> For the Yakilautti family

[1] (both biological and honorary)

[2] and for the many students

[3] who suffered through earlier drafts of this book

[4] and the many more students

[5] who will suffer later drafts

R Crash Course

for Biologists

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Boring legal stuff ...

R Crash Course for Biologists
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R Crash Course for Biologists

Contents

Preface

Think of a Biologist. Who do you see? Take a minute to write down some characteristics in your mind. Try to be specific: gender, skin, age, height, hair, clothes, personality. Who do you see?

Now think of a *computer programmer* or *data scientist*. Write down their characteristics.

How do these people differ in your mind? Can you imagine them being the same person? Can you picture yourself in both roles?

The goal of this book is to bridge these two worlds. In writing this book, I assume you are a practising biologist or a student of biology, or you are just motivated by biological phenomena. It doesn't matter if you are a recent high school graduate entering into a biology undergraduate program, a graduate student embarking on an independent research dissertation, or a senior scientist with specialized expertise in the science of life. As long as you are interested in learning how to code, this book is written for you.

The goal of this book is to provide a 'how-to' guide to connect you to the world of data science. We focus on the fundamentals of the R programming language and its applications in biology. In writing this book, I assume you do not have much coding experience. Whether you are a new biology student or a seasoned professional, this book was written for you.

There are many great introductions to the R coding language available in print and online. But these tend to be general and abstract, sometimes going on tangents that are not so relevant to what you want to do as a biologist.

What makes this a different, is that it is written with the biologist in mind. Specifically, my goal was to write the book that I wish I had access to as an undergraduate student learning how to collect and analyze data. With the benefit of hindsight, I've tried to cut out all the programming details that haven't been of much use to me as a data scientist, and focus on the most common methods. I've tried to connect to biological questions and examples as much as possible, without getting too sidetracked with biological details.

This decision-making progress is based on my research and teaching experience in a range of topics in Biology and Health Sciences at Queen's University – Environmental Science, Epidemiology, Genomics, Ecology, and Evolution.

A comprehensive coding volume would require thousands of printed pages and take decades to master. In choosing the content for this book, I have focused on everything that I wish I knew when I first started learning to program in R. Many of the functions and packages included here were not available when I started, but have some exceptional functionality. I continue to add new tricks and techniques that I find useful.

0.1 Is this book for you?

Maybe you are curious about coding for data analysis but you aren't sure if you want to invest the time and energy you will need to become competent in these methods. Many students in biology programs do not receive strong quantitative skills training in math, statistics, or computer science. In fact, many of us choose to go into biology programs because we are scared of the quantitative focus of the 'hard' sciences like physics and chemistry. Only much later do we realize how valuable these skills can be for investigating biological phenomena. Modern biology is defined by 'big data' sources including high-throughput sequencing, real-time environmental measurements, satellite imaging, animal tracking, human health monitoring, etc. Along with more traditional types approaches, these data are increasingly made available in online databases that are too big to navigate manually. Coding is not simply helpful to biologists – it's becoming essential.

To help demonstrate the tremendous value of coding, I focus on examples drawn from real biological studies. I try to provide real-world examples of how one can apply programming tools and techniques to curate, analyze, and visualize biological data. These tend to be areas in which I have researched and published papers – opportunities that were presented to me because of my ability to analyze data in a reproducible and open framework. However, a key theme is that these skills are highly transferable, not only across the biological sciences but to other disciplines.

Here are a few examples of the diversity of data, analyses, and visualizations in my own collaborations, which all use similar methods in R:

1. A paper examining rapid evolution of flowering time, published in Science: https://doi.org/10.1126/science.1242121
2. A *de novo* genome assembly: https://doi.org/10.1093/g3journal/jkab339
3. A meta-analysis of evolution of invasive species: https://doi.org/10.1111/mec.13162
4. Tracking COVID-19 outbreaks using whole-genome sequencing: https://doi.org/10.1038/s41598-021-83355-1
5. A study of metabolites in nasal swabs that can differentiate COVID-19 from other viral infections in human patients: https://www.nature.com/articles/s41598-022-14050-y

6. An analysis of 3,429 herbarium images and >1 million weather records to reconstruct evolution of an invasive plant: https://www.pnas.org/doi/full/10.1073/pnas.2107584119
7. A model of species range limits

0.2 Why R?

In Biology, there are two dominant programming languages: **Python** and **R**. Thousands of hours have been wasted arguing the merits of one programming language over another. The truth is that there is a lot of similarity and it's very easy to to move from one to the other.

There are many other programming languages used in Biology. **C/C#/C++** and **Java** are popular in computer science because they provide a high level of control, but this comes at a cost of abstraction and a steeper learning curve. Bash programming in **Unix/Linux/GNU** is all but necessary for high-performance computing on remote servers, but in biology it is most often used to automate file management and to run programs written in other languages. **Julia** is gaining momentum for mathematical modellers, but it is still in its infancy. **PERL** was popular for bioinformatics but is not as common as Python.

We focus on R because it is more commonly used in published statistical analyses in Biology, and it is a bit easier to learn. As you will see, it is very easy to walk through the fundamentals and generate graphs and statistical analyses within just a few hours of tutorial. This comes at a cost of slower run-times and less flexibility than Python, but this is usually not a problem for beginners. In fact, it is possible to use R to run Python code (or C++ or many other languages). More importantly, concepts like data objects, function and packages are conceptually very similar between R and Python, making it easy to move from one language to the other. The truth is that they are both good languages and anyone who tells you that language A is better than B is simply showing their ignorance about language B.

0.3 Advice

If you've completed a few years of any undergraduate program in biology, then you've probably developed a good approach to study various subjects in Biology. Maybe it involves reading the textbook, attending lectures, and making notes that you review before the big test. Coding is different.

If this is your first attempt to learn how to code, then it's important to understand HOW to learn to code. You won't learn by reading this textbook. You need to take **participate** and actively take control of your learning by typing along with the examples in this book.

Consider that R is a programming *language*. When I teach this content at the senior undergraduate and junior graduate level, I often begin with a poll of students to see who has learned to speak more than one language. I then ask:

Question: How did you become fluent in a second language?

Some common themes in the answers tend to be:

- Immerse yourself
- Study, read, listen
- Try something new, fail, correct errors, repeat
- Practice, practice, practice!

How do you become fluent in a programming language? Pretty much the same way:

- Immerse yourself
- Study, read, and **type everything out**!
- Try something new, fail, correct errors, repeat
- Practice, practice, practice!

Learning a new language is not easy. Learning a programming language is not easy either. Here are a few specific tips to become fluent in R:

1. **Get organized and PLAN**. Use a personal calender and schedule sufficient time to deal with error messages. This is important to accept, though it can be difficult: troubleshooting your code often takes more time than planning and writing it!
2. **Apply what you learn**. You will start to develop a toolbox of coding techniques from day one. Look for opportunities to apply them whenever you can. Even if it takes a lot longer to code than to use other methods, the extra time is worth it in the long run. Take time to think about what coding tools you can apply.

3. **Experiment**. Try new things, make mistakes, solve problems.

4. **Devote time**. Set aside large blocks of time (2+ hours), to **immerse yourself** in your coding lessons or project.

5. **Focus**. Turn off your notifications. Eliminate distractions. Put your phone and computer on 'airplane mode'. Do whatever it takes to work without interruption. Get some good headphones with white noise or instrumental sounds (no lyrics) to block out distractions. Here are some things I listen to, depending on mood:
   a. Baroque/Classical
   b. Smooth Jazz
   c. Electronic (ambient, house, lofi)
   d. https://coffitivity.com/

6. **Learn to Troubleshoot**.
   a. If you get stuck, Google: "How do I ______ in R". Look for answers from a website called Stack Overflow
   b. If you can't figure out what an error means, paste it into Google. Again, look for answers from Stack Overflow

7. **Socialize**. Find a coding support group or find a few others to form your own group. Discuss problems and successes. Read other people's code to see how they tackle problems. Rarely is there one single 'right' way to code something.

8. **Git 'er done**. When you are starting out, the 'right' way to code is whatever it takes to get the code to do what you want. Don't let perfection be the enemy of the good: messy code that works is 100% better than efficient code that never runs.

9. **Improve**. As you get more comfortable you can start to think about cleaner, clearer, more efficient ways to code. As you advance, look for ways to do the same thing faster and with fewer lines of code.

10. **Embrace Failure**. I can't stress this enough. Even after 10+ years of programming experience, most of my code does not work on the first try, and most of my time is spent dealing with error messages and unexpected output.

11. **Read** the documentation for the function or package you are using. Don't worry if you don't understand everything. Be sure to take the time to read it slowly and try to understand as much as you can. Try searching online

for terms or phrases that are not familiar to you. You will come across these again in the future, so you are investing time now for future payoff. In addition to the built-in help in R, often the repository on R-CRAN.org or Bioconductor will include 'vignettes' or tutorials with worked examples.

0.4 Learn By Doing!

As you work through these self-tutorials, don't just read them. I can't stress this enough: take the time to type out the commands in your R (Studio) console and make sure you get the same output. The simple act of typing it out will send messages to your brain saying "hey, this is an important thing to remember." If you get an error, even better! Read the error carefully, then compare what you typed to what is in the tutorial. Once you find what is different, you will learn what that error means.

About 70-90% of coding time is dealing with errors, and the same is true for learning to code. This can be difficult for us to accept because our experience in biology programs is quite different.

0.5 What to Expect

Learning to code is a lifelong journey. There is always more to learn and new ways to improve. The beginning of the journal might be broken up into three overlapping stages, depending on the level of training you have already received:

1. **Utter bewilderment** – reading code is like reading a foreign language. All these letters and symbols are meaningless to you.
2. **Understanding** – you can look at a function and have a decent idea of what it does and how to use it, but you don't understand most of the parameters. You usually rely on default parameters.
3. **Competence** – you can write your own code from scratch, without needing to look up examples, and you are able to carefully review and apply parameters. You rarely trust default parameters, especially for more complicated functions.
4. **Expertise** – you write your own functions and help others to troubleshoot code, analysis pipelines, etc. Maybe you even have your own published R package or algorithms.

Don't confuse *understanding* with *competence* – this is a common mistake that students make. It's relatively easy to learn how to understand code that is shown to you, but it's quite another skill to learn the names and parameters of useful functions and apply them to solve problems or answer questions. That doesn't mean you need to memorize every function – though memorization can help. A good strategy to move from understanding to competence is to make the extra time and effort to type out the code that is shown to you, even when you can look at it and understand what it does. As noted above, the act of typing out the code is what will help to solidify it in your brain.

0.6 Translational Coding

There is often a mismatch between the knowledge acquired through a university degree and the skills that employers need in their workforce. That is, newly minted university students have a lot of knowledge and skills for learning, but often struggle with goals laid out by employers or in entrepreneurial endeavours or thesis/dissertation research.

In the computing world, the disconnect between learning and application can happen when students have acquired knowledge of coding algorithms and tools, but learn to apply these tools only when working within a 'sandbox' created for teaching purposes. The sandbox is a clean and well-groomed programming environment with pre-loaded software and examples, curated by the educator. The sandbox lacks the messiness and ambiguity that define real-world applications, and the student never faces these uncomfortable but highly relevant challenges. The sandbox approach is commonly used in both university settings and online courses (e.g. Udemy, Coursera, Datacamp, Skillshare).

A typical teaching sandbox will probably include pre-installed software with 'clean' data defined by a well-defined data structure without errors or missing observations. It will probably have a clear and singular path from problem to solution. This approach has the advantage of efficiency – both for the educator and for the learner. The learner can be guided to move efficiently through key learning objectives while minimizing unexpected bugs or problems that can slow progress and take significant time for educators to deal with. The sandbox creates a more homogeneous experience that is more efficient for tracking progress and assigning grades. The trade-off is that sandbox learning does a poor job preparing you for the messy realities of coding with real data in the real world.

An alternative to the sandbox approach is translational coding, which borrows the term from translational medicine. Translational medicine is a multidisciplinary hybrid between research and application that directly connects medical researchers to the needs of patients. Similarly, translational coding tries to directly connect coding skills and tools to the needs of potential employers.

This will not be pleasant for you, the learner, at first. The sandbox approach is popular with learners because it is relatively quick and painless with minimal time needed for researching, planning, debugging, and other forms of problem solving. There is value to learning to work quickly and efficiently, but there is also value in learning to deal with problems that arise in the real-world. This includes dealing with errors at every stage, from installing software to problems hidden among thousands of lines of data or code. This can be frustrating at first, and it will absolutely slow down your progress. There are three key things to remember when this happens:

1. Every error, problem, or roadblock is a **learning opportunity**. Every problem and assignment will have specific goals and challenges that are explicitly laid out by the tutorial, assignment or practice problem. These are the challenges that every learner must overcome to complete the task. In addition, there are *implicit* challenges that may be unique or shared by only a few learners – a particular typo in the code, an error importing or saving, an unidentified error in your dataset. These implicit problems may feel ‘unfair’ because not every learner has to deal with the same problems at the same time. Over time however, these will tend to average out so that everyone will make similar mistakes just at different times.
2. You can learn to **budget your time** to deal with these implicit, unforeseen errors. And this is an important and highly-transferrable skill! Start a problem or assignment as soon as possible. Give yourself time to take a break and come back to a problem when you get stuck. When you estimate how long an assignment will take, don’t just look at the *explicit* goals. Remember to also add time for the *implicit* challenges, which will take much longer to complete.
3. **Time devoted to a new problem pays off in the future**. Most of your time will be spent the first time you encounter a problem. If you take the time to read the error or warning, think about it, and investigate it, then you will know how to recognize and deal with it in the future. Once you learn to recognize and solve a particular problem, you will know how to recognize and deal with it in the future. In this way, implicit challenges tend to balance out among learners over time. Some learners will encounter a problem early and struggle while others move ahead, until they encounter the same problem, evening the playing field.

The most important thing is to **embrace the challenge**! Don’t let yourself get discouraged.

Now, let’s get coding…

1 Setup

1.1 R

Before you begin these tutorials, you should install the latest version of R: https://cran.r-project.org/

Versions are available for Windows, MacOS and Linux operating systems. Immediately we can see one of the advantages of learning to code in R – we can move code across computing platforms quite easily, as long as R is installed there.

1.2 R Studio

You should also install R Studio: https://rstudio.com/products/rstudio/download/#download

R Studio is an **Integrated Development Environment (IDE)**. Once you install R Studio, go ahead and run the program.

You will see several helpful *tabs*, probably arranged across four windows. Several windows have more than one tab at the top, which you can click to access. Here is a quick overview of the more useful ones (some of this will make more sense after you work through the first few chapters of the tutorial):

- **Environment** keeps track of all of the objects in your programming environment. If this doesn't make sense now, it will later.
- **History** keeps track of the code you have run.
- **Files** similar to the Finder (MacOS) or File Explorer (Windows), starting with the *working directory*.
- **Plots** are where your plots are created
- **Packages** show which packages you have installed, and which have been loaded.
- **Help** provides documentation for R functions
- **Console**…

1.3 Console

One of the most important tabs is the console. It's usually the main tab that opens on the left when you first start R Studio. You'll see a little chevron > with a cursor after it. That's the R Console and it's the part that actually runs the R program.

1.3.1 R Script

To run an R script, you can just type functions into the console. However, it is very hard to keep track of everything you do if you only use the console. In R Studio you can click `File-->New File-->R Script`. This will open a new tab window called **Untitled**. This is called a **script**, but it's really just a text file, with a **.R** suffix, that you can use to keep track of your R program. Try typing something into your R script – don't worry for now if it is just some random text. Note that you can **Save** this file.

Nothing happens (yet). To run the script, you have to send the text from the script tab to the console tab. There are a few ways you could do this:

1. Copy and paste manually. This works fine, but there are more effeicient options
2. Highlight the code you want to run and click the **Run** button on the top-right corner of the script tab. The run button sends the highlighted text from the script to the console.
3. If you click the **Run** button without highlighting text, it will send whatever text is on the same *line* as your cursor
4. If you press **Ctl + Enter** (Windows) or **Cmd + Return** (Mac) it will do the same thing – this is the shortcut for the **Run** button
5. There are other options if you press the tiny triangle next to the **Run** button, including **Run All**. This is the equivalent of running one line at a time.
6. **Ctl/Cmd + Shift + Enter/Return** is a shortcut for **Run All**

1.4 Packages

Packages in R contain functions – small programs that you can run. One really good package is called `tidyverse`. The `tidyverse` package contains a lot of useful functions for working with different types of data, including visualizations. You'll need to make sure you are connected to the internet and that your connection to the internet won't be interrupted during the download.

> WARNING! This may take a long time to run

To install the packages, open R Studio and look for the **Console** tab. Type this into your console:

```
install.packages("tidyverse")
```

Next, install ‘devtools:

```
install.packages("devtools")
```

2 Fundamentals

2.1 Introduction

This chapter provides a rapid breakdown of the core functionality of R. There is a lot to cover in a very short time. You may be tempted to skip over some of these sections, but this chapter forms the foundation of future chapters. If you don't have a solid foundation, you will have trouble building your coding skills. Remember that you can only learn coding through repetition. Take the extra time and make the effort to type out each code and run it in your console.

