. We assume that the observations are independent of each other, and the errors (that part of the data not explained by an observation's group mean) follow a normal distribution with the same variance for all the observations. The null hypothesis states that the means of all the groups are equal, against an alternative that at least one of the means differs from the others. We can test the null hypothesis by taking the ratio of the variance calculated in the two ways described above, and comparing it to an F distribution with appropriate degrees of freedom (more on that later).

In R , ANOVAs can be performed with the aov command. When you are performing an ANOVA in R, it's very important that all of the grouping variables involved in the ANOVA are converted to factors, or R will treat them as if they were just independent variables in a linear regression.

As a first example, consider once again the wine data frame. The Cultivar variable represents one of three different varieties of wine that have been studied. As a quick preliminary test, we can examine a dotplot of Alcohol versus Cultivar:


It does appear that there are some differences, even though there is overlap. We can test for these differences with an ANOVA:
> wine.aov = aov(Alcohol~Cultivar,data=wine)
> wine.aov
Call:
aov(formula = Alcohol ~ Cultivar, data = wine)

Terms:
Cultivar Residuals

```
Sum of Squares 70.79485 45.85918
Deg. of Freedom 2 175
Residual standard error: 0.5119106
Estimated effects may be unbalanced
> summary(wine.aov)
    Df Sum Sq Mean Sq F value Pr(>F)
Cultivar 2 70.795 35.397 135.08< 2.2e-16 ***
Residuals 175 45.859 0.262
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

The summary function displays the ANOVA table, which is similar to that produced by most statistical software. It indicates that the differences among the means are statistically significant. To see the values for the means, we can use the aggregate function:

```
> aggregate(wine$Alcohol,wine['Cultivar'],mean)
    Cultivar x
1 1 13.74475
2 2 12.27873
3 3 13.15375
```

The default plots from an aov object are the same as those for an lm object. They're displayed below for the Alcohol/Cultivar ANOVA we just calculated:


### 15.2 Multiple Comparisons

In the previous example, notice that the test for Cultivar is simply answering the question "Are there any significant differences among the cultivars?". This is because the F-test which is used to determine significant is based on the two different ways of calculating the variance, not on any particular differences among the means. Having seen that there is a significant effect for Cultivar in the previous example, a natural questions is "Which cultivars are different from each other". One possibility would be to look at all possible t-tests between the levels of the cultivar, i.e. do t-tests for 1 vs. 2,1 vs. 3 , and 2 vs. 3 . This is a very bad idea for at least two reasons:

1. One of the main goals of ANOVA is to combine together all our data, so that we can more accurately estimate the residual variance of our model. In the previous example, notice that there were 175 degrees of freedom used to estimate the residual variance. Under the assumptions of ANOVA, the variance of the dependent variable doesn't change across the different levels of the independent variables, so we can (and should) use the estimate from the ANOVA for all our tests. When we use a t-test, we'll be estimating the residual variance only using the observations for the two groups we're comparing, so we'll have fewer degrees of freedom, and less power in determining differences.
2. When we're comparing several groups using t-tests, we have to look at all possible combinations among the groups. This will sometimes result in many tests, and we can no longer be confident that the probability level we use for the individual tests will hold up across all of those comparisons we're making. This is a well-known problem in statistics, and many techniques have been developed to adjust probability values to handle this case. However, these techniques tend to be quite conservative, and they may prevent us from seeing differences that really exist.

To see how probabilities get adjusted when many comparisons are made, consider a data set on the nitrogen levels in 5 varieties of clover. We wish to test the hypothesis that the nitrogen level of the different varieties of clover is the same.

```
> clover = read.table('http://www.stat.berkeley.edu/classes/s133/data/clover.txt',header
> clover.aov = aov(Nitrogen~Strain,data=clover)
> summary(clover.aov)
\begin{tabular}{lrrrrr} 
& Df & Sum Sq & Mean Sq F value & Pr \((>F)\) \\
Strain & 5 & 847.05 & 169.41 & 14.370 & \(1.485 e^{-06}\)
\end{tabular}\(\quad * * *\)
---
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
```

Let's say that we want to look at all the possible t-tests among pairs of the 6 strains. First, we can use the combn function to show us all the possible 2-way combinations of the strains:

```
> combs = combn(as.character(unique(clover$Strain)),2)
> combs
\(\left.\begin{array}{lllllll}{[, 1]} & {[, 2]} & {[, 3]} & {[, 4]} & {[, 5]} & {[, 6]} & {[, 7]}\end{array}\right][, 8] ~ 子\)
    [,9] [,10] [,11] [,12] [,13] [,14] [,15]
[1,] "3DOK5" "3DOK4" "3DOK4" "3DOK4" "3DOK7" "3DOK7" "3DOK13"
[2,] "COMPOS" "3DOK7" "3DOK13" "COMPOS" "3DOK13" "COMPOS" "COMPOS"
```

Let's focus on the first column:

```
> x = combs[,1]
> tt = t.test(Nitrogen~Strain,data=clover)
> names(tt)
[1] "statistic" "parameter" "p.value" "conf.int" "estimate"
[6] "null.value" "alternative" "method" "data.name"
```

This suggests a function which would return the probability for each combination of cars:

```
> gettprob = function(x)t.test(Nitrogen~Strain,data=clover[clover$Strain %in% x,])$p.val
```

We can get the probabilities for all the tests, and combine them with the country names for display:

```
> probs = data.frame(t(combs),probs=apply(combs,2,gettprob))
> probs
    X1 X2 probs
1 3DOK1 3DOK5 1.626608e-01
2 3DOK1 3DOK4 2.732478e-03
3 3DOK1 3DOK7 2.511696e-02
4 3DOK1 3DOK13 3.016445e-03
5 3DOK1 COMPOS 1.528480e-02
6 3DOK5 3DOK4 5.794178e-03
7 3DOK5 3DOK7 7.276336e-02
8 3DOK5 3DOK13 1.785048e-03
9 3DOK5 COMPOS 3.177169e-02
10 3DOK4 3DOK7 4.331464e-02
11 3DOK4 3DOK13 5.107291e-01
12 3DOK4 COMPOS 9.298460e-02
13 3DOK7 3DOK13 4.996374e-05
14 3DOK7 COMPOS 2.055216e-01
15 3DOK13 COMPOS 4.932466e-04
```

These probabilities are for the individual t-tests, each with an alpha level of 0.05 , but that doesn't guarantee that the experiment-wise alpha will be .05 . We can use the p.adjust function to adjust these probabilities:

```
> probs = data.frame(probs,adj.prob=p.adjust(probs$probs,method='bonferroni'))
> probs
            X1 X2 probs adj.prob
1 3DOK1 3DOK5 1.626608e-01 1.000000000
2 3DOK1 3DOK4 2.732478e-03 0.040987172
3 3DOK1 3DOK7 2.511696e-02 0.376754330
4 3DOK1 3DOK13 3.016445e-03 0.045246679
5 3DOK1 COMPOS 1.528480e-02 0.229272031
6 3DOK5 3DOK4 5.794178e-03 0.086912663
7 3DOK5 3DOK7 7.276336e-02 1.000000000
8 3DOK5 3DOK13 1.785048e-03 0.026775721
9 3DOK5 COMPOS 3.177169e-02 0.476575396
10 3DOK4 3DOK7 4.331464e-02 0.649719553
11 3DOK4 3DOK13 5.107291e-01 1.000000000
12 3DOK4 COMPOS 9.298460e-02 1.000000000
13 3DOK7 3DOK13 4.996374e-05 0.000749456
14 3DOK7 COMPOS 2.055216e-01 1.000000000
1 5 ~ 3 D O K 1 3 ~ C O M P O S ~ 4 . 9 3 2 4 6 6 e - 0 4 ~ 0 . 0 0 7 3 9 8 6 9 9 ~
```

Notice that many of the comparisons that seemed significant when using the t-test are no longer significant. Plus, we didn't take advantage of the increased degrees of freedom. One technique that uses all the degrees of freedom of the combined test, while still correcting for the problem of multiple comparisons is known as Tukey's Honestly Significant Difference (HSD) test. The TukeyHSD function takes a model object and the name of a factor, and provides protected probability values for all the two-way comparisons of factor levels. Here's the output of TukeyHSD for the clover data:

```
> tclover = TukeyHSD(clover.aov,'Strain')
> tclover
    Tukey multiple comparisons of means
        95% family-wise confidence level
Fit: aov(formula = Nitrogen ~ Strain, data = clover)
$Strain
\begin{tabular}{lrrrr} 
& diff & lwr & upr & p adj \\
3DOK13-3DOK1 & -15.56 & -22.27416704 & -8.845833 & 0.0000029 \\
3DOK4-3DOK1 & -14.18 & -20.89416704 & -7.465833 & 0.0000128 \\
3DOK5-3DOK1 & -4.84 & -11.55416704 & 1.874167 & 0.2617111 \\
3DOK7-3DOK1 & -8.90 & -15.61416704 & -2.185833 & 0.0048849 \\
COMPOS-3DOK1 & -10.12 & -16.83416704 & -3.405833 & 0.0012341 \\
3DOK4-3DOK13 & 1.38 & -5.33416704 & 8.094167 & 0.9870716 \\
3DOK5-3DOK13 & 10.72 & 4.00583296 & 17.434167 & 0.0006233 \\
3DOK7-3DOK13 & 6.66 & -0.05416704 & 13.374167 & 0.0527514
\end{tabular}
```

```
COMPOS-3DOK13 5.44 -1.27416704 12.154167 0.1621550
3DOK5-3DOK4 9.34 2.62583296 16.054167 0.0029837
3DOK7-3DOK4 5.28 -1.43416704 11.994167 0.1852490
COMPOS-3DOK4 4.06 -2.65416704 10.774167 0.4434643
3DOK7-3DOK5 -4.06 -10.77416704 2.654167 0.4434643
COMPOS-3DOK5 -5.28 -11.99416704 1.434167 0.1852490
COMPOS-3DOK7 -1.22 -7.93416704 5.494167 0.9926132
> class(tclover)
[1] "multicomp" "TukeyHSD"
> names(tclover)
[1] "Strain"
> class(tclover$Strain)
[1] "matrix"
```

These probabilities seem more reasonable. To combine these results with the previous ones, notice that tclover\$Strain is a matrix, with row names indicating the comparisons being made. We can put similar row names on our earlier results and then merge them:

```
> row.names(probs) = paste(probs$X2,probs$X1,sep='-')
> probs = merge(probs,tclover$Strain[,'p adj',drop=FALSE],by=0)
> probs
```

|  | Row.names | X1 | X2 | probs | adj.prob | p adj |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| 1 | 3DOK13-3DOK1 | 3DOK1 | 3DOK13 | 0.0030164452 | 0.045246679 | $2.888133 \mathrm{e}-06$ |
| 2 | 3DOK4-3DOK1 | 3DOK1 | 3DOK4 | 0.0027324782 | 0.040987172 | $1.278706 \mathrm{e}-05$ |
| 3 | 3DOK5-3DOK1 | 3DOK1 | 3DOK5 | 0.1626608271 | 1.000000000 | $2.617111 \mathrm{e}-01$ |
| 4 | 3DOK7-3DOK1 | 3DOK1 | 3DOK7 | 0.0251169553 | 0.376754330 | $4.884864 \mathrm{e}-03$ |
| 5 | 3DOK7-3DOK4 | 3DOK4 | 3DOK7 | 0.0433146369 | 0.649719553 | $1.852490 \mathrm{e}-01$ |
| 6 | 3DOK7-3DOK5 | 3DOK5 | 3DOK7 | 0.0727633570 | 1.000000000 | $4.434643 \mathrm{e}-01$ |
| 7 | COMPOS-3DOK1 | 3DOK1 | COMPOS | 0.0152848021 | 0.229272031 | $1.234071 \mathrm{e}-03$ |
| 8 | COMPOS-3DDK13 | 3DOK13 | COMPOS | 0.0004932466 | 0.007398699 | $1.621550 \mathrm{e}-01$ |
| 9 | COMPOS-3DOK4 | 3DOK4 COMPOS | 0.0929845957 | 1.000000000 | $4.434643 \mathrm{e}-01$ |  |
| 10 | COMPOS-3DOK5 | 3DOK5 | COMPOS | 0.0317716931 | 0.476575396 | $1.852490 \mathrm{e}-01$ |
| 11 | COMPOS-3DOK7 | 3DOK7 | COMPOS | 0.2055215679 | 1.000000000 | $9.926132 \mathrm{e}-01$ |

Finally, we can display the probabilities without scientific notation as follows:

```
> format(probs,scientific=FALSE)
    Row.names X1 X2 probs adj.prob p adj
1 3DOK13-3DOK1 3DOK1 3DOK13 0.0030164452 0.045246679 0.000002888133
2 3DOK4-3DOK1 3DOK1 3DOK4 0.0027324782 0.040987172 0.000012787061
3 3DOK5-3DOK1 3DOK1 3DOK5 0.1626608271 1.000000000 0.261711120046
4 3DOK7-3DOK1 3DOK1 3DOK7 0.0251169553 0.376754330 0.004884863746
5 3DOK7-3DOK4 3DOK4 3DOK7 0.0433146369 0.649719553 0.185248969392
```

| 6 | 3DOK7-3DOK5 | 3DOK5 | 3DOK7 | 0.0727633570 | 1.000000000 | 0.443464260597 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| 7 | COMPOS-3DOK1 | 3DOK1 | COMPOS | 0.0152848021 | 0.229272031 | 0.001234070633 |
| 8 | COMPOS-3DOK13 | 3DOK13 | COMPOS | 0.0004932466 | 0.007398699 | 0.162154993324 |
| 9 | COMPOS-3DOK4 | 3DOK4 | COMPOS | 0.0929845957 | 1.000000000 | 0.443464260597 |
| 10 | COMPOS-3DOK5 | 3DOK5 | COMPOS | 0.0317716931 | 0.476575396 | 0.185248969392 |
| 11 | COMPOS-3DOK7 | 3DOK7 | COMPOS | 0.2055215679 | 1.000000000 | 0.992613208547 |

By using all of the data to estimate the residual error, Tukey's HSD method actually reports some of the probabilities as even lower than the t-tests.

### 15.3 Two-Way ANOVA

To express the idea of an interaction in the R modeling language, we need to introduce two new operators. The colon (:) is used to indicate an interaction between two or more variables in model formula. The asterisk (*) is use to indicate all main effects and interactions among the variables that it joins. So, for example the term $\mathrm{A} * \mathrm{~B}$ would expand to the three terms A, B, and A:B. As an example of a two-way ANOVA, consider a study to determine the effects of physical activity on obesity. Subjects were rated for their physical activity on a three point scale with $1=$ not very active, $2=$ somewhat active, and $3=$ very active. In addition, the race (either 1 or 2) of the participant was recorded, along with their Body Mass Index (BMI). We want to answer the following three questions:

1. Were the means for BMI the same for the two races?
2. Were the means for BMI the same for the three activity levels?
3. Is the effect of activity level different depending on race?, or equivalently Is the effect of race different depending on activity level?

The first two questions can be answered by looking at the race and activity main effects, while the third question describes the race by activity interaction. The data can be found at http://www.stat.berkeley.edu/classes/s133/data/activity.csv. Here are the R statements to run the ANOVA:

```
> activity = read.csv('activity.csv')
> activity$race = factor(activity$race)
> activity$activity = factor(activity$activity)
> activity.aov = aov(bmi~race*activity,data=activity)
> summary(activity.aov)
                Df Sum Sq Mean Sq F value Pr(>F)
\begin{tabular}{lrrrrll} 
race & 1 & 3552 & 3552 & 102.5894 & \(<2 \mathrm{e}-16\) & \(* * *\) \\
activity & 2 & 2672 & 1336 & 38.5803 & \(<2 \mathrm{e}-16 \quad * * *\) \\
race:activity & 2 & 301 & 151 & 4.3508 & 0.01303 & \(*\) \\
Residuals & 1865 & 64574 & 35 & & &
\end{tabular}
```

```
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

Notice that there are two degrees of freedom for activity - this means two parameters will be estimated in order to explain activity's effect on bmi. Unlike linear regression, where only a single parameter is estimated, and the only relationship that can be fit is a linear one, using two parameters (to account for the three levels of activity) provides more flexibility than would be possible with linear regression.