> **I can't stress this enough: It is important that you physically participate and code along with the examples. Type everything out. The physical act of typing into R and troubleshooting any errors you get is a crucial part of the learning process.**

It's very likely you will sometimes get a different result, such as a warning or error message. Don't get frustrated! Think of it as an opportunity to work on you debugging skills. Check to make sure you don't have any typos, like the letter `l` and the number `1`, or \ vs `/`, or missing spaces or other changes that may be hard to spot visually. If you are getting a warning, read it carefully.

2.2 R Basics

Make comments inside your code with the hash mark `#`. When you type this character, it tells the R program to ignore everything that comes after it.

Documentation is an important part of coding. It takes a bit of extra time to write, but it will save you a lot of time. Careful documentation will be essential when coding collaboratively, even if your collaborator is you when you wrote code six months back.

It's ok to play around with code to get it working, but once you have a piece you are happy with, be sure to go back and add documentation.

Later, we will see how to use R markdown to provide more attractive documents for reproducible analysis. But for dedicated programs, you can get creative with characters to help make long documentation more readable:

```
# Use hastags to make comments - not read by the R console
# Use other characters and blank lines to improve readability:
# -------------------------
# My first R script
# Today's Date
# -------------------------
# Add a summary description of what the script does
# This script will...
# And annotate individual parts of the script
```

> Did you type this out? If not, you missed something important. Go back to the beginning of the book and read more carefully.

2.2.1 Basic Math

You can do basic mathematical equations in R. Many of us choose to become biologists because we aren't comfortable with mathematical equations, only to find out later how important math is for biology! As we'll see later, coding can help to demystify mathematical equations. Let's start with some basics:

> *Yes, type these out!*

```
10+2 # add
```

```
## [1] 12
```

```
10-2 # subtract
```

```
## [1] 8
```

```
10*2 # multiply
```

```
## [1] 20
```

```r
10/2 # divide
```

```
## [1] 5
```

```r
10^2 # exponent
```

```
## [1] 100
```

> **Tip**: To get more practice, use R instead of your calculator app whenever you need to calculate something. It seems silly to go through the trouble to open R Studio to calculate a few numbers, but it will get you comfortable using R and R Studio, which will pay off in the long run..

2.2.2 Objects & Functions

Objects and **functions** are the bread and butter of the R programming language. An object can take many forms, but is generally an input or output. This could include a letter or a number, or a set of letters or numbers, or a set of letters and numbers, or more structured types of objects that link together different kinds of information.

Objects are manipulated with **functions**. Each function has a unique name followed by a set of parentheses, which are used to define input and **parameters** that are used by the function.

In fact, there is a function called `function()`. Yes, there is a function in R called *function*, and you can use it to write your own custom functions, but we'll save that for later.

For now, just remember that functions have brackets. Brackets are used to define input and parameters that the function uses to produce output.

> **Warning**: Do not put a space between the function name and the opening bracket or you will generate an error.

2.2.3 `c()`

The **concatenate** function `c()` is a very simple yet important and common function in R. Use it to group items together.

```
c(1,2,3,5)
```

```
## [1] 1 2 3 5
```

In this function, the numbers 1, 2, 3, and 5 are the input parameters.

The output is an **object** called a **vector** that contains four **elements**. The `c()` function takes four separate objects (elements) and combines them into a new object (vector). If this seems weird, take a few minutes to think it through because this difference will be important later.

Think of a vector as part of a row or column in a spreadsheet, and an element as one of the cells. We can also have more complex obects that are equivalent to entire spreadsheets, or a combination of multiple spreadsheets and other kinds of structured data.

2.2.4 Math Functions

Here are some functions for common mathematical calculations. Type these out and then try channging some of the numbers in brackets to get a feel for them:

```
abs(-10) # absolute value
```

```
## [1] 10
```

```
sqrt(10-1) # square root (with subtraction)
```

```
## [1] 3
```

```
log(10) # natural log
```

```
## [1] 2.302585
```

```
log10(10) # log base 10
```

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

```
exp(1) # power of e
```

```
## [1] 2.718282
```

```
sin(pi/2) # sine function
```

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

```
asin(1) # inverse sine
```

```
## [1] 1.570796
```

```
cos(pi) # cosine
```

```
## [1] -1
```

```
acos(-1) # inverse cosine
```

```
## [1] 3.141593
```

```
tan(0) # tangent
```

```
## [1] 0
```

```
atan(0) # inverse tangent
```

```
## [1] 0
```

> Note that `pi` is a special object containing the digits of pi. Try typing `pi` in the R Studio Console and pressing **`Enter`**.

2.2.5 Round/Truncate

We can use R for rounding and truncating numbers.

```
round(pi, digits=3) # standard rounding to 3 digits
```

```
## [1] 3.142
```

```
floor(pi) # round down to closest whole number
```

```
## [1] 3
```

```
ceiling(pi) # round up to closest whole number
```

```
## [1] 4
```

```
signif(pi, digits=2) # round to keep 2 significant digits
```

```
## [1] 3.1
```

> **Pro-tip**: round() with digits=3 is a great function to use in your reports, manuscripts, theses, etc.

Later, we'll look at how to generate reports that incorporate code (e.g. statistical analyses) that you can quickly update with new data. Rounding the output of your R code with round() makes for much cleaner, and more readable reports.

2.2.6 Logic Operators

An **operator** is used to compare values. We'll use these a lot when we start writing our own custom programs and functions. It also comes in handy for sub-setting your data.

```
1 > 2 # greater than
```

```
## [1] FALSE
```

```r
1 < 2 # less than
```

```
## [1] TRUE
```

```r
1 <= 2 # less than or equal to
```

```
## [1] TRUE
```

```r
1 == 1 # equal to
```

```
## [1] TRUE
```

```r
1 == 2 | 1 == 1 # | means 'OR'
```

```
## [1] TRUE
```

```r
1 == 2 & 1 == 1 # & means 'AND'
```

```
## [1] FALSE
```

```r
1 == 1 & 1 == 1
```

```
## [1] TRUE
```

We can also use `!` as a negation/inverse operator

```r
1 != 1 # not equal to
```

```
## [1] FALSE
```

2.2.7 Group Comparisons

Instead of the vertical bar character `|`, you can use `%in%` with `c()` to check a large number of values.

```
1 %in% c(1,2,3,4,5,6,7,8,9,10)
```

```
## [1] TRUE
```

2.2.8 Congrats!

Before we move on to the next section, take a second to look back at all the coding skills you've already learned: documenting code, basic math, working with objects and functions, combining objects, some advanced math functions, and comparing objects. Well done!

Seriously, you already know enough write your own R program! Try it!

1. Make a new file: `File-->New File-->R Script`
2. Write some code – try to use as many concepts above as you can.
3. Don't forget your documentation!
4. Save the file
5. Run the file and look at the output
6. Debug your error and warning messages.
7. Show off your program to your friends a family

You are a coder now! Let's take your skills to the next level.

2.3 Use ? for HELP

Whenever you are learning a new function, you should use `?` and carefully read about all the parameters and outputs. The explanations can be a bit technical, which is intimidating at first. But after enough practice you will start to understand more and more of the descriptions. Let's break it down:

```
?round
```

> **Note**: In R Studio, the help will open in a separate 'Help' tab (lower, right panel in the default view)

2.3.1 Description

The description gives a general overview of the function. In this case, `round()` is one of a set of related functions, which are all described together in the same help file

2.3.2 Usage

This shows the general form of the function.

2.3.3 Arguments

This explains the ‘arguments’ of the function, which are the input values and parameters. In the case of `round` the arguments include a numeric vector `x` as input and `digits` as a parameter.

2.3.4 Value

This help doesn’t have a **Value** subheading, but more complex functions do. For example, try `?lm` to see the help for linear models. Values are objects created by the function as output. For example, the model `coefficients` and `residuals` are separate objects of a linear model created by the `lm()` function.

2.3.5 Details

This explains the function(s) in greater detail, and is worth reading the first few times you use a function

2.3.6 Examples

This section gives examples as reproducible code, which you can copy-paste right into your terminal to try.

To conclude, always read the help **carefully** when you first use a function. It’s normal to keep referring to the help every time you use a function that you aren’t too familiar with. It’s also normal that you might not understand everything in the help file. Just do your best and be persistent and over time it will start to make more sense to you. You will find these get easier as you read about more functions and try to apply whatever you can understand.

2.4 Random Numbers

The ability to quickly and efficiently generate random numbers has a lot of useful applications for biologists. What are some examples?

1. Generating random numbers for an experimental design
2. Simulating 'noise' or stochastic processes in a population or other biological system
3. Developing a null model for statistical significance testing
4. Exploring 'parameter space' in a Maximum Likelihood model or a Markov Chain Monte Carlo simulation

It is very easy to generate some random numbers in R, from a variety of different sampling distributions.

These are covered in more detail in the Distributions Tutorial, which is part of a different book (R Stats Crash Course for Biologists). For now, we'll just focus on generating random numbers.

2.4.1 Uniform

Perhaps the simplest random number is a whole number (i.e. no decimal) drawn from a **uniform distribution**, meaning that each number has an equal probability of being selected.

```
runif(n=10, min=0, max=1)
```

```
##  [1] 0.16393352 0.66795602 0.38344108 0.44853423 0.48684766 0.98423853
##  [7] 0.10302963 0.06513989 0.57559656 0.17175667
```

> Note that your randomly chosen numbers will be different from the ones randomly chosen here.

The `runif()` function here uses 3 parameters:

1. `n` – the number of random values to generate
2. `min` – the minimum value that can be chosen
3. `max` – the maximum value that can be chosen.

We'll talk more about parameters later.

2.4.2 Gaussian

One of the most common random distributions in biology is the **Gaussian distribution** with a given `mean` and `sd` (standard deviation). Rational numbers (i.e. with decimal) closer to the mean are more likely to be chosen, with sd defining probability of sampling a value far above or below the mean value.

```
rnorm(10, mean=0, sd=1)
```

```
##  [1]  1.67881119 -0.93474079 -0.27787545  1.27962082 -1.90465711 -1.09506584
##  [7] -1.00034249 -0.33707271  1.27437382 -0.02151392
```

> **Side note**: Look what we did here. We wrote `10` instead of `n=10` and the function still works! In fact, we can get away with:

```
rnorm(10,0,1)
```

```
##  [1] -0.5991280  0.6867562 -0.3446526  0.5076155 -1.7059862 -0.2326348
##  [7] -0.9726856  1.4600686  1.3997361 -0.9333766
```

You can figure out the order by reading more detail about the function, but we'll get to that later. When you are starting out, it's a good idea to type the extra characters to specify the parameter names to avoid bugs in your code. It also makes the code more readable to others.

2.4.3 Poisson

A **poisson distribution** includes only whole numbers with a parameter `lambda`, which is analogous to the mean in the normal distribution.

Poisson distributions are common for count data in biology – seed or egg number, for example.

```
rpois(10, lambda=10)
```

```
##  [1] 10  4 12 12  6 12 10  9 12  9
```

2.4.4 Binomial

The **binomial distribution** is useful for binary outcomes – variables with only two possibilities, which can coded as 0 or 1 (or true/false). The `size` parameter is the number of events (e.g. number of coin flips), and the `prob` parameter is the probability of getting a 1.

Binomial distributions are commonly used in population genetics (e.g. sampling alleles with different frequencies).

```
rbinom(10, size=1, prob=0.5)
```

```
##  [1] 0 1 1 1 1 0 1 0 1 0
```

```
rbinom(10, size=10, prob=0.5)
```

```
##  [1] 4 5 4 3 6 8 6 4 7 4
```

2.4.5 Other

Here are a few other random distributions you might be familiar with:

Distribution	R function
Chi-Squared	`chisq()`
t	`t()`
F	`F()`
Exponential	`exp`
Log-Normal	`Lognormal`
Logistic	`Logistic`

2.5 `set.seed()`

Fun fact: random numbers generated by a computer are not truly random. Instead, the numbers involve a calculation from a starting number called a **seed**. The seed might be the current Year/Month/Day/Hour/Minute/Second/Millisecond, which means the 'random' number could be determined by somebody who knows the equation and the time it was executed.

In practice, computer-generated random numbers are much more 'random' than numbers 'randomly' chosen by a human mind.

We can also take advantage of a computer's pseudo-random number generation by setting the **seed** number. This can help with testing and debugging our code, and for writing code for research that is 100% reproducible. With the same seed, anyone can generate the exact same "random" numbers. We do this with the `set.seed()` function.

Compare these outputs:

```r
runif(5)
```

```
## [1] 0.49206068 0.85187873 0.12648966 0.05102828 0.66389254
```

```r
runif(5)
```

```
## [1] 0.8481760 0.1176348 0.5150773 0.8494982 0.9557773
```

```r
set.seed(3)
runif(5)
```

```
## [1] 0.1680415 0.8075164 0.3849424 0.3277343 0.6021007
```

```r
set.seed(3)
runif(5)
```

```
## [1] 0.1680415 0.8075164 0.3849424 0.3277343 0.6021007
```

```r
set.seed(172834782)
runif(5)
```

```
## [1] 0.13729290 0.18587365 0.01860484 0.88440060 0.21414154
```

```r
set.seed(172834782)
runif(5)
```

```
## [1] 0.13729290 0.18587365 0.01860484 0.88440060 0.21414154
```

```r
runif(5)
```

```
## [1] 0.19787402 0.84870074 0.27303904 0.12225215 0.08365613
```

See how the same ‘random’ numbers are generated with the same seed?

3 Combining objects

Returning now to the concatenation function, we saw how to use use `c()` to concatenate single objects.

```r
c(1,2,5)
```

```
## [1] 1 2 5
```

We can also *nest* functions, for example we can use `c()` inside of another concatenate function.

```r
c(c(1,2,5),50)
```

```
## [1]  1  2  5 50
```

If we need to concatenate a range of numbers, we can simplify with the colon `:`

```
c(1:10)
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10
```

```
c(100:90)
```

```
##  [1] 100  99  98  97  96  95  94  93  92  91  90
```

```
c(-1:1)
```

```
## [1] -1  0  1
```

> **Question**: How could you use this to generate a set of numbers from -1.0 to 1.0 in increments of 0.1? You have all the coding knowledge you need to do this. You just have to try combining two of the things you have learned so far.

Hint: Think about how many elements should be in the vector, and what kind of math operation you could use.

3.1 Sequence

Alternatively, you can also use `seq()` to generate more complicated sequences

```
seq(-1, 1, by = 0.1)
```

```
##  [1] -1.0 -0.9 -0.8 -0.7 -0.6 -0.5 -0.4 -0.3 -0.2 -0.1  0.0  0.1  0.2  0.3  0.4
## [16]  0.5  0.6  0.7  0.8  0.9  1.0
```

```
seq(-1, 1, length=7)
```

```
## [1] -1.0000000 -0.6666667 -0.3333333  0.0000000  0.3333333  0.6666667  1.00000
```

3.2 Rows and Columns

As noted above, the output of `c()` with two or more elements is a **vector** object that is conceptually similar to a set of rows or columns in a spreadsheet.

Use `cbind()` to bind columns and `rbind()` to bind rows. The result is a two-dimensional **matrix**, which is conceptually similar to a spreadsheet of `n` rows by `c` columns.

```
cbind(1:10,10:1)
```

```
##       [,1] [,2]
##  [1,]    1   10
##  [2,]    2    9
##  [3,]    3    8
##  [4,]    4    7
##  [5,]    5    6
##  [6,]    6    5
##  [7,]    7    4
##  [8,]    8    3
##  [9,]    9    2
## [10,]   10    1
```

```
rbind(1:10,10:1)
```

```
##      [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
## [1,]    1    2    3    4    5    6    7    8    9    10
## [2,]   10    9    8    7    6    5    4    3    2     1
```

> What are `n` (number of rows) and `c` (number of columns) for each of the above examples?

3.2.1 Congrats, again!

Okay, let's take a quick breather from writing code. You have been typing along, right? If not, go back and type out the code. It really is so important if you want to learn this!

We are about to enter into the realm of **object-oriented programming**, but first we need to cover a few basic concepts.

3.3 Data Types

Programming languages like R use different data types.

It's very important to understand data types in order to properly encode and analyze data in R. Here is an overview of the main data types:

Type	Example	Description
`string`	`"String"`	Strings are the most common and versatile data type. They can be defined with single `''` or double `""` quotation marks. The downside of strings is that you typically can't do mathematical functions with them.
`numeric` (**float**)	`12.421`	Numeric variables are numbers and come in a few flavours. Floats are rational numbers.
`numeric` (**integer**)	`12`	Integers are numeric objects that store whole numbers, and may be positive or negative (no decimal).
`complex`	`0+12.43i`	Complex numbers include real and imaginary numbers.
`logical`	`T` or `TRUE`	Logical (aka **Boolean**) variables are either `TRUE` or `FALSE`, which can be shortened to `T` and `F` (**Note** the use of capital letters only). NOTE: `TRUE` is a *logical* data type but `"TRUE"` and `'TRUE'` are *strings*.
`factors`	any	Factors are a special type of data that may include strings and/or numbers but have a limited number of classes. Factors are often used to code groups in statistical models.

Note that computers cannot store irrational (i.e. infinite, non-repeating) numbers, instead they have encoded as fractions or equations and rounded to some (tiny) decimal place.

Why does it matter? It's very common to have errors in statistical analyses caused by the wrong kind of data. Here is a very common example of a big coding error in Biology:

Imagine you have an experiment set up with three experimental groups coded as `1`, `2` and `3`.

Question: What data type should these be?

Answer: These should be coded and analyzed as **factors** NOT **numeric** variables. Running statistical anlayses in R on numeric objects that should be factors will give completely different (and wrong!) statistical results.

More generally, you should keep these data types in mind. Consider memorizing them, or even just printing or writing them out and pasting them on your wall. When you get to a point where you are collecting your own data or working with other data sources, you will need to think carefully about what data type each observation should be coded as. This is called **data coding** and it is one of the most important steps in any data analysis pipeline.

3.4 Objects & Variables

R supports **Object-Oriented Programming (OOP)**, which is a programming style that defines and manipulates **objects**

An **object** in R can be a lot of things, but to understand some of the key objects, let's start by thinking about a spreadsheet (example Microsoft Excel).

A spreadsheet has individual cells or elements (boxes) organized into rows (e.g., numbers) and columns (e.g., letters), and may have multiple sheets (tabs). Any of these can be coded objects in R. Objects can also be more complicated types of text files. In biology, we might have DNA (or RNA or protein) sequence data, or matrices of species community data, or time series, or the output of a statistical test. All of these can be coded as objects in R.

Variables are objects that can change value. In R, we use can assign variables using <- or =. Almost everything you need to know about R to be a prolific data scientist in biology involves manipulating object variables with functions!

3.4.1 Cells (elements)

The most basic object is a single value. For example, a string:

```
X<-"string"
```

> **Question**: Why no output?

Answer: When we wrote: `X<-"string"` R created the object called **X**, so no output is produced.

There are a few options To see the contents of `X`:

```
print(X)
```

```
## [1] "string"
```

```
paste(X)
```

```
## [1] "string"
```

```
X
```

```
## [1] "string"
```

`print()` Is most generic and versatile for providing feedback while running complex scripts (e.g. during loops, Bash scripts, etc)

`paste()` Converts objects to a string, we'll come back to this.

Generally `print()` or `paste()` are preferred over calling the object directly.

OR, we can put the whole thing in brackets, which saves a line of code:

```
(X<-"string")
```

```
## [1] "string"
```

Which one should you use? It's ok to use the bracket methods for simple scripts and reports, but use `print()` for more complicated analysis pipelines, especially those that run through a scheduler on remote computers.

3.4.2 Vector

A vector is a one-dimensional array of cells. This could be part of a row or column in our spreadsheet example.

Each cell within the vector has an ‘address’ – a number corresponding to the cell ranging from 1 to N, where N is the number of cells.

The number of cells in a vector is called the **length** of the vector.

All items in a vector must be of the same data type. If you mix data types, then the whole vector will be formatted to the most inclusive type. For example, if you include a string with any other format, then the whole vector will be treated as a string:

```
Xvec<-c(1.1829378, X, 1:10, "E", "Computational Biology", 100:90)
Xvec
```

```
##  [1] "1.1829378"             "string"                "1"
##  [4] "2"                     "3"                     "4"
##  [7] "5"                     "6"                     "7"
## [10] "8"                     "9"                     "10"
## [13] "E"                     "Computational Biology" "100"
## [16] "99"                    "98"                    "97"
## [19] "96"                    "95"                    "94"
## [22] "93"                    "92"                    "91"
## [25] "90"
```

Similarly, a vector containing integer and rational numbers is a vector of all rational numbers:

```
c(1,2,3,1.23)
```

```
## [1] 1.00 2.00 3.00 1.23
```

> **Protip**: A common problem when importing data to R occurs when a column of numeric data includes at least one text value (e.g. “missing” or “< 1”). R will treat the entire column as text rather than numeric values. Watch for this when working with real data!

If you want to mix data types without converting them, you can use a **list** object, which is described later. But first we will need to get comfortable working with the more basic data types.

3.4.2.1 Subset a Vector Each cell within a vector has a specific address. Just as text message with the correct email address can find its way to your computer, you can find an element in a vector using its address. Remember that in R, addresses start with the number 1 and increase up to the total number of elements.

R uses square brackets `[]` to subset a vector based on the element addresses.

```
Xvec[1]
```

```
## [1] "1.1829378"
```

```
Xvec[13]
```

```
## [1] "E"
```

```
Xvec[1:3]
```

```
## [1] "1.1829378" "string"    "1"
```

3.4.3 Matrices

A matrix is a 2-D array of cells, equivalent to one sheet in a spreadsheet program. The `matrix()` function can convert a vector to a matrix.

```
Xmat<-matrix(Xvec,nrow=5)
Xmat
```

```
##      [,1]        [,2] [,3]                    [,4] [,5]
## [1,] "1.1829378" "4"  "9"                     "99" "94"
## [2,] "string"    "5"  "10"                    "98" "93"
## [3,] "1"         "6"  "E"                     "97" "92"
## [4,] "2"         "7"  "Computational Biology" "96" "91"
## [5,] "3"         "8"  "100"                   "95" "90"
```

Be sure to understand what happened here. Compare this `Xmat` object to the `Xvec` object, above. See how we have re-arranged the elements of a one-dimensional vector into a two-dimensional matrix? **Note**: these two objects need the same number of elements – 1×25 for `Xvec` and 5×5 for `Xmat`.

3.4.3.1 Subset a Matrix Did you notice the **square brackets** along the top and left side? Do you see how the **rows** have numbers *before* the comma and **columns** have numbers *after* the comma?

These show the address of each element in the matrix. We can subset with square brackets, just like we did with vectors. Since there are two dimensions, we need to specify two numbers using the syntax `[row,column]`.

For example, if we want to select the element from the 3rd column of the 1st row:

```
Xmat[1,3]
```

```
## [1] "9"
```

Or leave it blank if you want the whole row or column:

```
Xmat[1,]
```

```
## [1] "1.1829378" "4"         "9"         "99"        "94"
```

```
Xmat[,3]
```

```
## [1] "9"                       "10"                      "E"
## [4] "Computational Biology" "100"
```

> **Protip**: Always remember "**rows** *before* and **columns** *after* the column: `[row,col]`

3.4.4 Arrays

Array is a general term to describe any object with N dimensions. We've already seen a few different examples:

Dimension	Object Name
0	Cell
1	Vector
2	Matrix

Dimension	Object Name
3+	Array

In R you can build arrays by adding as many dimensions as you need using the `array()` function.

```
Xarray<-array(0, dim=c(3,3,2)) # 3 dimensions
Xarray
```

```
## , , 1
##
##      [,1] [,2] [,3]
## [1,]    0    0    0
## [2,]    0    0    0
## [3,]    0    0    0
##
## , , 2
##
##      [,1] [,2] [,3]
## [1,]    0    0    0
## [2,]    0    0    0
## [3,]    0    0    0
```

Notice how 3rd dimension is sliced to print out in 2D. Another way to conceptualize this array is to think of two matrices with the same dimension (rows-by-columns). The element of each matrix can be addressed by its `[row,col]` but we need a third dimension do distinguish between the two matrices. You can see this in the output above each matrix: `,,,1` vs `,,,2`. Together, this array has three dimensions: `[row,col,matrix]`.

> **Question**: If we add a third matrix with the same number of rows and columns, how many dimensions would you need to pull out a specific cell element in R? What if there were 10 or 100 instead of three?

Answer: Three! In all cases, this is still a 3-dimensional array, and we can access any element as above: `[row,col,matrix]`. All we are changing is the matrix number from 2 to 3 to 10 to 100!

Higher-order arrays are possible, but a bit tricky to read on a 2-dimensional screen, and very hard to conceptualize.

Here's an example of a six-dimensional array.

```
Xarray<-array(rnorm(64), dim=c(2,2,2,2,2,2))
```

Once you get the hang of it, it's easy to subset. Just think of each dimension, separated by commas.

```
Xarray[1:2,1:2,1,1,1,1]
```

```
##           [,1]       [,2]
## [1,] -1.718987  0.3487603
## [2,]  1.779268 -0.3523615
```

```
Xarray[1:2,1,1,1:2,1,1]
```

```
##           [,1]      [,2]
## [1,] -1.718987 0.8664164
## [2,]  1.779268 1.2394975
```

> **Question**: Why are these numbers not the same?

Answer: Look at the `array[]` function and compare to the 6-D array to understand how this works. Each function captures a different 2-dimensional subspace of the 6-dimensional array

If these higher-dimension arrays are too abstract, don't worry. They are important for neural networks, machine learning, and multivariate data (e.g. quantitative genetics, community ecology). Luckily, most of what you need to know you can extrapolate from your intuition about 2-dimensional and 3-dimensional space. Just make sure you understand the similarities and differences among cells/elements, vectors and matrices before you moe on.

3.5 Matrix Algebra

R is pretty handy for matrix calculations that would be very time-consuming to do by hand or even in a spreadsheet program.

As an example, let's create some numeric vectors that we can play with. First, a simple vector object called X containing the numbers 1 through 10.

```
X<-c(1:10)
X
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10
```

Second, a vector called Y containing the numbers 0.5 to 5 in 0.5 increments. Note how we can do this using some simple math:

```
Y<-c(1:10*0.5)
Y
```

```
##  [1] 0.5 1.0 1.5 2.0 2.5 3.0 3.5 4.0 4.5 5.0
```

3.5.1 Basic Operations

Probably the most common calculation for these X and Y objects is just to cycle through each element of each vector and multiply them together. For example, if X is a vector of leaf length measurements and Y is a vector of leaf width measurements, then we might want to calculate leaf area by multiplying each length by its corresponding width.

In R we just use the standard multiplication operator * on a vector, just like we would do for two individual numbers.

```
X * Y
```

```
##  [1]  0.5  2.0  4.5  8.0 12.5 18.0 24.5 32.0 40.5 50.0
```

Addition, subtraction, division, and exponents are similar.

```
X + Y
```

```
##  [1]  1.5  3.0  4.5  6.0  7.5  9.0 10.5 12.0 13.5 15.0
```

```
X / Y
```

```
##  [1] 2 2 2 2 2 2 2 2 2 2
```

```
X ^ Y
```

```
##  [1] 1.000000e+00 2.000000e+00 5.196152e+00 1.600000e+01 5.590170e+01
##  [6] 2.160000e+02 9.074927e+02 4.096000e+03 1.968300e+04 1.000000e+05
```

Just as we apply operators to vectors, we can also apply functions to vectors. When we do this, the same function is applied to each individual cell of the vector.

```
log(X)
```

```
##  [1] 0.0000000 0.6931472 1.0986123 1.3862944 1.6094379 1.7917595 1.9459101
##  [8] 2.0794415 2.1972246 2.3025851
```

```
exp(Y)
```

```
##  [1]   1.648721   2.718282   4.481689   7.389056  12.182494  20.085537
##  [7]  33.115452  54.598150  90.017131 148.413159
```

3.5.2 Matrix Multiplication

Vectors, matrices, and higher-order arrays have multiple elements. Because of this, there are more than one ways to multiply the elements in one object with the elements in the other. This is going to get a bit abstract but matrix multiplication has broad applications in biology, from gene expression and molecular biology to community ecology and image analysis.

There are more options than simply multiplying each corresponding element. For example, we can multiply each element in the vector `X` by each element in the vector `Y`. This will create a matrix. Let's make an example with the first 4 elements of `X` and the first 3 elements of `Y`.

3.5.2.1 Outer product.

Another way to multiply together two vectors or matrices is to multiply individual elements in different combinations. In the outer product we work across columns of the first object, multiplying by rows of the second object. It's easier to understand by example:

```
Z<-X[1:4] %o% Y[1:3]
Z
```

```
##      [,1] [,2] [,3]
## [1,]  0.5    1  1.5
## [2,]  1.0    2  3.0
## [3,]  1.5    3  4.5
## [4,]  2.0    4  6.0
```

Note how the first column is each value of `X` (1-4) multiplied by the first value of `Y` (0.5), and the second column is multiplied by the second value of `Y` (1). Similarly, the first row is each value of `Y` multiplied by the first value of `X` (1), etc. What happens if we reverse the order?

```
YoX<-Y[1:3] %o% X[1:4]
YoX
```

```
##      [,1] [,2] [,3] [,4]
## [1,]  0.5    1  1.5    2
## [2,]  1.0    2  3.0    4
## [3,]  1.5    3  4.5    6
```

> **Question**: How does the `Z` matrix object differ from `YoX`?

Answer: We have switched the rows and columns, which is called a **transpose**

3.5.2.2 Transpose

In R, we can transpose matrices with the `t()` function

```
t(YoX)
```

```
##      [,1] [,2] [,3]
## [1,]  0.5    1  1.5
## [2,]  1.0    2  3.0
## [3,]  1.5    3  4.5
## [4,]  2.0    4  6.0
```

3.5.2.3 By convention

To multiply two vectors together with the outer product, we arrange the first vector as rows, and the second vector as columns, and then multiply each pair of values together to fill in the matrix.

We can extend this to multiply two objects that are 2-dimensional matrices instead of 1-dimensional vectors. However, this gets tricky for the outer product because instead of generating a 2-D matrix from two 1-D vectors, we will generate a 4-D array from the outer product of two 2-D matrices.

3.5.2.4 Dot Product

Another way to multiply two arrays is with the dot product. To do this, we multiply matrices we match the element of each **row** in the **first** object with each **column** in the *second* object, and sum them together: (e.g. `X[1]*Y[1]+X[2]*Y[2]...`).

It's easy to extend from two vectors to two matrices, just by multiplying out elements in each row of the first object by elements in the second object.

```
X %*% Y
```

```
##       [,1]
## [1,] 192.5
```

```
sum(X*Y) == X %*% Y
```

```
##      [,1]
## [1,] TRUE
```

3.5.2.5 Other Operations

There are a few other important matrix operations that are useful for biological data and modelling/simulations. The **cross-product** is a complicated formula that is easy to calculate in R

```
crossprod(X[1:4],Z) # Cross product
```

```
##      [,1] [,2] [,3]
## [1,]   15   30   45
```

```r
crossprod(Z) # Cross product of Z and t(Z)
```

```
##      [,1] [,2] [,3]
## [1,]  7.5   15 22.5
## [2,] 15.0   30 45.0
## [3,] 22.5   45 67.5
```

The **Identity Matrix** is a special matrix with 1 on the diagonal and 0 on the off-diagonal. We can create it with the `diag()` function

```r
diag(4) # Identity matrix, 4x4 in this case
```

```
##      [,1] [,2] [,3] [,4]
## [1,]    1    0    0    0
## [2,]    0    1    0    0
## [3,]    0    0    1    0
## [4,]    0    0    0    1
```

We can also use the `diag()` function on an existing matrix, to pull out all of the values on the diagonal, resulting in a vector

```r
diag(Z) # Diagonal elements of Z
```

```
## [1] 0.5 2.0 4.5
```

Some of these calculations can get a bit tricky – especially when we move to 2D matrices instead of vectors. You'll want to consult or review a matrix algebra textbook if you are going to apply these, but that's getting too advanced for this book. For now, the important thing is just to know that these options are available if you need them in the future.

3.5.2.6 Matrix Math Summary

Operator	Name
`*`	Multiply elements

Operator	Name
`%*%`	Dot Product
`%o%`	Outer product
`t()`	Transpose
`crossprod()`	Cross-product
`diag(4)`	Identity of 4x4 matrix
`diag(M)`	Diagonal elements of matrix M

3.6 PCA

One popular use-case for matrix calculation is the principal components analysis (PCA). The PCA is covered in much more detail in the PCA Tutorial in the R Intro Stats for Biologists textbook.

Briefly, PCA is a form of **supervised machine learning**. It uses matrix math to re-scale a bunch of **correlated** vectors (e.g. measurements) so that they can be mapped to an equal number of **independent** PC axes. For example, if you measure tail fin lengths and body lengths of 100 fish, then you can code the data as two vectors. These values will probably be correlated since bigger fish have bigger tails. We can re-scale these two *dependent* (i.e. correlated) vectors as two *independent* (i.e. uncorrelated) principal components.

In the above example, PC1 is a measure of larger fish, whereas PC2 is a measure of tail fin size relative to body size.