To see if the analysis was reasonable, we can look at the default plots:

```
> plot(activity.aov)
```

The graphs appear below:


There seems to some deviation from normality when looking at the Normal Q-Q plot (recall that, if the residuals did follow a normal distribution, we would see a straight line.) When this situation arises, analyzing the logarithm of the dependent variable often helps. Here are the same results for the analysis of $\log (\mathrm{bmi})$ :

```
> activity1.aov = aov(log(bmi) ~race*activity,data=activity)
> summary(activity1.aov)
    Df Sum Sq Mean Sq F value Pr(>F)
race 1 4.588 4.588 100.3741 < 2.2e-16 ***
activity 2 3.251 1.625 35.5596 6.98e-16 ***
```

```
race:activity 2 0.317 0.158 3.4625 0.03155 *
Residuals 1865 85.240 0.046
---
Signif. codes: 0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
> plot(activity1.aov)
```



The Q-Q plot looks better, so this model is probably more appropriate. We can see both main effects as well as the interaction are significant. To see what's happening with the main effects, we can use aggregate:

```
> aggregate(log(activity$bmi),activity['race'],mean)
    race x
1 3.122940
2 2 3.222024
aggregate(log(activity$bmi),activity['activity'],mean)
    activity x
1 1 3.242682
2 2 3.189810
3 3 3.109518
```

Race 2 has higher values of BMI than race 1, and BMI decreases as the level of activity increases.

To study the interaction, we could use aggregate, passing both race and activity as the second argument:

```
> aggregate(log(activity$bmi),activity[c('race','activity')],mean)
    race activity x
1 1 1 3.161119
2 2 1 3.298576
3 1 2 3.140970
4 2 2 3.230651
5 1 3 3.084426
6 2 3 3.143478
```

The arrangement of the output from tapply may be more helpful:

```
> tapply(log(activity$bmi),activity[c('race','activity')],mean)
    activity
race 1 2 3
    1 3.161119 3.140970 3.084426
    2 3.298576 3.230651 3.143478
```

It's usually difficult to judge relationships like this from a table. One useful tool in this case is an interaction plot. An interaction plot has one point for each combination of the factors defined by an interaction. The $x$-axis represents the levels of one of the factors, and the $y$-axis represents the mean of the dependent variable, and a separate line is drawn for each level of the factor not represented on the x-axis. While it wouldn't be too hard to produce such a plot with basic commands in R, the process is automated by the interaction.plot function. The first argument to this function is the factor to appear on the x-axis; the second is the factor which will define the multiple lines being drawn, and the third argument is the dependent variable. By default, interaction.plot uses the mean for its display, but you can provide a function of your own choosing through the fun= argument. For the activity data, we can produce an interaction plot with the following code:

```
> with(activity,interaction.plot(activity,race,log(bmi)))
```

Here's the plot:


It can be seen that the interaction is due to the fact that the slope of the line for race 2 is steeper than the line for race 1 .

### 15.4 Another Example

This example has to do with iron retention in mice. Two different treatments, each at three different levels, were fed to mice. The treatments were tagged with radioactive iron, so that
the percentage of iron retained could be measured after a fixed period of time. The data is presented in a table as follows:

| Fe2+ |  |  |  | Fe3+ |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| high | medium | low | high | medium | low |
| 0.71 | 2.20 | 2.25 | 2.20 | 4.04 | 2.71 |
| 1.66 | 2.93 | 3.93 | 2.69 | 4.16 | 5.43 |
| 2.01 | 3.08 | 5.08 | 3.54 | 4.42 | 6.38 |
| 2.16 | 3.49 | 5.82 | 3.75 | 4.93 | 6.38 |
| 2.42 | 4.11 | 5.84 | 3.83 | 5.49 | 8.32 |
| 2.42 | 4.95 | 6.89 | 4.08 | 5.77 | 9.04 |
| 2.56 | 5.16 | 8.50 | 4.27 | 5.86 | 9.56 |
| 2.60 | 5.54 | 8.56 | 4.53 | 6.28 | 10.01 |
| 3.31 | 5.68 | 9.44 | 5.32 | 6.97 | 10.08 |
| 3.64 | 6.25 | 10.52 | 6.18 | 7.06 | 10.62 |
| 3.74 | 7.25 | 13.46 | 6.22 | 7.78 | 13.80 |
| 3.74 | 7.90 | 13.57 | 6.33 | 9.23 | 15.99 |
| 4.39 | 8.85 | 14.76 | 6.97 | 9.34 | 17.90 |
| 4.50 | 11.96 | 16.41 | 6.97 | 9.91 | 18.25 |
| 5.07 | 15.54 | 16.96 | 7.52 | 13.46 | 19.32 |
| 5.26 | 15.89 | 17.56 | 8.36 | 18.40 | 19.87 |
| 8.15 | 18.30 | 22.82 | 11.65 | 23.89 | 21.60 |
| 8.24 | 18.59 | 29.13 | 12.45 | 26.39 | 22.25 |

Thus, before we can perform analysis on the data, it needs to be rearranged. To do this, we can use the reshape function. Since there are two different sets of variables that represent the change in the factors of the experiment, we first read in the data (skipping the header), and create two groups of variables in our call to reshape:

```
> iron0 = read.table('iron.txt',skip=5,nrows=18)
> names(iron0) = c('Fe2high','Fe2medium','Fe2low','Fe3high','Fe3medium','Fe3low')
> iron1 = reshape(iron0,varying=list(1:3,4:6),direction='long')
> head(iron1)
    time Fe2high Fe3high id
1.1 1 0.71 2.20 1
2.1 1 1.66 2.69 2
3.1 1 2.01 3.54 3
4.1 1 2.16 3.75 4
5.1 1 2.42 3.83 5
6.1 1 2.42 4.08 6
```

After examining the data, it can be seen that the low, medium, and high values have been translated into values 1,2 , and 3 in the variable time. The id variable is created to help us see which line each observation came from, which is not relevant in this case, since the table was just used to present the data, and the values in the table don't represent repeated measures on the same experimental unit.