PCA and other ordination methods are widely used in biology, from community ecology and microbiome studies to morphometrics, population genetics, metagenomics and gene expression. Of course there are many applications outside of biology too! For now, just know that it is easy to run a PCA using the `princomp()` function. In most cases, we would want to scale the vectors to have a mean of 0 and standard deviation of 1. Equivalently, we can use the `cor=T` parameter to use the correlation matrix in the calculations.

```
princomp(Z, cor=T)
```

```
## Call:
## princomp(x = Z, cor = T)
##
## Standard deviations:
```

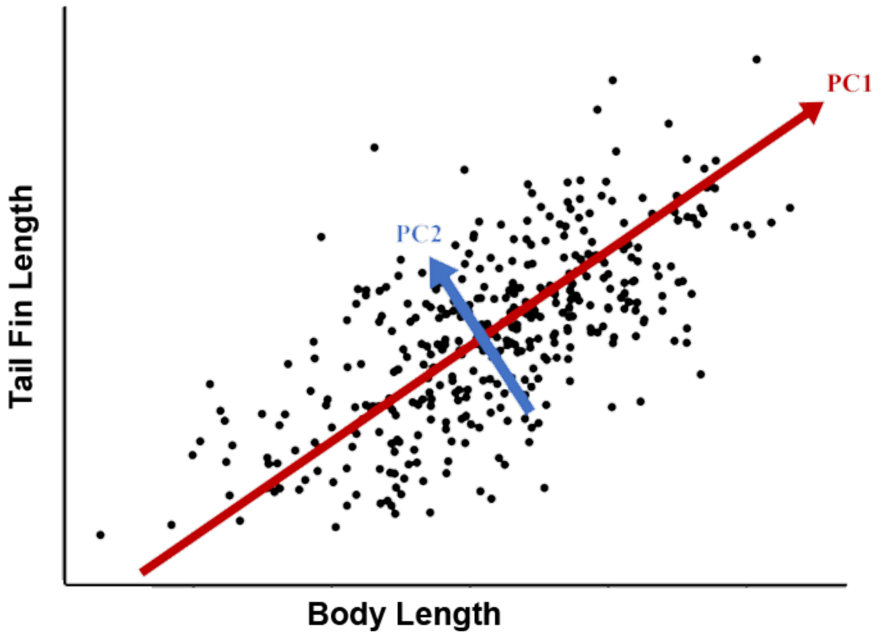


Figure 1: PCA of fish size

```
##       Comp.1       Comp.2       Comp.3
## 1.732051e+00 4.214685e-08 0.000000e+00
##
##  3  variables and  4 observations.
```

3.7 Lists

Matrices and higher-order arrays generally all have the same data type and sub-dimension. For example, if you want to combine two separate 2D matrices into a single 3-D array, then the individual matrices have to have the same number of rows and columns. They should also have the same data type, or else everything will be converted to the most inclusive type, as noted above.

Often we may want to link different types of information together while still maintaining their different data types. Think of a record in a database where you may have information about an organism's taxonomic classification (factors) height (numeric), weight (numeric), general notes and observations (string), number of scales (integer), and maybe a photograph (numeric matrix) and a DNA sequence (string vector). This wouldn't fit neatly into an array format. Instead, we can use a **list** object.

Lists are useful for mixing data types, and can combine different dimensions of cells, vectors, and higher-order arrays.

Each element in a list needs a name:

```
MyList<-list(name="SWC",potpourri=Xvec,numbers=1:10)
MyList
```

```
## $name
## [1] "SWC"
##
## $potpourri
##  [1] "1.1829378"             "string"                "1"
##  [4] "2"                     "3"                     "4"
##  [7] "5"                     "6"                     "7"
## [10] "8"                     "9"                     "10"
## [13] "E"                     "Computational Biology" "100"
## [16] "99"                    "98"                    "97"
## [19] "96"                    "95"                    "94"
## [22] "93"                          "92"                          "91"
## [25] "90"
##
## $numbers
##  [1]  1  2  3  4  5  6  7  8  9 10
```

> **Important**: Many of the statistical functions and other tools in R use list objects to store output. Taking some time now to think about how lists work will save time later when you need to interpret output of R functions.

3.7.1 Subset

There are a few different ways to subset a list object. We can subset by name using the `$` character

```
MyList$numbers # Use $ to subset by name
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10
```

Or we can **slice** using square brackets.

```
MyList[3] # A 'slice' of MyList
```

```
## $numbers
##  [1]  1  2  3  4  5  6  7  8  9 10
```

This is similar to the way we used `[]` in vectors and matrices BUT note the inclusion of the name `$numbers` at the top of the output.

With lists, we have another option, to **extract** using double square brackets.

```
MyList[[3]] # An 'extract' of MyList
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10
```

> What's the difference between `[]` and `[[]]`?

This is a bit tricky, but if you invest some time now to understand, you will save yourself a lot of headaches troubleshooting error messages in your code. Do your future-self a favour and take some time to understand this…

First, Look carefully at the output above; notice how the `[]` includes `$numbers` but the `[[]]` includes only the values? This is important if you want to use the slice:

```
2*MyList[3]
```

```
## Error in 2 * MyList[3]: non-numeric argument to binary operator
```

```
2*MyList[[3]]
```

```
##  [1]  2  4  6  8 10 12 14 16 18 20
```

> Note the error generated in the first case

The second case is just a pure vector of numbers, that's why we can multiply each value by two. The first case is still connected to a list object, with the `$numbers` indicating that we are looking at the *numbers* element of the list. This is part of a larger object, so R returns an error when we try to multiply a number.

In other words, the `$numbers` heading is part of the sliced object created with `[]` but NOT the extracted object created with `[[]]`.

3.7.2 Function Output

> **Protip**: Many analysis functions in R output as lists (e.g. statistical packages).

For example, the output of `princomp`:

```
princomp(Z)
```

```
## Call:
## princomp(x = Z)
##
## Standard deviations:
```

```
##       Comp.1       Comp.2       Comp.3
## 2.091650e+00 2.980232e-08 0.000000e+00
##
##  3  variables and  4 observations.
```

```
names(princomp(Z))
```

```
## [1] "sdev"     "loadings" "center"   "scale"    "n.obs"    "scores"   "call"
```

```
princomp(Z)$center
```

```
## [1] 1.25 2.50 3.75
```

```
princomp(Z)$scale
```

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

Look at the help `?princomp` and scroll down to the **Value** subheading. See how these corresponde to `names(princomp(z))`? These values are stored as a list object with each element corresonding to a part of the list object denoted by `$`.

3.8 `print()` and `paste()`

As noted earlier, the `print` function is the go-to function for printing output to the user. The `paste` function is useful for combining things together.

Paste is a versatile function for manipulating output:

```
paste("Hello World!") # Basic string
```

```
## [1] "Hello World!"
```

```
paste("Hello","World!") # Concatenate two strings
```

```
## [1] "Hello World!"
```

Sometimes we need to convert numbers to strings. `paste` is an easy way to do this:

```
paste(1:10) # Paste numbers as strings
```

```
##  [1] "1"  "2"  "3"  "4"  "5"  "6"  "7"  "8"  "9"  "10"
```

```
paste(1:10)[4]
```

```
## [1] "4"
```

Note how each number above is a separate cell in a vector of strings.

Use `as.numeric` to convert strings back to numbers.

```
as.numeric(paste(1:10)) # Convert back to numbers
```

```
##  [1]  1  2  3  4  5  6  7  8  9 10
```

We can also use the `collapse` parameter to condense a multi-cell vector into a single cell. Reading the help for new functions reveals a lot of great treasures like this!

```
paste(1:10,collapse=".")
```

```
## [1] "1.2.3.4.5.6.7.8.9.10"
```

> **Question**: What happens if we paste objects of different length?

```
paste(c("Hello","World"),1:10,sep="-")
```

```
##  [1] "Hello-1"  "World-2"  "Hello-3"  "World-4"  "Hello-5"  "World-6"
##  [7] "Hello-7"  "World-8"  "Hello-9"  "World-10"
```

Answer: The shorter vector gets re-cycled until every element of the longer vector is pasted.

It is not uncommon to nest a paste function within a print function when communicating output in a more complex R script.

```
print(paste("Hello",1:10,sep="-"))
```

```
##  [1] "Hello-1"  "Hello-2"  "Hello-3"  "Hello-4"  "Hello-5"  "Hello-6"
##  [7] "Hello-7"  "Hello-8"  "Hello-9"  "Hello-10"
```

This would be useful if you were running a program, maybe on a remote high-performance computer where you submit your jobs to a sceduler and you want your program to keep notes about its progress, or generate other notes or feedback. The output of `paste` is not shown on the screen if used inside of a loop, whereas the output of `print` is. More about loops below.

3.9 External Files

So far we've done everything within the R environment. If we quit R, then everything we have made will be removed from memory and we'll have to start all over – unless you are typing this out in a `.R` file that you made in R Studio.

For larger projects and reproducible analysis, it is useful to save and load data from external files.

3.9.1 Working Directory

The **working directory** is the place on your computer where R looks to load or save your files. You can figure out what your current working directory is with the `getwd()` function.

```
getwd()
```

Note: The output is specific to your computer, so it isn't shown here

3.9.2 Absolute Path

The directory shown in `getwd()` is called an **absolute path**. A path is just computer jargon for the way you get to your working directory, like walking down a path in your computer, turning into the correct directory or folder each time until you reach your destination. The absolute means that it is a location that is unchanging. The problem, for reproducible research, is that the location is specific to your user profile on your computer.

You can set an absolute path with `setwd()`. Here's one example:

```
setwd("C:/Users/ColauttiLab/Documents")
```

> Did you type out the above line? You should if you have been following the instructions! If you haven't, go back to where you stopped and type everything out to reinforce it in your brain. Remember, going through and typing everything out is one of the most effective ways to learn to code.

If you have been typing along, you should have an error message, unless you are working in Windows and for some reason have a *ColauttiLab* username. Now try changing to a different directory on your computer.

If you are a mac user, your directory is probably similar, but without the `C:`:

```
setwd("/Users/ColauttiLab/Documents")
```

Again, you will get an error unless you replace the above with a directory that exists on your own computer.

This is why you should NEVER USE ABSOLUTE PATH NAMES in your code. It is not reproducible code!

Don't worry, there is a better way…

3.9.3 Relative Path

In the **absolute path** example above, we first go to the **root** directory, which is the most basic level (or the C: drive in the case of Windows). From the root directory we first click on the **Users** folder, then the **ColauttiLab** folder, and finally the **Documents** folder.

In R, we can just provide a path name as text rather than clicking through all the different folders each time. But as we have seen, the problem with absolute path names is that they are often unique to each user.

Instead of an absolute path, we should use a **relative path** in our code. The relative path in R is denoted with a period, often followed by a forward slash.

For example, if we have a folder called `Data` inside our `Documents` folder, and our current working directory is one of the two examples above, we can use a relative path name to set the `Data` folder as the working directory. Before you type this out, you should make a folder called `Data` inside of your current working directory, or else you will get an error.

```
setwd("./Data")
```

The `.` means *inside of my current directory* and the `/Data` means *move into the Data folder*. This is the coding equivalent of double-clicking the data Folder in your Windows File Explorer or Mac OS Finder.

Now try running this code:

```
getwd()
setwd("..")
getwd()
```

Compare the working directories. The `..` means *go to the parent directory* (i.e. directory containing the current working directory).

The neat thing about relative directories is that it makes it easy to share complex R code between Windows, MacOS and Linux/Unix. In fact, the syntax used by R is the same as Unix, GNU, and Linux.

3.9.4 R Studio Projects

Working with relative paths can get a little bit confusing, especially if you start using `setwd()`. A good way to avoid confusion is to make an R project in R Studio

`File-->New Project-->New Directory-->New Project`

Then make a name for your project and choose where you want to save it on your computer.

Now quit R studio and look inside the new directory that you just created on your computer. You will see a file with the name of your project followed by `.Rproj`

This file is an R project file, and you can double-click on it to open the project. Now here's the cool part: Start R Studio by double-clicking the `.Rproj` *project file* instead of opening the *R Studio App* directly. This should open R Studio, but you will see that the project folder will be your default relative path, which you can check with `getwd()`.

There are lots of good reasons to do this, which become more obvious as you progress as a coder and start working on collaborative projects. For now, think of your project folder as your self-contained programming pipeline. In principle, you want to be able to send this file to somebody else to run on another computer without making any changes to the code. You can do this if you learn how to use relative path names.

3.9.5 Import Data

Download this data file and save it in a directory called `Data` inside of your new project folder:

https://colauttilab.github.io/RCrashCourse/FallopiaData.csv

Now open the file with a text editor and take a look at it.

The `.csv` suffix stands for 'Comma Separated Values'. This is really just a regular old text file with different columns separated by commas and different rows separated by each line of text (i.e. hit 'Enter' to add a new row). You can see this if you try opening the file in a simple text editor (e.g. Notepad for Windows or textEdit for MacOS).

> You can easily create a .csv by choosing the *Save As* or *Export* in most spreadsheet programs (e.g. MS Excel), and choosing CSV as the output format.

To import this data into R, we can use the `read.csv` command and save it as an object.

Often we have column names as the first row, so we include the parameter `header=T` to convert the first row to column names.

Data without column names would have data on the first row, so we would want `header=F` or else our first row of data would be treated as column names.

```
MyData<-read.csv("Data/FallopiaData.csv",header=T)
```

Important: In R, objects created by `read.csv` and other `read.?` functions are special objects called `data.frame` objects.

3.9.6 `data.frame`

A `data.frame` is a special type of object in R that is similar to a 2D matrix, but with with additional indexing information for rows/columns of data. This format is partly why R is so useful for writing a quick, reproducible data analysis.

There are a number of useful functions for inspecting a `data.frame` object.

The indices used for column names can accessed with the `names()` function

```
names(MyData)
```

```
##  [1] "PotNum"       "Scenario"     "Nutrients"    "Taxon"        "Symphytum"
##  [6] "Silene"       "Urtica"       "Geranium"     "Geum"         "All_Natives"
## [11] "Fallopia"     "Total"        "Pct_Fallopia"
```

There are also a number of functions to quickly inspect the data.frame:

1. Show the first six rows of data

```
head(MyData)
```

```
##   PotNum Scenario Nutrients Taxon Symphytum Silene Urtica Geranium Geum
## 1      1      low       low japon      9.81  36.36  16.08     4.68 0.12
## 2      2      low       low japon      8.64  29.65   5.59     5.75 0.55
## 3      3      low       low japon      2.65  36.03  17.09     5.13 0.09
## 4      5      low       low japon      1.44  21.43  12.39     5.37 0.31
## 5      6      low       low japon      9.15  23.90   5.19     0.00 0.17
## 6      7      low       low japon      6.31  24.40   7.00     9.05 0.97
##   All_Natives Fallopia Total Pct_Fallopia
## 1       67.05     0.01 67.06         0.01
## 2       50.18     0.04 50.22         0.08
## 3       60.99     0.09 61.08         0.15
## 4       40.94     0.77 41.71         1.85
## 5       38.41     3.40 41.81         8.13
## 6       47.73     0.54 48.27         1.12
```

2. Show the last six rows

```
tail(MyData)
```

```
##     PotNum     Scenario Nutrients Taxon Symphytum Silene Urtica Geranium Geum
## 118    143 fluctuations      high bohem      5.06  12.81  23.82     3.64 0.16
## 119    144 fluctuations      high bohem     19.93  21.07   6.08     2.80 0.43
## 120    145 fluctuations      high bohem      4.89  32.93   6.30     9.64 0.00
## 121    147 fluctuations      high bohem      7.84  31.16  13.61     6.58 0.03
## 122    148 fluctuations      high bohem      4.15  38.70  23.59     5.11 1.36
## 123    149 fluctuations      high bohem      1.72  10.41  23.48     8.51 0.43
##     All_Natives Fallopia Total Pct_Fallopia
## 118       45.49    21.31 66.80        31.90
## 119       50.31     0.00 50.31         0.00
## 120       53.76     2.36 56.12         4.21
## 121       59.22     3.74 62.96         5.94
## 122       72.91     5.89 78.80         7.47
## 123       44.55    19.70 64.25        30.66
```

3. Check the dimension – the number of rows and columns

```
dim(MyData)
```

```
## [1] 123  13
```

4. Check the number of rows only

```
nrow(MyData)
```

```
## [1] 123
```

5. Check the number of columns only

```
ncol(MyData)
```

```
## [1] 13
```

6. Interrogate the **structure** of the data

```
str(MyData)
```

```
## 'data.frame':    123 obs. of  13 variables:
##  $ PotNum      : int  1 2 3 5 6 7 8 9 10 11 ...
##  $ Scenario    : chr  "low" "low" "low" "low" ...
##  $ Nutrients   : chr  "low" "low" "low" "low" ...
##  $ Taxon       : chr  "japon" "japon" "japon" "japon" ...
##  $ Symphytum   : num  9.81 8.64 2.65 1.44 9.15 ...
##  $ Silene      : num  36.4 29.6 36 21.4 23.9 ...
##  $ Urtica      : num  16.08 5.59 17.09 12.39 5.19 ...
##  $ Geranium    : num  4.68 5.75 5.13 5.37 0 9.05 3.51 9.64 7.3 6.36 ...
##  $ Geum        : num  0.12 0.55 0.09 0.31 0.17 0.97 0.4 0.01 0.47 0.33 ...
##  $ All_Natives : num  67 50.2 61 40.9 38.4 ...
##  $ Fallopia    : num  0.01 0.04 0.09 0.77 3.4 0.54 2.05 0.26 0 0 ...
##  $ Total       : num  67.1 50.2 61.1 41.7 41.8 ...
##  $ Pct_Fallopia: num  0.01 0.08 0.15 1.85 8.13 1.12 3.7 0.61 0 0 ...
```

We can use this to see column headers, types of data contained in each column, and the first few values in each column.

> **Protip**: `str()` is also useful for inspecting other objects, like the output of functions used for statistics or plotting

Pay careful attention to integer `int` vs numeric `num` vs `factor` columns in the `str()` output. These are the data types assigned to each column. As noted earlier, a common source of error students make when starting to analyzing data is using the wrong data *type*.

Here's an example of data types gone rogue: In an analysis of variance (ANOVA), you want a `factor` as a predictor and a `num` or `int` as a response. But in linear regression you want `int` or `num` as a predictor instead of `factor`. If you code your factor (e.g. treatment) as a number (e.g. 1-4) then R will treat it as an integer when you import the data. When you run a linear model with the `lm` function, you will be running a regression rather than ANOVA! As a result, you will estimate a slope rather than the difference between group means.

3.9.6.1 Summary Always check your data types (e.g. using `str`) when you first import the data.

3.9.7 Subset

The `data.frame` object can be subset, just like a matrix object.

```
MyData[1,] # Returns first row of data.frame
```

```
##   PotNum Scenario Nutrients Taxon Symphytum Silene Urtica Geranium Geum
## 1      1      low       low japon      9.81  36.36  16.08     4.68 0.12
##   All_Natives Fallopia Total Pct_Fallopia
## 1       67.05     0.01 67.06         0.01
```

```
MyData[1,1] # Returns first value of data.frame
```

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

In addition to numbers, you can subset a column by its header.

```
MyData[1:4,"PotNum"] # Returns values in "PotNum" column
```

```
## [1] 1 2 3 5
```

```
MyData$PotNum[1:4] # A shortcut to subset the column
```

```
## [1] 1 2 3 5
```

Note how we also include 1:4 to show only the first 4 elements, which reduces the output to a more manageable level. If you aren't sure why, try running the above without 1:4 to see the difference.

We can also subset the data based on particular row values. For example, we can find only the records in the *extreme* treatment scenario.

```
subset(MyData,Scenario=="low") # Subset
```

```
##    PotNum Scenario Nutrients Taxon Symphytum Silene Urtica Geranium Geum
## 1       1      low       low japon      9.81  36.36  16.08     4.68 0.12
## 2       2      low       low japon      8.64  29.65   5.59     5.75 0.55
## 3       3      low       low japon      2.65  36.03  17.09      5.13 0.09
## 4       5      low       low japon      1.44  21.43  12.39      5.37 0.31
## 5       6      low       low japon      9.15  23.90   5.19      0.00 0.17
## 6       7      low       low japon      6.31  24.40   7.00      9.05 0.97
## 7       8      low       low japon     19.53  29.93   0.00      3.51 0.40
## 8       9      low       low japon      6.08  18.25   8.44      9.64 0.01
## 9      10      low       low japon      5.69  35.23   4.84      7.30 0.47
## 10     11      low       low japon     15.58  20.81   2.81      6.36 0.33
## 11     12      low       low japon     11.38  28.67   9.79      5.04 0.56
## 12     14      low       low japon      2.92  27.11   6.25      9.50 0.05
## 13     16      low       low bohem     12.99  18.02   9.51      7.52 0.36
## 14     17      low       low bohem      4.90  29.52   1.36      0.00 0.19
## 15     18      low       low bohem      3.51  27.61   8.14      3.81 0.21
## 16     19      low       low bohem      7.49  32.14   5.70      6.93 0.01
## 17     20      low       low bohem     11.16  25.58   1.80      5.10 0.07
## 18     22      low       low bohem      0.76  22.66   9.85     10.60 0.74
## 19     23      low       low bohem      7.53  33.14   9.42      9.02 0.02
## 20     24      low       low bohem      5.74  28.12  14.69      7.55 0.48
## 21     25      low       low bohem      8.91  32.99   7.35      3.79 0.18
## 22     26      low       low bohem     13.25  18.11   0.00      0.00 0.10
## 23     28      low       low bohem     10.59  18.78   7.19      6.73 0.17
## 24     29      low       low bohem     11.48  19.89   5.84      3.86 0.13
## 25     30      low       low bohem     10.35  26.64  20.07      2.05 0.58
##    All_Natives Fallopia Total Pct_Fallopia
## 1        67.05     0.01 67.06         0.01
## 2        50.18     0.04 50.22         0.08
## 3        60.99     0.09 61.08         0.15
## 4        40.94     0.77 41.71         1.85
## 5        38.41     3.40 41.81         8.13
## 6        47.73     0.54 48.27         1.12
## 7        53.37     2.05 55.42         3.70
## 8        42.42     0.26 42.68         0.61
## 9        53.53     0.00 53.53         0.00
## 10       45.89     0.00 45.89         0.00
## 11       55.44     3.58 59.02         6.07
## 12       45.83    11.83 57.66        20.52
## 13       48.40     0.58 48.98         1.18
## 14       35.97     0.00 35.97         0.00
## 15       43.28     0.00 43.28         0.00
## 16       52.27     0.00 52.27         0.00
## 17        43.71     2.21 45.92          4.81
## 18        44.61     0.00 44.61          0.00
## 19        59.13     0.00 59.13          0.00
## 20        56.58     2.39 58.97          4.05
## 21        53.22     2.14 55.36          3.87
## 22        31.46     0.00 31.46          0.00
## 23        43.46     0.00 43.46          0.00
## 24        41.20     3.45 44.65          7.73
## 25        59.69     0.00 59.69          0.00
```

3.9.8 New Columns

It's easy to add new columns to a data frame. For example, to add a new column that is the sum of two others:

```
MyData$NewTotal<-MyData$Symphytum + MyData$Silene + MyData$Urtica
names(MyData)
```

```
##  [1] "PotNum"        "Scenario"      "Nutrients"     "Taxon"         "Symphytum"
##  [6] "Silene"        "Urtica"        "Geranium"      "Geum"          "All_Natives"
## [11] "Fallopia"      "Total"         "Pct_Fallopia" "NewTotal"
```

Notice the new column added to the end. Let's look at the first 10 values:

```
print(MyData$NewTotal[1:10])
```

```
##  [1] 62.25 43.88 55.77 35.26 38.24 37.71 49.46 32.77 45.76 39.20
```

3.10 Other Functions

There are a few more useful functions for inspecting your data.

3.10.1 `unique`

Find all the unique values within a vector using `unique`.

```
unique(MyData$Nutrients)
```

```
## [1] "low"  "high"
```

3.10.2 `duplicated`

Look at each value in a vector and return a `TRUE` if it is duplicated and `FALSE` if it is unique.

```
duplicated(MyData$Nutrients)
```

```
##   [1] FALSE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [13]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [25]  TRUE FALSE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [37]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [49]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [61]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [73]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [85]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
##  [97]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
## [109]  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE  TRUE
## [121]  TRUE  TRUE  TRUE
```

3.10.3 `aggregate`

Quickly calculate means of one column of data (`NewTotal`) for each value of another column with groups (`Nutrients`).

```
aggregate(MyData$NewTotal,list(MyData$Nutrients), mean)
```

```
##   Group.1        x
## 1    high 46.51173
## 2     low 42.76800
```

The ~ provides an alternative way to write this function. In R the ~ usually means *by* and it is often used in statistical models.

```
aggregate(NewTotal ~ Nutrients, data=MyData, mean)
```

```
##   Nutrients NewTotal
## 1      high 46.51173
## 2       low 42.76800
```

For the code above, we can say "aggregate `NewTotal` *by* `Nutrients` grouping".

The nice thing about doing it this way is that we preserve the column name. Compare the column names here: *Nutrients* and *NewTotal*, vs above: *Group.1* and *x*.

We can also use this to calculate means across different combinations of two or more grouping columns.

```
aggregate(NewTotal ~ Nutrients*Taxon*Scenario, data=MyData, mean)
```

```
##    Nutrients Taxon     Scenario NewTotal
## 1       high bohem      extreme 45.24833
## 2       high japon      extreme 45.31500
## 3       high bohem fluctuations 43.89545
## 4       high japon fluctuations 44.77692
## 5       high bohem      gradual 45.36923
## 6       high japon      gradual 50.43417
## 7       high bohem         high 52.04273
## 8       high japon         high 45.69417
## 9        low bohem          low 41.75231
## 10       low japon          low 43.86833
```

Note that `mean` is just the `mean()` function in R. We can use other functions, like the standard deviation `sd`:

```
aggregate(NewTotal ~ Nutrients, data=MyData, sd)
```

```
##   Nutrients  NewTotal
## 1      high 11.175885
## 2       low  8.227402
```

3.10.4 `tapply`

`tapply` works similarly, but using a `list()` function

For example, we can calculate means of each `Nutrients` group:

```
tapply(MyData$NewTotal, list(MyData$Nutrients), mean)
```

```
##     high      low
## 46.51173 42.76800
```

Compare this output with `aggregate` above. Here, the groups are the column names.

3.10.5 `sapply` & `lapply`

The `sapply` and `lapply` functions are similar in principle to `tapply`, but are used to apply a function repeatedly and output the result as a vector (`sapply`) or list object (`lapply`).

Here's an example, where we can summarize the `class` of each column in our `data.frame`

```
lapply(MyData, class)[1:3]
```

```
## $PotNum
## [1] "integer"
##
## $Scenario
## [1] "character"
##
## $Nutrients
## [1] "character"
```

```
sapply(MyData, class)[1:3]
```

```
##      PotNum    Scenario   Nutrients
##   "integer" "character" "character"
```

Compare the above with:

```
class(MyData)
```

```
## [1] "data.frame"
```

```
class(MyData$Taxon)
```

```
## [1] "character"
```

3.11 Tidyverse

Most of the methods above for managing and summarizing data are the *classic* or *base R* functions. More recently, the **tidyverse** group of functions has gained popularity and these functions have a lot of advantages over the classic tools, particularly for complex data management.

For example, it is easy to string together multiple steps into a single 'pipe' of data reorganization. The Data Science Tutorial/Chapter introduces the `dplyr` package as an introduction to the `tidyverse`.

3.12 Save

Just as we can load FROM external files, we can save TO external files. We just change `read` to `write`. For a CSV file:

```
## Calulate means
NutrientMeans<-tapply(MyData$NewTotal,list(MyData$Nutrients),mean)
## Save means as .csv file
write.csv(NutrientMeans,"MyData_Nutrient_Means.csv", row.names=F)
```

> NOTE: the default for write.csv adds a column of row names (i.e. numbers) to the output file. To avoid this, use row.names=F

You should see a file called *MyData_Nutrients_Means.csv* in your working directory.

3.12.1 Output Foler

Larger projects may generate a lot of different output files, which you may want to organize in an `Output` folder inside of your project folder. Saving to this folder is easy for relative path names, just add `./Data/` before the file name in your `write.csv()` function. Just make sure the folder exists before you try to save to it!

```
write.csv(NutrientMeans,"./Data/MyData_Nutrient_Means.csv", row.names=F)
```

3.13 Flow control

Think of your data analysis as a stream flowing from the raw data at the headwaters down to the river mouth, exiting as a full analysis with graphics, statistical analyses, and biological interpretation.

There are different ways we can control the flow of the water. The simplest is just to write a sequence of lines of code, with the output of one line of code forming the input of the next. A pseudo-code example might be:

```
A<-functionA()
B<-functionB(A)
C<-functionC(B)
```

But sometimes we may want to do the same function or analysis only if the input meets certain criteria. Or we may want to reiterate the same analysis multiple times on different inputs. This is where more advanced flow control comes in handy.

To start, let's make up a couple of objects to play with:

```
X<-21
Xvec<-c(1:10,"string")
```

3.13.1 `if`

The `if` statement uses an **operator** (see above) to asses whether the value is `TRUE` or `FALSE`:

```r
if(X > 100){ # Is X greater than 100?
  print("X > 100") # If TRUE
} else {
  print("X <= 100") # If FALSE
}
```

```
## [1] "X <= 100"
```

A common ‘rookie’ mistake is to leave out a bracket or use the wrong type of bracket. Use regular brackets for the *if function* `if()` followed by two sets of curly brackets containing the code to run `{run if true}else{run if false}`.

Break up across multiple lines to improve readability. Note that you don’t need an `else{}` part if you just want to do nothing when `FALSE`.

```r
if(X > 0){print ("yup")}
```

```
## [1] "yup"
```

3.13.2 ifelse

The `ifelse` is a more compact version for simple comparisons. The following code does the same as above.

```r
ifelse(X > 100,"X > 100", "X <= 100")
```

```
## [1] "X <= 100"
```

3.13.3 nested if

You can also nest `if` and ifelse‘ statements to account for more outcomes. Conceptually think of it as a bifurcating tree, starting at the top (root) and then splitting in two for every if statement.

```
if(X > 100){
  print("X > 100")
  if(X > 200){
    print("X > 200")
  }
} else {
  if(X == 100){
    print("X = 100")
  } else {
    print("X < 100")
  }
}
```

```
## [1] "X < 100"
```

Don't get intimidated. It just takes time to work through all of the possibilities. Try to draw a bifurcating diagram to represent each true/false outcome for the above code.

3.13.4 `for` loop

A loop does the same thing over and over again until some condition is met. In the case of a `for` loop, we set a 'counter' variable and loop through each value of the counter variable. Here are a few examples:

1. Loop through numbers from 1 to 5

```
for (i in 1:5){
  print(paste(X,i,sep=":"))
}
```

```
## [1] "21:1"
## [1] "21:2"
## [1] "21:3"
## [1] "21:4"
## [1] "21:5"
```

2. Loop through the elements of a vector directly

```r
for (i in Xvec){
  print(i)
}
```

```
## [1] "1"
## [1] "2"
## [1] "3"
## [1] "4"
## [1] "5"
## [1] "6"
## [1] "7"
## [1] "8"
## [1] "9"
## [1] "10"
## [1] "string"
```

3. Use an index object to index the elements of a vector

```r
for (i in 1:length(Xvec)){
  print(Xvec[i])
}
```

```
## [1] "1"
## [1] "2"
## [1] "3"
## [1] "4"
## [1] "5"
## [1] "6"
## [1] "7"
## [1] "8"
## [1] "9"
## [1] "10"
## [1] "string"
```

Note that in each case there is a vector and we loop through each cell in the vector. The `i` keeps track of the cell value in each iteration of the loop.

Loops can be tricky, and the only way to really learn them is to practice as much as possible. Whenever you find yourself writing similar code more than 2 or 3 times, challenge yourself to try to re-write it as a loop.

In addition to looping through a vector, it can often be useful to include a counter variable. This can be especially useful for more complicated loops, but one important thing to watch out for is what part of the loop you want to update the counter variable. USUALLY it will be either

1. At the end, by setting the initial value to 1 before the loop gegins

```
count1<-1
count10<-1

for(i in 1:5){
  print(paste("count1 =",count1))
  print(paste("count10 =",count10))
  count1<-count1+1
  count10<-count10*10
}
```

```
## [1] "count1 = 1"
## [1] "count10 = 1"
## [1] "count1 = 2"
## [1] "count10 = 10"
## [1] "count1 = 3"
## [1] "count10 = 100"
## [1] "count1 = 4"
## [1] "count10 = 1000"
## [1] "count1 = 5"
## [1] "count10 = 10000"
```

2. At the beginning, setting the initial value to 0

```
countbefore<-0
countafter<-0

for(i in 1:5){
  countbefore<-countbefore+1
  print(paste("before =",countbefore))
  print(paste("after =",countafter))
  countafter<-countafter+1
}
```

```
## [1] "before = 1"
## [1] "after = 0"
## [1] "before = 2"
## [1] "after = 1"
## [1] "before = 3"
## [1] "after = 2"
## [1] "before = 4"
## [1] "after = 3"
## [1] "before = 5"
## [1] "after = 4"
```

Read through the outputs above carefully to make sure you understand how the loops work. When you are confident you understand, then write a new loop and write down the predicted output. Run the loop to check if you were right.

3.13.5 Nested Loops

Counters are particularly valuable when you have a nested loop, which is just one loop inside of another.

In the example below, we are first looping through a vector of length 3, tracked with `i`. Then **for each i** we do a second loop, tracked by `j`.

This time, try to predict the output BEFORE you run the loop. Write it down, then run the loop to check your answer.

```r
LoopCount<-0
for(i in 1:3){
  for(j in 1:2){
    LoopCount<-LoopCount+1
    print(paste("i = ",i))
    print(paste("j = ",j))
    print(paste("Loop =",LoopCount))
  }
}
```

```
## [1] "i =  1"
## [1] "j =  1"
## [1] "Loop = 1"
## [1] "i =  1"
## [1] "j =  2"
## [1] "Loop = 2"
## [1] "i =  2"
## [1] "j =  1"
## [1] "Loop = 3"
## [1] "i =  2"
## [1] "j =  2"
## [1] "Loop = 4"
## [1] "i =  3"
## [1] "j =  1"
## [1] "Loop = 5"
## [1] "i =  3"
## [1] "j =  2"
## [1] "Loop = 6"
```

3.13.6 `while` loop

The `while` is another kind of loop, but instead of looping through a predefined set of variables, we iterate until some condition is met inside of the loop. This is called the **exit condition**.

Often, the `while` loop is used in optimization algorithms, where many calculations are run until some optimum or threshold value is reached.

One common coding error associated with `while` loops is that the exit condition is never reached, causing your computer to run an infinite loop.

Here's a simple while loop, which will continue until `count` is greater than or equal to `X`.

```
count<-0
while (count < X){
  print(count)
  count<-count+1
}
```

```
## [1] 0
## [1] 1
## [1] 2
## [1] 3
## [1] 4
## [1] 5
## [1] 6
## [1] 7
## [1] 8
## [1] 9
## [1] 10
## [1] 11
## [1] 12
## [1] 13
## [1] 14
## [1] 15
## [1] 16
## [1] 17
## [1] 18
## [1] 19
## [1] 20
```

3.14 Packages

As noted above, **functions** in R use brackets `()` and generally have **input** and **output** objects as well as **parameters** that affect their behaviour.