Next, we eliminate the id column, rename the column named "time and further reshape the data to represent the two treatments:

```
> iron1$id = NULL
> names(iron1)[1] = 'level'
> iron = reshape(iron1,varying=list(2:3),direction='long')
> head(iron)
\begin{tabular}{lrrrr}
\multicolumn{4}{c}{ level } & time \\
Fe2high & id \\
1.1 & 1 & 1 & 0.71 & 1 \\
2.1 & 1 & 1 & 1.66 & 2 \\
3.1 & 1 & 1 & 2.01 & 3 \\
4.1 & 1 & 1 & 2.16 & 4 \\
5.1 & 1 & 1 & 2.42 & 5 \\
6.1 & 1 & 1 & 2.42 & 6
\end{tabular}
```

All that's left is to remove the id column and to rename time and Fe2high:

```
> iron$id = NULL
> names(iron)[2:3] = c('treatment','retention')
> head(iron)
    level treatment retention
1.1 1 1 0.71
2.1 1 1 1 1.66
3.1 1 1 1 2.01
4.1 1 1 2.16
5.1 1 1 1 2.42
6.1 1 1 2.42
```

Once the data has been reshaped, it's essential to make sure that the independent variables are correctly stored as factors:

```
> sapply(iron,class)
    level treatment retention
"integer" "integer" "numeric"
```

Since treatment and level are not factors, we must convert them:

```
> iron$treatment = factor(iron$treatment,labels=c('Fe2+', 'Fe3+'))
> iron$level = factor(iron$level,labels=c('high','medium','low'))
> head(iron)
```

|  | level | treatment | retention |
| :--- | ---: | ---: | ---: |
| 1.1 | high | Fe2+ | 0.71 |
| 2.1 | high | $\mathrm{Fe} 2+$ | 1.66 |
| 3.1 | high | $\mathrm{Fe} 2+$ | 2.01 |
| 4.1 | high | $\mathrm{Fe} 2+$ | 2.16 |
| 5.1 | high | $\mathrm{Fe} 2+$ | 2.42 |
| 6.1 | high | $\mathrm{Fe} 2+$ | 2.42 |

Now we can perform the ANOVA:

```
> iron.aov = aov(retention ~ level*treatment,data=iron)
> summary(iron.aov)
    Df Sum Sq Mean Sq F value Pr(>F)
level 2 983.62 491.81 17.0732 4.021e-07 ***
treatment }1\begin{array}{llllll}{1}&{62.26}&{62.26}&{2.1613}&{0.1446}
level:treatment }\begin{array}{llrrrr}{2}&{8.29}&{4.15}&{0.1439}&{0.8661}
Residuals 102 2938.20 28.81
```

Before proceeding further, we should examine the ANOVA plots to see if the data meets the assumptions of ANOVA:


Both the normal Q-Q plot and the scale-location plot indicate problems similar to the previous example, and a log transformation is once again suggested. This is not unusual when data is measured as percentages or ratios.

```
> ironl.aov = aov(log(retention) ~ level*treatment,data=iron)
> par(mfrow=c(2,2))
> plot(ironl.aov)
```



The plots look much better, so we'll continue with the analysis of the $\log$ of retention.

|  | Df Sum Sq Mean Sq F value | Pr $(>F)$ |  |  |  |  |
| :--- | ---: | ---: | ---: | ---: | :---: | :---: |
| level | 2 | 15.588 | 7.794 | 22.5241 | $7.91 e-09$ | $* * *$ |
| treatment | 1 | 2.074 | 2.074 | 5.9931 | 0.01607 | $*$ |
| level:treatment | 2 | 0.810 | 0.405 | 1.1708 | 0.31426 |  |
| Residuals | 102 | 35.296 | 0.346 |  |  |  |
| --- |  |  |  |  |  |  |
| Signif. codes: | 0 | $* * *$ | 0.001 | $* * 0.01 * 0.05$ | 0.1 | 1 |

Since there were only two levels of treatment, the significant treatment effect means the two treatments were different. We can use the TukeyHSD function to see if the different levels of the treatment were different:

```
> TukeyHSD(ironl.aov,'level')
    Tukey multiple comparisons of means
        95% family-wise confidence level
Fit: aov(formula = log(retention) ~ level * treatment, data = iron)
$level
            diff lwr upr p adj
medium-high 0.5751084 0.24533774 0.9048791 0.0002042
low-high 0.9211588 0.59138806 1.2509295 0.0000000
low-medium 0.3460503 0.01627962 0.6758210 0.0373939
```

It appears that the high level had much lower retention values than the other two levels:

```
> aggregate(log(iron$retention),iron['level'],mean)
```

```
    level x
1 high 1.420526
2 medium 1.995635
3 low 2.341685
```

Although there was no significant interaction, an interaction plot can still be useful in visualizing what happens in an experiment:

```
> interaction.plot(iron$level,iron$treatment,log(iron$retention))
```



### 15.5 More Complex Models

When working with the wine data frame, we've separated the categorical variable (Cultivar) from the continuous variable for pedagogical reasons, but the aov function can accomodate both in the same model. Let's add the Cultivar variable to the regression model we've previously worked with:

```
> wine.new = lm(Alcohol Cultivar+Malic.acid+Alkalinity.ash+Proanthocyanins+Color.intensi
> summary(wine.new)
```

Call:
lm(formula $=$ Alcohol ~ Cultivar + Malic.acid + Alkalinity.ash +
Proanthocyanins + Color.intensity + OD.Ratio + Proline, data $=$ wine)
Residuals:

| Min | $1 Q$ | Median | 3Q | Max |
| ---: | ---: | ---: | ---: | ---: |
| -1.13591 | -0.31737 | -0.02623 | 0.33229 | 1.65633 |