All of the functions in this tutorial are automatically loaded when you start R, but there are many more functions available. For example, our lab developed the `baRcodeR` package for creating unique identifier codes with printable barcodes and data sheets to help with sample management and data collection. You may find this helpful for labelling and tracking samples in your own work: https://doi.org/10.1111/2041-210X.13405

A **package** in R is a set of functions grouped together. For example, the `stats` package is automatically loaded when you run R and contains many useful functions. You can see what package a function belongs to at the beginning of the help file:

```
?cor
```

The package is shown in curly brackets at the top of the help file. In this case, we see *cor {stats}* telling us that the `cor` function is part of the `stats` package. You can see which packages are loaded if you click on the **Packages** tab in **R Studio** (by default it is in the bottom-right window). The loaded packages are shown with check marks.

3.14.1 Installing

There are many more packages available that are not yet installed on your computer. You will need to install a new package before you can use it. You only have to do this once, but it is a good idea to update the package frequently, especially when you update to a new version of R. This ensures that you are using the most recent version of the package.

Packages are installed with `install.packages()`, with the package indicated with single or double quotation marks. When you run this code may be prompted to choose a repository, in which case choose one that is geographically close to you.

```
install.packages('baRcodeR')
```

Note that **installing** a package just downloads it from an online **repository** (remote computer) and saves to your personal computer.

3.14.2 Loading

To use a package that you already have installed, you can access it two ways.

1. You can load the package using the `library()` function, giving you access to all of the functions contained within it:

```
library(baRcodeR)
make_labels()
```

This method is more common, especially when you will use multiple functions from the same package, or use the same functions multiple times.

2. You can use `::` to call a function without loading the whole package

```
baRcodeR::make_labels()
```

This translates to *Run the `make_labels` function from the `baRcodeR` library*. This method is convenient if you just want to use one function from a large library.

Another reason to go with the second method is that some packages have **functions with the same names**. Let's say you load two packages `pkgA` and `pkgB` that have different functions but both are called `cor`. When you run the `cor` function, R will assume you want the one from whichever package was most recently loaded using the `library()` function.

To avoid confusion, you can use the second method to specify which function to run:

```
pkgA::cor()
pkgB::cor()
```

3.14.2.1 Library vs Package

The terms **library** and **package** are often used interchangeably. Technically, the **package** is the collection of functions whereas the **library** is the specific folder where the R packages are stored. A library may contain more than one package.

For the most part, you just need to know that a package and a library are a collection of functions.

3.15 Readable code

Now that you've learned how to code, let's take a few minutes to think about best practices. It's important to make your code readable and interpretable by collaborators, peer reviewers, and yourself 6 months from now. There are lots of opinions on this but here are a few basic suggestions:

1. Add documentation to explain what you are doing
2. Add spacing between parameters to improve readability
3. Add spacing on either side of <- when making objects
4. Break long functions into multiple lines; add the line break after a comma
5. Follow these additional suggestions for object/column/file names
   a. Try to keep your names short and concise but meaningful
   b. Use underscore _ to improve readability
   c. Always start object names with a letter, never a number or symbol d. Avoid symbols completely

Bad	Good
`sum(X,na.rm=T)`	`sum(X, na.rm=T)`

Bad	Good
`X`	`Mass`
`Days.To.First.Flower`	`Flwr_Days` or `FDays`
`10d.Height`	`Ht10d`
`Length*Width`	`LxW`

Break up longer code across multiple lines:

Bad:

```
MyObject<-cor(c(1,2,NA,5,9,8,1,2,5,2,6,3),c(2,2,6,3,6,8,3,NA,2,4,5,1),...)
```

Good:

```
MyObject <- cor(c(1,2,NA,5,9,8,1,2,5,2,6,3),
                c(2,2,6,3,6,8,3,NA,2,4,5,1),
                method="spearman", na.rm=T)
```

To take your code to the next level, look into the Tidyverse Style Guide

4 Quick Visualizations

4.1 Overview

Visualizing data is a key step in any analysis. R provides powerful and flexible graphing tools, whether you are just starting to understand the structure of your data, or polishing off the perfect figure for publication in a 'tabloid' journal like Science or Nature.

In this tutorial, you will learn how to make quick graphs with the `ggplot()` function from the `ggplot2` package. We will go over some options for customizing the look and layout that will allow you to produce professional-grade graphs. In the next chapter you will learn some additional tricks and resources for developing your graphing skills even further.

By the time you are finished these two self-tutorials, you will have all the resources you need to make **publication-ready graphics**!

Both `ggplot` functions come from the `ggplot2` package. Developed by Hadley Wickham and the same team as R Studio, `ggplot2` is part of the Tidyverse group of helpful R packages.

> **Note** I don't know what happened to ggplot1…

Once you have mastered these tutorials, you might want to continue to expand your `ggplot` repertoire by reading through additional examples in the `ggplot2` documentation http://docs.ggplot2.org/current/

WARNING: There is a learning curve for graphing in R! Learning visualizations in R can feel like a struggle at first, and you may ask yourself: *Is it worth my time?*

If you already have experience making figures with point-and-click graphics programs, you may ask yourself: *Why deal with all these coding errors when I can just generate a quick figure in a different program?*

There are a few good reasons to invest the time to get over the learning curve and use R for all your graphing needs.

1. You will get much faster with practice.
2. You have much more control over every aspect of your figure.
3. Your visualization will be **reproducible**, meaning anyone with the data and the code can reproduce every aspect of your figure, from each individual data point down to the specific axis labels.

The third point is worth some extra thought. Everybody makes mistakes, whether you are graphing with R or a point-and-click graphics program. If you make a mistake in a point-and-click program, you may produce a graph that is incorrect with no way to check! If you make an error in R you will either get an error message telling you, or you will have reproducible code that you can share with somebody who can check your work – even if that *somebody* is you, six months in the future. In this way, **reproducibility is quality** – a nice looking but non-reproducible figure is a low-quality figure.

In addition to quality and scientific rigour, there is a more practical reason to value reproducible code. Consider what happens as you collect new data or find a mistake in your original data that needs to be corrected. With a point-and-click program you have to make the graph all over again. With R, you just rerun the code with the new input and get the updated figures and analyses! Later, we will learn how to incorporate code for figures along with statistical analysis into fully reproducible reports with output as `.html` (Website), `.pdf` (Adobe Acrobat), and `.docx` (Microsoft Word)

4.2 Graphical Concepts

Before we dive into coding for visualizations, there are a few universal graphing concepts that are important to understand in order to create publication-ready graphics in R: file formats, pixel dimension, screen vs print colours, and accessibility.

4.2.1 Vector vs. Raster

There are many different **file formats** that you can use to save individual graphs. Each format has a different suffix or extension in the file name: .jpg, .png, .pdf, etc. Once saved, you can send these to graphics programs for minor tweaks, or you can send them directly to academic journals for final publication.

Importantly, file formats for visualizations fall into two main classes: **Raster** and **Vector**.

Raster files save graphs in a 2-dimensional grid of data corresponding to pixel location and colour. Imagine breaking up your screen into a large `data.frame` object with each pixel represented by a cell, and the value of each cell holding information about the colour and intensity of the pixel. You are probably quite familiar with this ‘pixel art’ format if you’ve ever worked with a digital photo or played a retro video game made before 1993. Some popular Raster file types include *JPEG/JPG, PNG, TIFF, and BMP*.

Vector files save information about shapes. Instead of tracking every single pixel, the data are encoded as colourd points mapped onto a two-dimensional plane, with points connected by straight or curved lines. To generate the image, the computer must plot out all of the points and lines, and then translate that information to pixels that display on your screen.

If you've ever drawn a shape in a program like Microsoft Powerpoint or Adobe Illustrator, you might have some sense of how this works. Some popular vector formats include *SVG, PDF, EPS, AI, PS*.

So, why does this matter?

In most cases, you should save your visualizations as **vector** files. *SVG* is a good choice, because it can be interpreted by web browsers and it is not proprietary. *PDF* and *EPS* are commonly used by publishers and can be viewed on most computers after insalling free software.

Saving your graphs as a *vector* format allows you (or the journal proof editor) to easily scale your image while maintaining crisp, clear lines. This is because the shapes themselves are tracked, so scaling just expands or contracts the x- and y-axes.

In contrast, if you expand a *raster* file, your computer has to figure out how to expand each pixel. This introduces blurriness or other artifacts. You have seen some images that look 'pixelated' – this happens when you try to expand the size of a lower-resolution figure. This also happens when a program compresses an image to save space – the computer program is trying to reduce the data content by reducing the dimensionality of the image.

In summary, **vector** images are generally a better format to use when saving your figures because you can rescale to any size and the lines will always be clean and clear. There are a few important exceptions, however.

1. **Photographs** – Photographs captured by a camera are saved in the *Raster* format and cannot be converted to vector without significant loss of information.
2. **Grid Data** – Raster data are convenient for plotting data that occurs in a grid. This includes most spatial data that is broken up into a geographic grid. However, you may often want to use the vector format for mapping/GIS data so that the overlapping geographical features (e.g. borders, lakes, rivers) remain in the vector format, even if an underlying data layer is a raster object (e.g. temperature in 1km squares).

3. **Large Data** – With some large data applications (e.g. 'omics' datasets) a graph may have many millions or billions of data points or lines. In these cases, the **vector** file would be too big to use in publication (e.g. several gigabytes). In this case you might opt for a high-resolution *Raster* file. On the other hand, you could graph your data using a density grid with colours corresponding to the density of points. In this case, you could use the *vector* format to maintain clean lines for the graph axes and labels.

The bottom line: you generally want to save your graphics as *SVG* or *PDF* files if you plan to publish them.

4.2.2 Resolution vs Dimension

In cases where you do need to use raster images in a publication, pay careful attention to the image's **Pixel Dimension**. You have probably heard about image *resolution*: For example, a 2 megapixel camera is better than a 1 megapixel camera; a 200 dpi (dots per inch) printer is better than 100 dpi. But when creating and saving raster images, it's not just the **resolution** that matters, the image **size** also determines the quality of the final image. The **size** and **resolution** of an image jointly determine its **Pixel Dimension**.

> For example, an image with 200 dpi that is 1 x 3 inches will have the same pixel dimension of an image with 100 dpi that is 2 x 6 inches. These images will look exactly the same if they are printed at the same size. The pixel dimension, not the resolution *per se*, determines how 'clean' vs pixelated an image looks.

4.2.3 Screen vs Print

Another important consideration is the intended audience and whether they will likely view your figures on a computer screen or printed page (or both). Each pixel of your screen has tiny lights that determine the specific colour that is reproduced. The pixels *emit* different wavelengths from your screen, which overlap in our eyes to produce the different colours that we see. In contrast, printed images get their colour from combinations of ink, which *absorb* different wavelengths of colour. This is a key distinction! One important consequence of this difference is that your computer monitor can produce a broader range of colours and intensities than a printed pages, and therefore some colours on your computer monitor can look very different in print. In print, the intensity of colours are limited by the intensity of the Cyan, Magenta and Yellow inks that are used to reproduce the images. This is called **CMYK printing**.

Some programs like *Adobe Illustrator* have options to limit the screen to display only those colours that can be reproduced with CMYK printing.

4.2.4 Accessibility

Another important consideration about your choice of colours involves your audience. Remember that many cultures have particular intuitions about colours that can cause confusion if your choice does not match these expectations. For example, in Western European cultures, the red spectrum colours (red, orange, yellow) are often associated with ‘hot’ or ‘danger’ while blue spectrum (blue, cyan, purple) are more associated with ‘cold’ or ‘calm’. Imagine how confusing it would be to look at a weather map that used blue for hot temperatures and red for cool temperatures.

In addition to **cultural biases**, a significant portion of the population has some form of **colour-blindness** that limits their ability to see certain colours. This article in Nature has a good explanation with tips for making inclusive figures: https://www.nature.com/articles/d41586-021-02696-z

Here is a simulation of colour blindness, written in R. Note how certain reds and blue/purple are indistinguishable. A good strategy is to use different **intensity** as well as different **spectra**.

There is also a more practical reason for this. It is common for scientists and students to print your manuscript or published article in black-and-white to read on public transit or during a group discussion. If you choose colours and shading that can be interpreted properly in black and white, then you will avoid confusion with this significant portion of your audience. The `viridis` package is a good tool for this. See: https://cran.r-project.org/web/packages/viridis/vignettes/intro-to-viridis.html

4.2.5 Slides

Some of the above information is covered and expanded in the *Introductory Slides*: https://colauttilab.github.io/RCrashCourse/Graphics_small.pdf

These slides cover:

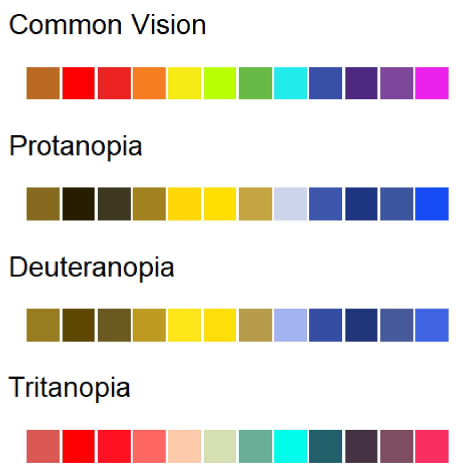


Figure 2: Simulated colourblind palettes

1. Graphing examples
2. Graphical concepts
3. `ggplot` grammar
4. anatomy of a `ggplot` graph

4.3 Getting Started

Install the `ggplot2` package using the `install.packages()` function the first time you want to use it. This installs it on your local computer, so you only need to do it once – though it is a good idea to re-install periodically to update to the most recent version.

```
install.packages("ggplot2")
```

Once it is installed, you still need to load it with the `library` function if you want to use it in your code.

```
library(ggplot2)
```

4.3.1 Data setup

We will again be working with the `FallopiaData.csv` dataset, which can be downloaded here: https://colauttilab.github.io/RCrashCourse/FallopiaData.csv, and saved to a folder called `Data` inside your project folder. Remember that you can find your current working folder with the `getwd()` function.

Now load the *.csv* file into R as a `data.frame` object:

```
MyData<-read.csv("./Data/FallopiaData.csv", header=T)
```

Alternatively, you can load the file right from the internet:

```
MyData<-read.csv(
  "https://colauttilab.github.io/RCrashCourse/FallopiaData.csv")
```

This dataset comes from the research group of Dr. Oliver Bossdorf at the University of Tuebingen in Tuebingen, Germany – a historic university in wonderful little town on the Neckar River. Let's inspect the `data.frame` that was created from the data, to see what kind of data we are working with.

```
str(MyData)
```

```
## 'data.frame':    123 obs. of  13 variables:
##  $ PotNum      : int  1 2 3 5 6 7 8 9 10 11 ...
##  $ Scenario    : chr  "low" "low" "low" "low" ...
##  $ Nutrients   : chr  "low" "low" "low" "low" ...
##  $ Taxon       : chr  "japon" "japon" "japon" "japon" ...
##  $ Symphytum   : num  9.81 8.64 2.65 1.44 9.15 ...
##  $ Silene      : num  36.4 29.6 36 21.4 23.9 ...
##  $ Urtica      : num  16.08 5.59 17.09 12.39 5.19 ...
##  $ Geranium    : num  4.68 5.75 5.13 5.37 0 9.05 3.51 9.64 7.3 6.36 ...
##  $ Geum        : num  0.12 0.55 0.09 0.31 0.17 0.97 0.4 0.01 0.47 0.33 ...
##  $ All_Natives : num  67 50.2 61 40.9 38.4 ...
##  $ Fallopia    : num  0.01 0.04 0.09 0.77 3.4 0.54 2.05 0.26 0 0 ...
##  $ Total       : num  67.1 50.2 61.1 41.7 41.8 ...
##  $ Pct_Fallopia: num  0.01 0.08 0.15 1.85 8.13 1.12 3.7 0.61 0 0 ...
```

The data come from a plant competition experiment involving two invasive species from the genus *Fallopia*. These species were grown in planting pots in competition with several other species. The first four columns give information about the pot and treatments (`Taxon` = species of *Fallopia*. The rest give biomass measurements for each species (header = Genus names).

4.4 Basic Graphs

Think back to the previous Chapter, and you will hopefully recall the different data types represented by the columns of our data. For graphing purposes, there are really just two main types of data: **categorical** and **continuous**. Putting these together in different combinations with `ggplot()` gives us different default graph types.

Each `ggplot()` function requires two main components:

1. The `ggplot()` function defines the input data structure. this usually includes a nested *aesthetic* function `aes()` to define the plotting variables and a `data=` parameter to define the input data.
2. the `geom_<name>()` function defines the output geometry

Note that the `<name>` denotes a variable name that differs depending on the geography used to map the data. This is covered in more detail in the next chapter. For now, we'll look at the most common *geoms*, based on input data type.

Let's look at the defaults for one or two variables of categorical or continuous variables.