## Coefficients:

|  | Estimate | Std. Error | t value $\operatorname{Pr}(>\|t\|)$ |  |
| :--- | ---: | ---: | ---: | ---: | ---: |
| (Intercept) | 12.9158487 | 0.4711149 | 27.415 | $<2 \mathrm{e}-16 * * *$ |
| Cultivar2 | -0.9957910 | 0.1776136 | -5.607 | $8.26 \mathrm{e}-08 \quad * * *$ |
| Cultivar3 | -0.6714047 | 0.2396380 | -2.802 | $0.00568 * *$ |
| Malic.acid | 0.0559472 | 0.0410860 | 1.362 | 0.17510 |
| Alkalinity.ash | -0.0133598 | 0.0134499 | -0.993 | 0.32198 |
| Pranthocyanins | -0.0561493 | 0.0817366 | -0.687 | 0.49305 |
| Color.intensity | 0.1135452 | 0.0270097 | 4.204 | $4.24 \mathrm{e}-05 * * *$ |
| OD.Ratio | 0.0494695 | 0.0987946 | 0.501 | 0.61721 |
| Proline | 0.0002391 | 0.0002282 | 1.048 | 0.29629 |

Signif. codes: $0{ }^{\prime * * * '} 0.001^{\prime * * '} 0.01^{\prime *} *^{\prime} 0.05$ '.' $0.1^{\prime}$ ' 1

Residual standard error: 0.4886 on 169 degrees of freedom
Multiple R-Squared: 0.6541, Adjusted R-squared: 0.6377
F-statistic: 39.95 on 8 and $169 \mathrm{DF}, \mathrm{p}$-value: $<2.2 \mathrm{e}-16$
One problem with the summary display for models like this is that it's treating our factor variable (Cultivar) as two separate variables. While that is the way it is fit in the model, it's usually more informative to combine the effects of the two variables as a single effect. The anova command will produce a more traditional ANOVA table:

```
> anova(wine.new)
Analysis of Variance Table
```

Response: Alcohol

|  | Df | Sum Sq Mean Sq | F value | $\operatorname{Pr}(>F)$ |  |  |
| :--- | ---: | ---: | ---: | ---: | :---: | :--- |
|  | 2 | 70.795 | 35.397 | 148.2546 | $<2.2 \mathrm{e}-16$ | $* * *$ |
| Cultivar | 1 | 0.013 | 0.013 | 0.0552 | 0.8146 |  |
| Malic.acid | 1 | 0.229 | 0.229 | 0.9577 | 0.3292 |  |
| Alkalinity.ash |  |  |  |  |  |  |
| Proanthocyanins | 1 | 0.224 | 0.224 | 0.9384 | 0.3341 |  |
| Color.intensity | 1 | 4.750 | 4.750 | 19.8942 | $1.488 \mathrm{e}-05$ | $* * *$ |
| OD.Ratio | 1 | 0.031 | 0.031 | 0.1284 | 0.7206 |  |
| Proline | 1 | 0.262 | 0.262 | 1.0976 | 0.2963 |  |
| Residuals | 169 | 40.351 | 0.239 |  |  |  |

The summary display contained other useful information, so you shouldn't hesitate to look at both.

Comparing these results to our previous regression, we can see that only one variable (Color.intensity) is still significant, and the effect of Cultivar is very significant. For this data set, it means that while we can use the chemical composition to help predict the Alcohol content of the wines, but that knowing the Cultivar will be more effective. Let's look at a reduced model that uses only Cultivar and Color.intensity to see how it compares with the model containing the extra variables:

```
> wine.new1 = lm(Alcohol~Cultivar+Color.intensity,data=wine)
> summary(wine.new1)
```

Call:
lm(formula = Alcohol ~ Cultivar + Color.intensity, data = wine)
Residuals:

| Min | 1Q | Median | 3Q | Max |
| ---: | ---: | ---: | ---: | ---: |
| -1.12074 | -0.32721 | -0.04133 | 0.34799 | 1.54962 |

Coefficients:

|  | Estimate | Error | t value | $\operatorname{Pr}(>\|t\|)$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: |
| (Intercept) | 13.14845 | 0.14871 | 88.417 | < 2e-16 | * |
| Cultivar2 | -1.20265 | 0.10431 | -11.530 | < 2e-16 | * |
| Cultivar3 | -0.79248 | 0.10495 | -7.551 | $2.33 \mathrm{e}-12$ | *** |
| Color.intensity | 0.10786 | 0.02434 | 4.432 | $1.65 \mathrm{e}-05$ | *** |
| Signif. codes: | $0^{\prime} * * * '$ | $1^{\prime} * *$ ' | $01^{\prime} *$ ' | 0.05 |  |

Residual standard error: 0.4866 on 174 degrees of freedom Multiple R-Squared: 0.6468, Adjusted R-squared: 0.6407 F-statistic: 106.2 on 3 and 174 DF, p-value: < 2.2e-16

The adjusted R-squared for this model is better than that of the previous one, indicating that removing those extra variables didn't seem to cause any problems. To formally test to see if there is a difference between the two models, we can use the anova function. When passed a single model object, anova prints an ANOVA table, but when it's passed two model objects, it performs a test to compare the two models:

```
> anova(wine.new,wine.new1)
Analysis of Variance Table
Model 1: Alcohol ~ Cultivar + Malic.acid + Alkalinity.ash + Proanthocyanins +
        Color.intensity + OD.Ratio + Proline
        Model 2: Alcohol ~ Cultivar + Color.intensity
        Res.Df RSS Df Sum of Sq F Pr(>F)
        1 169 40.351
        2 174 41.207 -5 <r-0.856 0.7174 0.6112
```

The test indicates that there's no significant difference between the two models.
When all the independent variables in our model were categorical model (the race/activity example), the interactions between the categorical variables was one of the most interesting parts of the analysis. What does an interaction between a categorical variable and a continuous variable represent? Such an interaction can tell us if the slope of the continuous variable is different for the different levels of the categorical variable. In the current model, we can test to see if the slopes are different by adding the term Cultivar:Color.intensity to the model:

```
> anova(wine.new2)
Analysis of Variance Table
```

Response: Alcohol

|  |  | Sum Sq | Mean Sq | F value |  | $\operatorname{Pr}(>F)$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Cultivar | 2 | 70.795 | 35.397 | 149.6001 |  | $2.2 \mathrm{e}-16$ | *** |
| Color.intensity | 1 | 4.652 | 4.652 | 19.6613 |  | . $644 \mathrm{e}-05$ | *** |
| Cultivar:Color.intensity | 2 | 0.509 | 0.255 | 1.0766 |  | 0.343 |  |
| Residuals | 172 | 40.698 | 0.237 |  |  |  |  |
| Signif. codes: $0^{\prime} * * * '$ | 0.001 | $1^{\prime} * * ' 0$ | $0.01{ }^{\prime} *$ ' | 0.05 '.' |  | . 1 , , 1 |  |

There doesn't seem to be a significant interaction.
As another example, consider a data set with information about experience, gender, and wages. Experience is recorded as number of years on the job, and gender is recorded as 0 or 1. To see if the slope of the line relating experience to wages is different for the two genders, we can proceed as follows:

```
> wages = read.delim('http://www.stat.berkeley.edu/classes/s133/data/wages.tab')
```

```
> wages$gender = factor(wages$gender)
> wages.aov = aov(wage ~ experience*gender,data=wages)
> anova(wages.aov)
Analysis of Variance Table
Response: wage
\begin{tabular}{lrrrrrl} 
& Df & Sum Sq Mean Sq F value & \(\operatorname{Pr}(>F)\) \\
experience & 1 & 106.7 & 106.69 & 4.2821 & 0.03900 & \(*\) \\
gender & 1 & 635.8 & 635.78 & 25.5175 & \(6.042 e^{-07}\) & \(* * *\) \\
experience:gender & 1 & 128.9 & 128.94 & 5.1752 & 0.02331 & \(*\) \\
Residuals & 530 & 13205.3 & 24.92 & & &
\end{tabular}
Signif. codes: 0 *** 0.001 ** 0.01 * 0.05 . 0.1 1
```

The significant probability value for experience:gender indicates that the effect of experience on wages is different depending on the gender of the employee. By performing two separate regressions, we can see the values for the slopes for the different genders: ¿ $\operatorname{coef}(\operatorname{lm}($ wage experience,data $=$ subset $($ wages, gender $==0)))$

```
(Intercept) experience
    8.62215280 0.08091533
```

¿ coef( $\operatorname{lm}($ wage experience,data=subset $($ wages, gender $==1)))$
(Intercept) experience
7.8571973680 .001150118

This indicates that there is a small increase in wages as experience increases for gender $==$ 0 , but virtually no increase for gender $==1$.

### 15.6 Constructing Formulas

For the examples we've looked at, there weren't so many terms in the model that it became tedious entering them by hand, but in models with many interactions it can quickly become a nuisance to have to enter every term into the model. When the terms are all main effects, you can often save typing by using a data= argument specifying a data set with just the variables you are interested in and using the period (.) as the right-hand side of the model, but that will not automatically generate interactions.

The formula function will accept a text string containing a formula, and convert it to a formula that can be passed to any of the modeling functions. While it doesn't really make sense for the wine data, suppose we wanted to add Cultivar and all the interactions between Cultivar and the independent variables to our original regression model. The first step is to create a vector of the variables we want to work with. This can usually be done pretty easily using the names of the data frame we're working with.

```
> vnames = names(wine)[c(3,5,10,11,13,14)]
```

For the main part of the model we need to join together these names with plus signs (+):

```
> main = paste(vnames,collapse=' + ')
```

The interactions can be created by pasting together Cultivar with each of the continuous variables, using a colon (:) as a separator, and then joining them together with plus signs:

```
> ints = paste(paste('Cultivar',vnames,sep=':'),collapse=" + ")
```

Finally, we put the dependent variable and Cultivar into the model, and paste everything together:

```
> mymodel = paste('Alcohol ~ Cultivar',main,ints,sep='+')
> mymodel
[1] "Alcohol ~ Cultivar+Malic.acid + Alkalinity.ash + Proanthocyanins + Color.intensity
```

To run this, we need to pass it to a modeling function through the formula function:

```
> wine.big = aov(formula(mymodel),data=wine)
> anova(wine.big)
Analysis of Variance Table
```