4.4.1 One Continuous

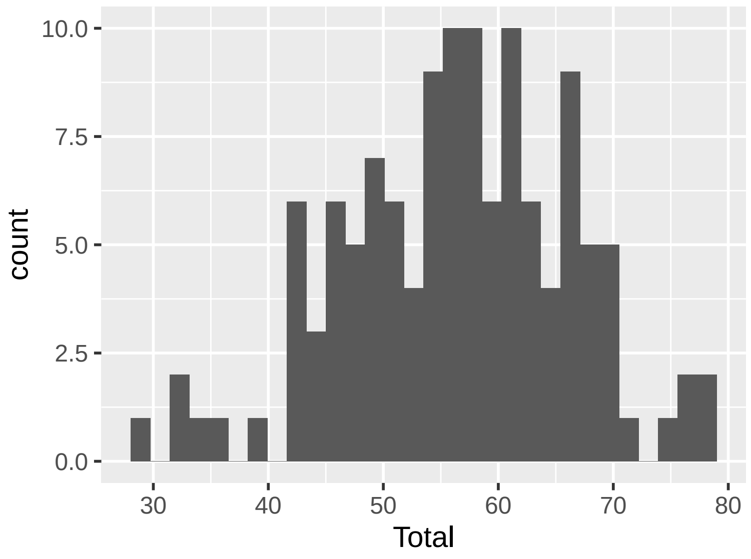
Usually when we only have a single continuous variable to graph, then we are interested in looking at the frequency distribution of values. This is called a **frequency histogram** . The frequency histogram shows the distribution of data – how many observations (y-axis) for a particular category (x-axis).

It is very common to plot histograms for all of your variables before running any kind of statistical model. This is because many statistical models make assumptions about the distribution of your input data. Looking at the histograms is a good way to look for potential coding errors (e.g. outliers) and whether data are generally normal or should be transformed to meet the assumptions of our statistical models.

Histogram

```
ggplot(aes(x=Total), data=MyData) + geom_histogram()
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



Note the two main components of our code: the `ggplot()` function defines the input data and the `geom_histogram()` function provides the mapping function.

You can also see we get a warning message about `stat_bin()`. With R we can distinguish *warning* messages from *error* messages.

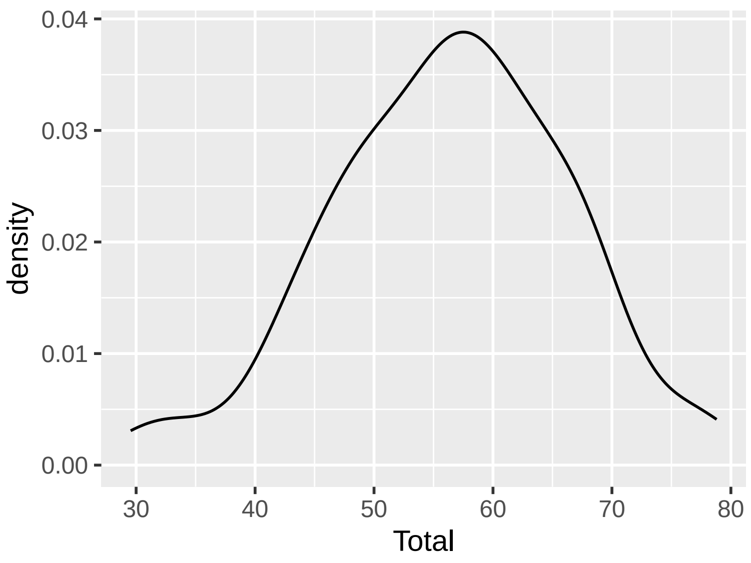
Error messages represent bigger problems and generally occur when the function doesn't run at all. For example, if we wrote `total` instead of `Total`, we would get an error because R is looking for an object called `total`, which is not the same as `Total` with a capital *T*.

Warning messages don't necessarily prevent the function from running, as in this case. However, it is still important to read the warning and understand if it is ok to ignore it. In this case, it is suggesting a different `binwidth` parameter. We'll come back to this later when we explore some of the different parameter options.

Density

A *density* geom is another way to graph the frequency distribution. Instead of bars, a smoothed curve is fit across the bins, and instead of 'count' data, an estimate of the probability is shown on the y-axis.

```
ggplot(aes(x=Total), data=MyData) + geom_density()
```



Notice that the y-axis says 'density', not probability? This curve is called a **probability density function** and we can calculate the probability of observing a value between two points along the x-axis by calculating the area under the curve for those two points. For example, the total area under the curve from Total=0 to Total > 80 should 1.

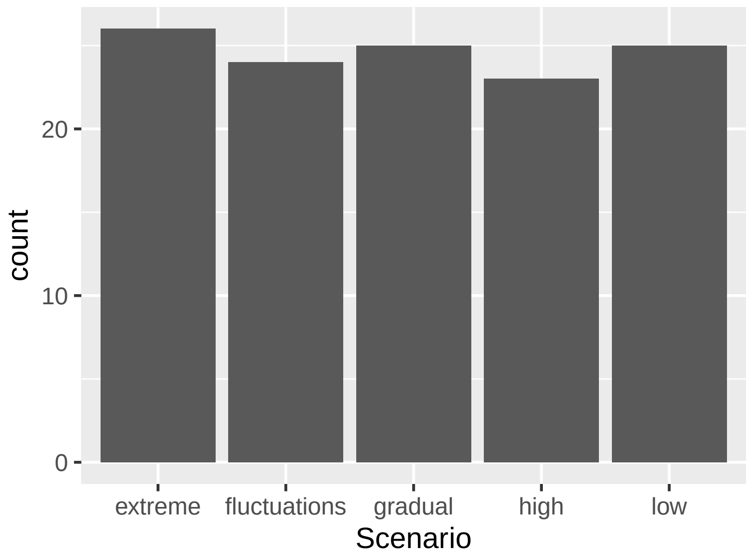
4.4.2 One Categorical

If we input one variable that is *categorical* rather than *continuous*, then we are often most interested in looking at the sample size for each category. In a classic ANOVA for example, you want to make sure you have a similar number of observations for each category.

Instead of `geom_histogram()` we use `geom_bar()`

Bar Graph

```
ggplot(aes(x=Scenario), data=MyData) + geom_bar()
```



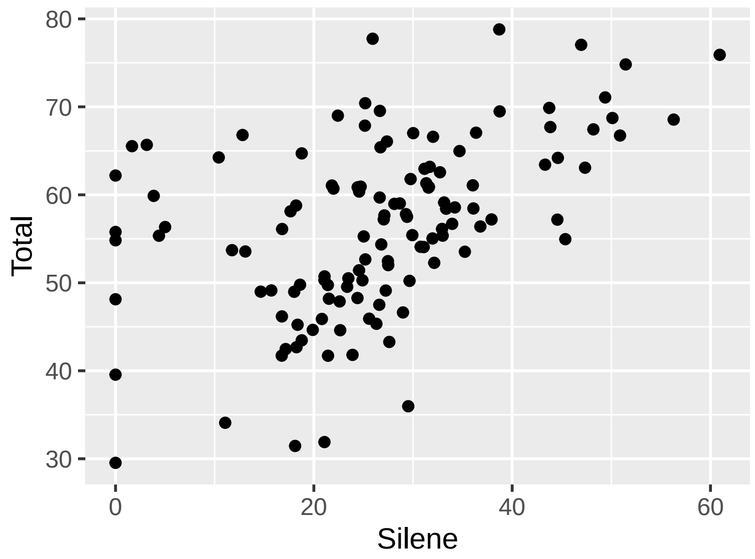
4.4.3 Two Continuous

If we have two continuous variables, we are most often interested int the classic **bivariate plot**, sometimes called a **scatter plot**.

The bivariate plot or scatter plot is the ‘meat and potatoes’ of data visualization. By plotting two variables we can see if they are independent (‘shotgun’ pattern) or have some degree of correlation (oval sloped up or down). We can also look for outliers, which would be seen as isolated points that are far away from the main ‘cloud’ of points.

Bivariate Plot

```
ggplot(aes(x=Silene, y=Total), data=MyData) + geom_point()
```



4.4.4 Two Categorical

Plotting two categorical variables is not so useful. Instead, we are better off plotting a summary table as described in detail the *Data Science Chapter*. Or, we can use the `length` function with `aggregate()` as introduced in the previous chapter:

```
aggregate(Total ~ Nutrients:Scenario, data=MyData, length)
```

```
##   Nutrients      Scenario Total
## 1      high       extreme    26
## 2      high fluctuations    24
## 3      high       gradual    25
## 4      high          high    23
## 5       low           low    25
```

OR we can use the handy `table()` function if we want to summarize the variables as rows and columns:

```
table(MyData$Scenario,MyData$Nutrients)
```

```
##
##               high low
##   extreme       26   0
##   fluctuations  24   0
##   gradual       25   0
##   high          23   0
##   low            0  25
```

In this case we can see that there is only one class of the “Low” *Nutrient* treatment, but four classes of “High” Nutrient treatments. In other words, all of the rows with “Low” Nutrient treatment also have the “Low” Scenario, and NONE of the rows with “High” Nutrient treatment have “Low” in the Scenario treatment. However, all groups have similar sample size of about 25. This is because the experiment compared low vs high nutrients, but also looked at different ways that high nutrients could be delivered.

4.4.5 Categorical by Continuous

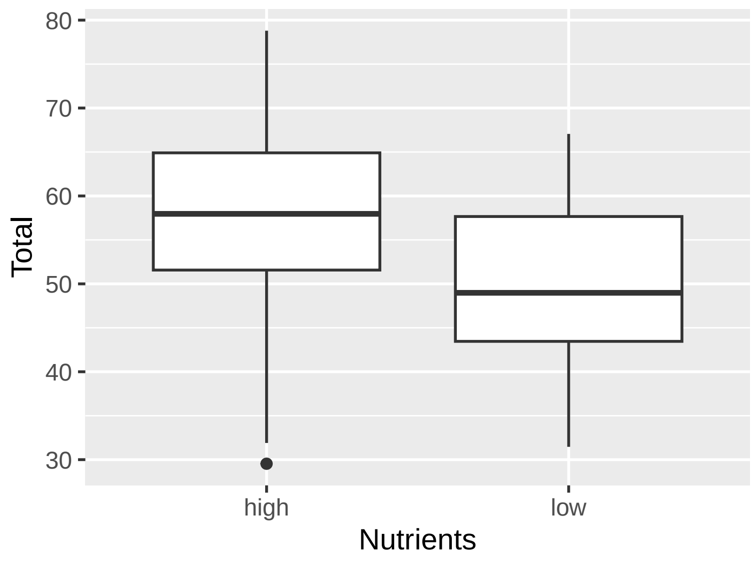
If we have a categorical and a continuous variable, we usually want to see the distribution of points for the two variables. There are a few ways to do this:

Categorical Scatter Plots

4.4.5.1 Box plot The box plot is a handy way to quickly inspect a few important characteristics of the data:

1. *median*: middle horizontal line (i.e. the 50th percentile)
2. *hinges*: top and bottom of the boxes showing the 75th and 25th percentiles, respectively
3. *whiskers*: vertical lines showing the highest and lowest values (excluding outliers, if present)
4. *outliers*: points showing outlier values more than 1.5 times the inter-quartile range (i.e. 1.5 times the distance from the 25th to 75th percentiles). Note that not all data sets will have outlier points.

```r
ggplot(aes(x=Nutrients, y=Total), data=MyData) + geom_boxplot()
```

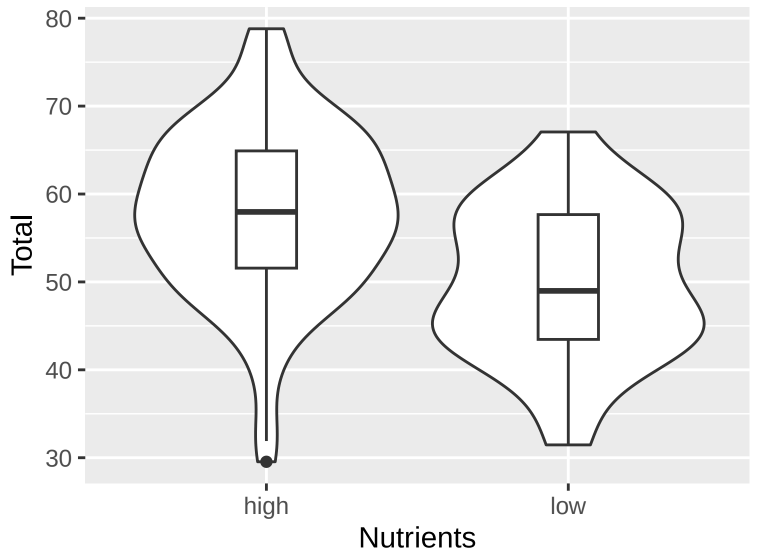


4.4.5.2 Violin plot

Violin plots or *Density strips* are another popular way to plot these type of data. The 'violin' or 'density' refers to the smoothed frequency distribution, which is similar the the `geom_histogram` we saw above, but imagine fitting a smoothed line along the top of each bar, and then turning it on its side and mirroring the image.

It can be very helpful to include both the violin and boxplot *geoms* on the same graph:

```r
ggplot(aes(x=Nutrients, y=Total), data=MyData) +
  geom_violin() + geom_boxplot(width=0.2)
```

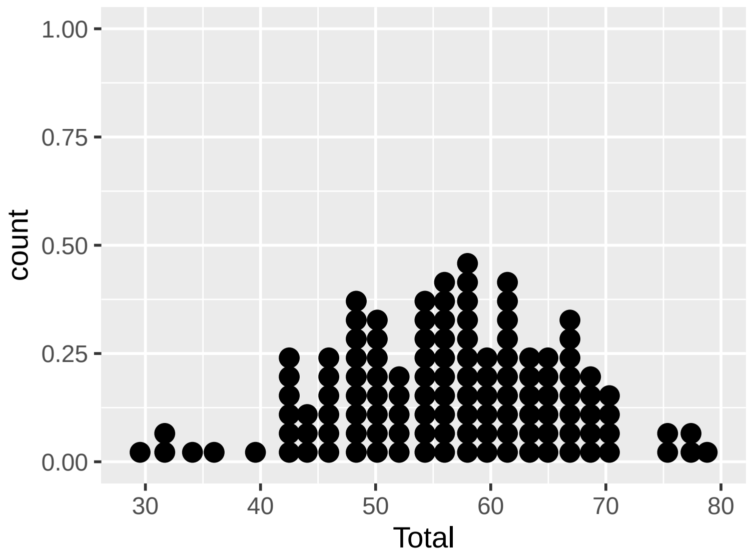


4.4.5.3 Dotplot The dotplot stacks points of similar value. It's particularly useful for smaller datasets where the smooting of the density function may be unreliable.

You can use dotplots for individual variables

```
ggplot(aes(x=Total), data=MyData) +
  geom_dotplot()
```

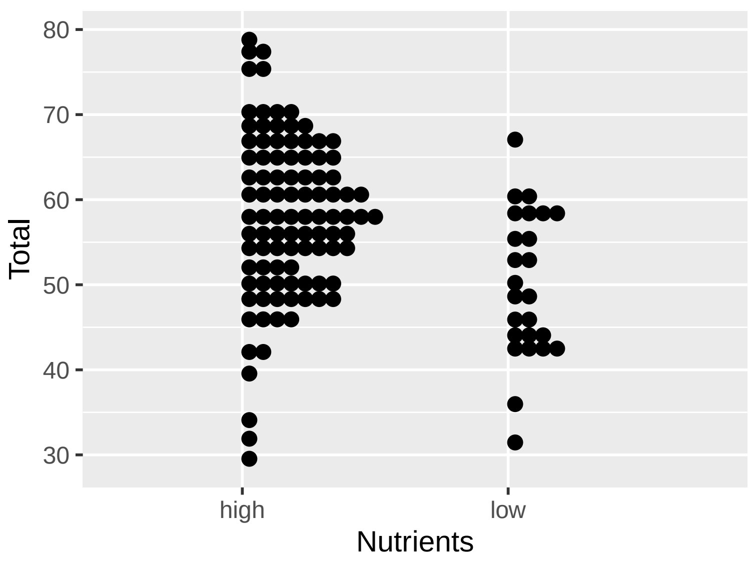
```
## Bin width defaults to 1/30 of the range of the data.
## Pick better value with `binwidth`.
```



Or for continuous x categorical (but note the parameters needed)

```
ggplot(aes(x=Nutrients, y=Total), data=MyData) +
  geom_dotplot(binaxis="y")
```

```
## Bin width defaults to 1/30 of the range of the data.
## Pick better value with `binwidth`.
```



4.4.6 Done!

That's it! That's all you need to start exploring your data! Load your data frame, and plot different combinations of variables to look at the distribution of values or the relationship between your variables.

Once you are comfortable producing these plots with different data types, you might start thinking about how to improve the appearance of your graphs. Once you understand these basic data types, you can explore how to customize and improve their appearance.

4.5 Basic Customization

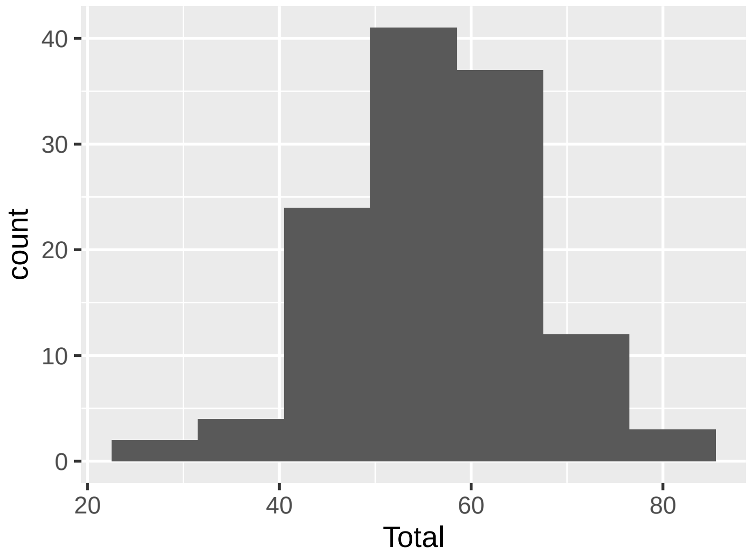
There are a number of parameters and other functions available with `ggplot()` that you can use to quickly customize your graphs. You may want to bookmark these and refer back to them when you work through the next chapter.

4.5.1 `binwidth`

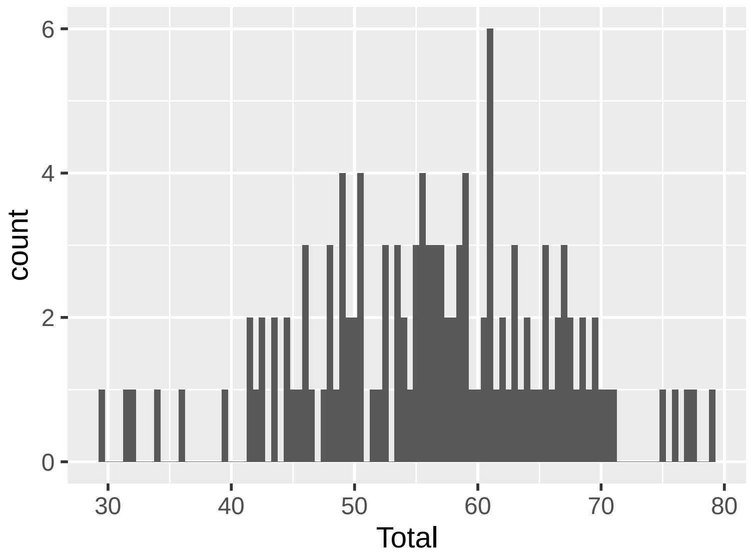
Use `binwidth` with the histogram graph type to alter the size of the 'bins' along the x-axis. A bin is defined by a range of values (x-axis). The bin count or frequency (y-axis) shows the number observations (or fraction) that fall within each bin range.

The `binwidth` defines the range of values (i.e. width) of each bin. Here are a couple of examples for comparison.