Response: Alcohol

|  |  | Sum Sq | Mean Sq | F value |  | $\operatorname{Pr}(>F)$ |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Cultivar | 2 | 70.795 | 35.397 | 154.1166 | $<$ | $2.2 \mathrm{e}-16$ | *** |
| Malic.acid | 1 | 0.013 | 0.013 | 0.0573 |  | 0.81106 |  |
| Alkalinity.ash | 1 | 0.229 | 0.229 | 0.9955 |  | 0.31993 |  |
| Proanthocyanins | 1 | 0.224 | 0.224 | 0.9755 |  | 0.32483 |  |
| Color.intensity | 1 | 4.750 | 4.750 | 20.6808 | 1. | .079e-05 | *** |
| OD.Ratio | 1 | 0.031 | 0.031 | 0.1335 |  | 0.71536 |  |
| Proline | 1 | 0.262 | 0.262 | 1.1410 |  | 0.28708 |  |
| Cultivar:Malic.acid | 2 | 0.116 | 0.058 | 0.2524 |  | 0.77727 |  |
| Cultivar:Alkalinity.ash | 2 | 0.876 | 0.438 | 1.9071 |  | 0.15194 |  |
| Cultivar: Proanthocyanins | 2 | 1.176 | 0.588 | 2.5610 |  | 0.08045 |  |
| Cultivar:Color.intensity | 2 | 0.548 | 0.274 | 1.1931 |  | 0.30602 |  |
| Cultivar:OD.Ratio | 2 | 0.415 | 0.207 | 0.9024 |  | 0.40769 |  |
| Cultivar: Proline | 2 | 1.160 | 0.580 | 2.5253 |  | 0.08328 |  |
| Residuals | 157 | 36.060 | 0.230 |  |  |  |  |
| Signif. codes: $0{ }^{\prime} * * *$ | . 001 | ${ }^{\prime} * *$ ' 0 | $0.01{ }^{\prime} *$ | 0.05 '.' | 0.1 | . ${ }^{\prime}$, 1 |  |

As expected there isn't anything too startling. If we wanted to investigate, say, the Cultivar: Proanthocyanins interaction, we could look at a scatter plot using separate colors for the points and corresponding best regression lines for each Cultivar:

```
> plot(wine$Proanthocyanins,wine$Alcohol,col=c('red','blue','green')[wine$Cultivar])
> abline(lm(Alcohol~Proanthocyanins,data=wine,subset=Cultivar==1),col='red')
> abline(lm(Alcohol~Proanthocyanins,data=wine,subset=Cultivar==2),col='blue')
> abline(lm(Alcohol~Proanthocyanins,data=wine,subset=Cultivar==3),col='green')
> legend('topleft',legend=levels(wine$Cultivar),pch=1,col=c('red','blue','green'))
```

The plot appears below:


### 15.7 Alternatives for ANOVA

Not all data is suitable for ANOVA - in particular, if the variance varies dramatically between different groups, the assumption of equal variances is violated, and ANOVA results may not be valid. We've seen before that log transformations often help with ratios or percentages, but they may not always be effective.

As an example of a data set not suitable for ANOVA, consider the builtin data set airquality which has daily measurements of ozone and other quantities for a 153 day period. The question to be answered is whether or not the average level of ozone is the same over the five months sampled.

On the surface, this data seems suitable for ANOVA, so let's examine the diagnostic plots that would result from performing the ANOVA:

```
> airquality$Month = factor(airquality$Month)
> ozone.aov = aov(Ozone NMonth,data=airquality)
> plot(ozone.aov)
```



There are deviations at both the low and high ends of the Q-Q plot, and some deviation from a constant in the Scale-Location plot. Will a log transformation help?

```
> ozonel.aov = aov(log(Ozone) ~Month,data=airquality)
> plot(ozonel.aov)
```



In this case, the transformation didn't really help.
It might be possible to find a more suitable transformation, but we can also use a statistical test that makes fewer assumptions about our data. One such test is the Kruskal-Wallis test. Basically, the test replaces the data with the ranks of the data, and performs an ANOVA on those ranks. It assumes that observations are independent from each other, but doesn't demand equality of variance across the groups, or that the observations follow a normal distribution. The kruskal.test function in R performs the test, using the same formula interface as aov.

```
> ozone.kruskal = kruskal.test(Ozone~Month,data=airquality)
> ozone.kruskal
Kruskal-Wallis rank sum test
data: Ozone by Month
Kruskal-Wallis chi-squared = 29.2666, df = 4, p-value = 6.901e-06
```

All that's reported is the significance level for the test, which tells us that the differences between the Ozone levels for different months is very significant. To see where the differences come from, we can use the kruskalmc function in the strangely-named pgirmess package. Unfortunately this function doesn't use the model interface - you simply provide the response variable and the (factor) grouping variable.

```
> library(pgirmess)
> kruskalmc(airquality$Ozone,airquality$Month)
Multiple comparison test after Kruskal-Wallis
p.value: 0.05
Comparisons
```

|  | obs.dif | critical.dif | difference |
| :--- | ---: | ---: | ---: |
| $5-6$ | 57.048925 | 31.85565 | TRUE |
| $5-7$ | 38.758065 | 31.59346 | TRUE |
| $5-8$ | 37.322581 | 31.59346 | TRUE |
| $5-9$ | 2.198925 | 31.85565 | FALSE |
| $6-7$ | 18.290860 | 31.85565 | FALSE |
| $6-8$ | 19.726344 | 31.85565 | FALSE |
| $6-9$ | 54.850000 | 32.11571 | TRUE |
| $7-8$ | 1.435484 | 31.59346 | FALSE |
| $7-9$ | 36.559140 | 31.85565 | TRUE |
| $8-9$ | 35.123656 | 31.85565 | TRUE |

Studying these results shows that months 6,7 , and 8 are very similar, but different from months 5 and 9.

To understand why this data is not suitable for ANOVA, we can look at boxplots of the Ozone levels for each month:

```
> boxplot(with(airquality,split(Ozone,Month)))
```



The variances are clearly not equal across months, and the lack of symmetry for months 5 and 6 brings the normal assumption into doubt.


[^0]:    xyplot(Diabetes~Prim_Care_Phys_Rate|CHSI_State_Name,data=risk,main='Diabetes vs. Physi