```
ggplot(aes(x=Total), data=MyData) + geom_histogram(binwidth=9)
```



```
ggplot(aes(x=Total), data=MyData) + geom_histogram(binwidth=0.5)
```



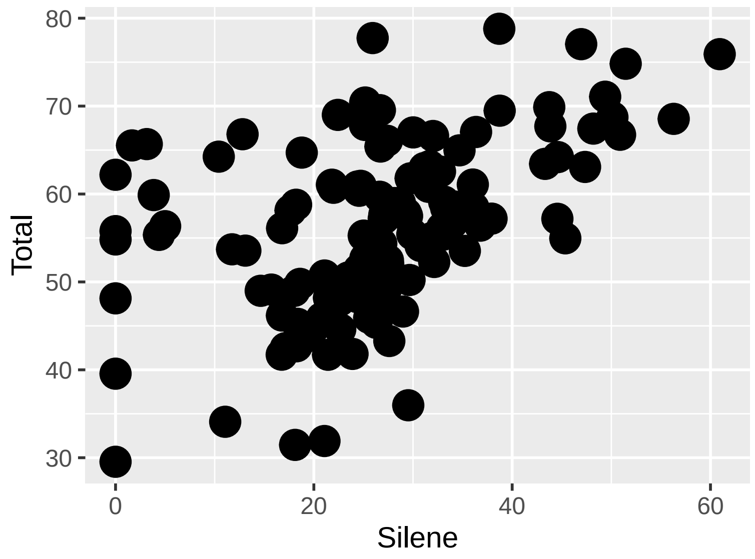
Note the difference in both the y-axis values and the width of the blocks along the x-axis.

4.5.2 `size`

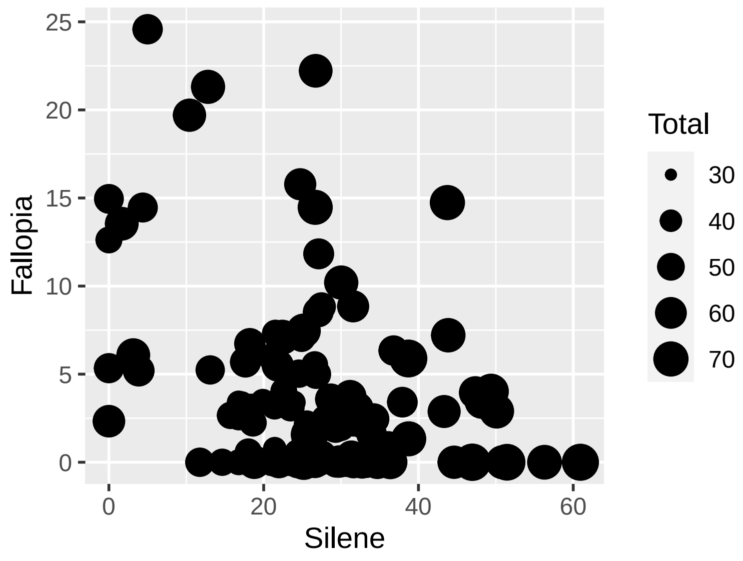
This controls the point size. Importantly, `size` values can be interpreted by R in two ways, which can cause some confusion:

1. As a **value**: To assign a specific size to all points. This is assigned in the `geom_point()` function
2. As a **vector**: Scale size based on a column of data (e.g. number of observations). This is defined in the `aes()` function.

```
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point(size=5)
```



```
ggplot(aes(x=Silene, y=Fallopia), data=MyData) +
  geom_point(aes(size=Total))
```



NOTE: The following code will produce the exact same graph.

```
ggplot(aes(x=Silene, y=Fallopia, size=Total), data=MyData) +
  geom_point()
```

Question: What do you think is the difference between putting an `aes` function inside of `ggplot()` vs inside of `geom_point()`?

Answer: It's important to understand the difference, even though in this specific example it doesn't change the graph:

1. If we put a variable in `aes()` inside of `ggplot()` then the parameter applies to ALL of the *geom* functions that follow it, but:
2. If we put a variable in `aes()` inside of a *geom* like `geom_point()`, then the parameter applies ONLY to that specific *geom*.

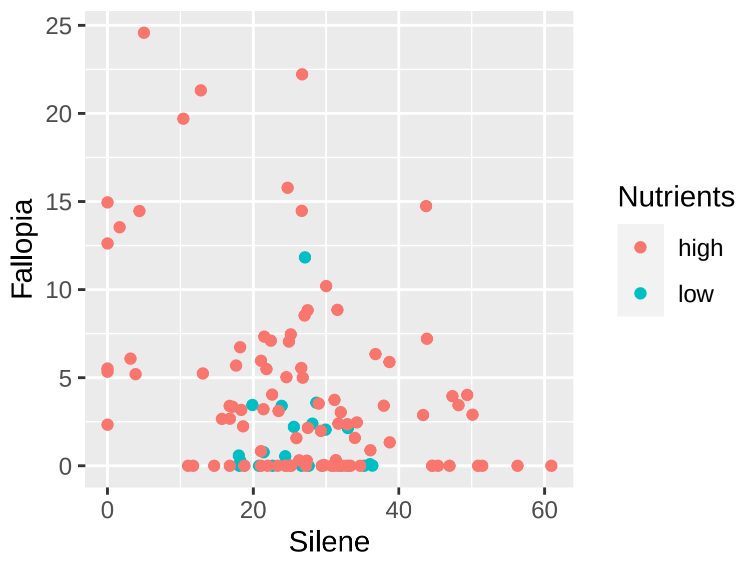
This becomes important in the next chapter, when we start to produce more complicated graphs with multiple, overlapping *geoms*.

4.5.3 `colour` (or `color`)

Another nice feature of `ggplot` is that you can use alternate English spelling for some of the parameters. For example, you can use *colour* or *color* add colour to your color graphs.

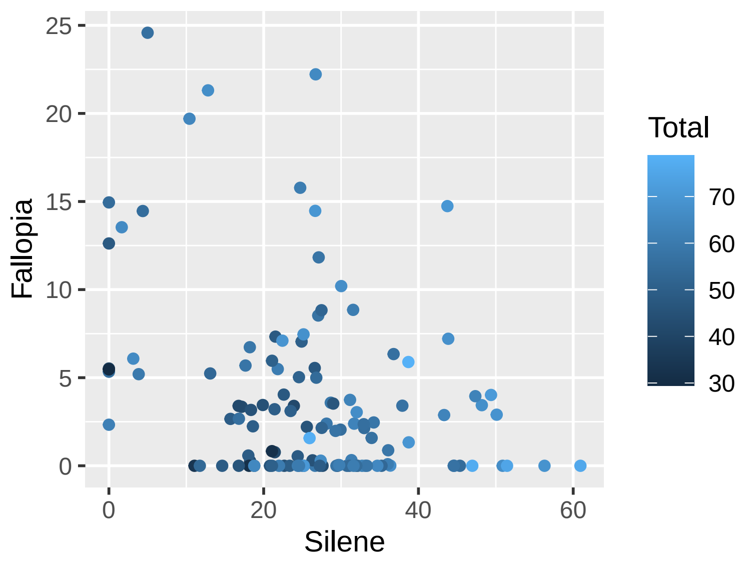
You can colour points based on a factor…

```
ggplot(aes(x=Silene, y=Fallopia), data=MyData) +
  geom_point(aes(colour=Nutrients))
```



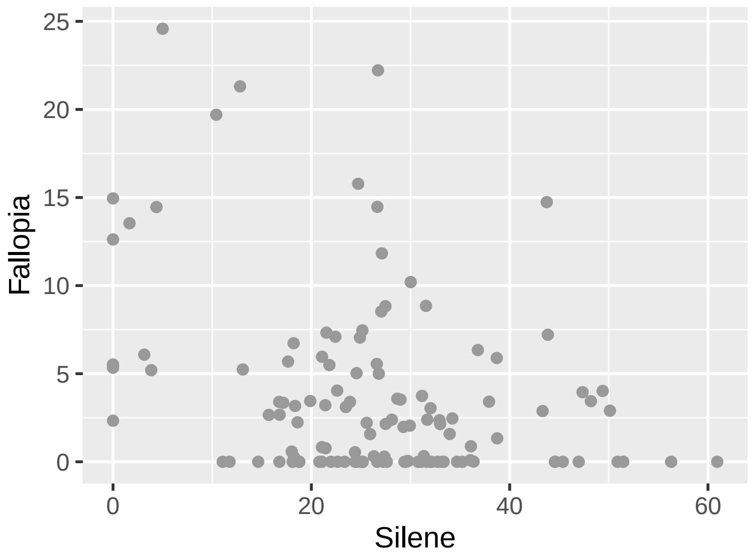
… or a continuous variable.

```
ggplot(aes(x=Silene, y=Fallopia), data=MyData) +
  geom_point(aes(colour=Total))
```



Or use a specific colour.

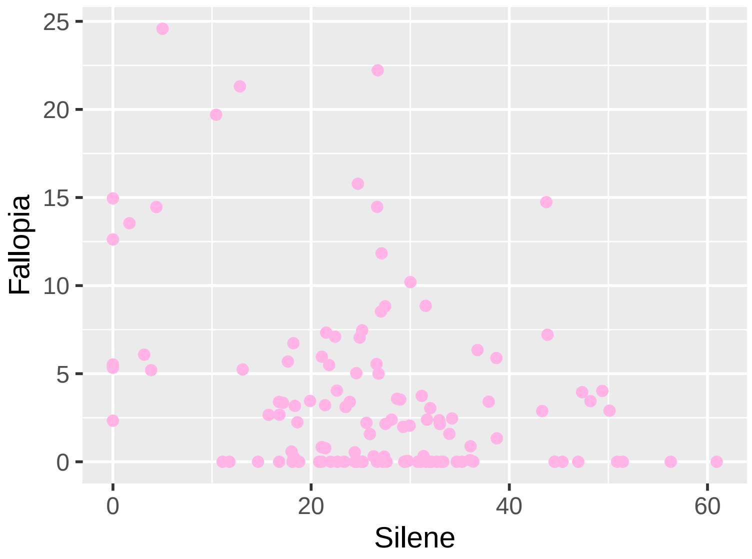
```
ggplot(aes(x=Silene, y=Fallopia), data=MyData) +
  geom_point(colour="grey60")
```



> **Protip**: Note that we only use the `aes()` function inside `geom_point()` or `ggplot()` functions if we are mapping columns of data.

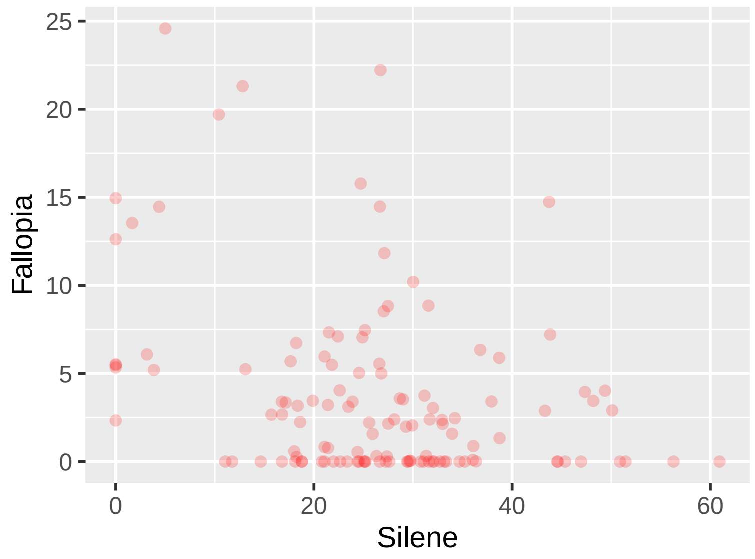
Several colours are available as strings (e.g. "red", "blue", "aquamarine", "coral", "grey20", "grey60"), but if you can't find one that you want, you can make just about any colour with the `rgb()` function. The `rgb` function takes three values corresponding to the intensity of red, green and blue light, respectively. Values range from 0 (no colour) to 1 (brightest intensity).

```
ggplot(aes(x=Silene, y=Fallopia), data=MyData) +
  geom_point(colour=rgb(1,0.7,0.9))
```



You can also add a 4th digit that defined **alpha** – an indication of opacity – also ranging from 0 (invisible) to 1 (completely opaque).

```
ggplot(aes(x=Silene, y=Fallopia), data=MyData) +
  geom_point(colour=rgb(1,0,0,0.2))
```



Some colouring systems use a 256-bit scale (0 to 255) instead of 0 to 1, which you can specify in the `rgb()` function with the `maxColorValue = 255` parameter. See `?rgb` for more information.

4.5.3.1 Hexadecimal Colour

Another common format for colour uses a **hexadecimal code**. In fact, the hexadecimal code is the output of the `rgb()` function that R uses for plotting:

```
rgb(0.1,0.3,1)
```

```
## [1] "#1A4DFF"
```

```
I(rgb(255,0,0, maxColorValue=255))
```

```
## [1] "#FF0000"
```

The **hexadecimal code** is a base-256 code that is common in computing. It uses the numerical digits 0-9 followed by the letters A (10) through F (15).

R uses a 6 OR 8-character **hexadecimal code**, starting with the hash mark **#** and usually in quotation marks.

The 6-character version uses two digits for each base colour: `#rrggbb`

> Note: 16 x 16 = 256 levels for each colour

The 8-digit code is similar, with the additional two digits at the end to define the level of alpha/transparency.

```
rgb(1,1,1,0.5)
```

```
## [1] "#FFFFFF80"
```

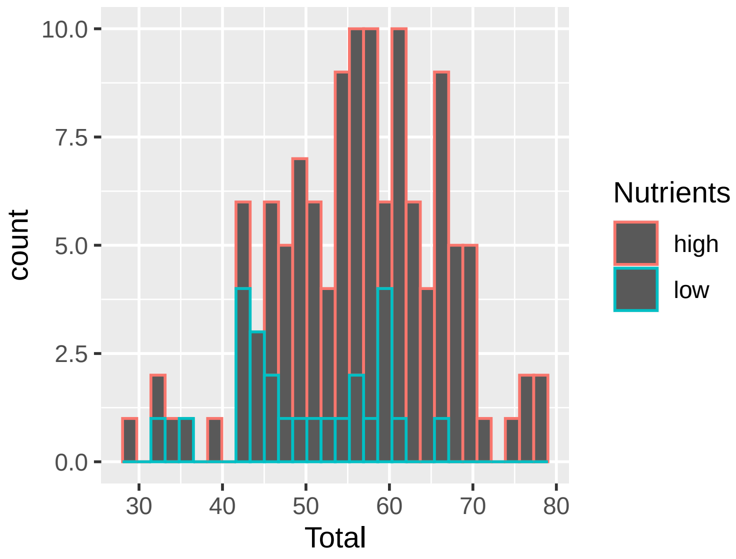
This can also be specified with the `alpha` parameter, below.

4.5.3.2 Histogram

Note what happens when we use the `colour` parameter for a histogram.

```
ggplot(aes(x=Total), data=MyData) +
  geom_histogram(aes(colour=Nutrients))
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



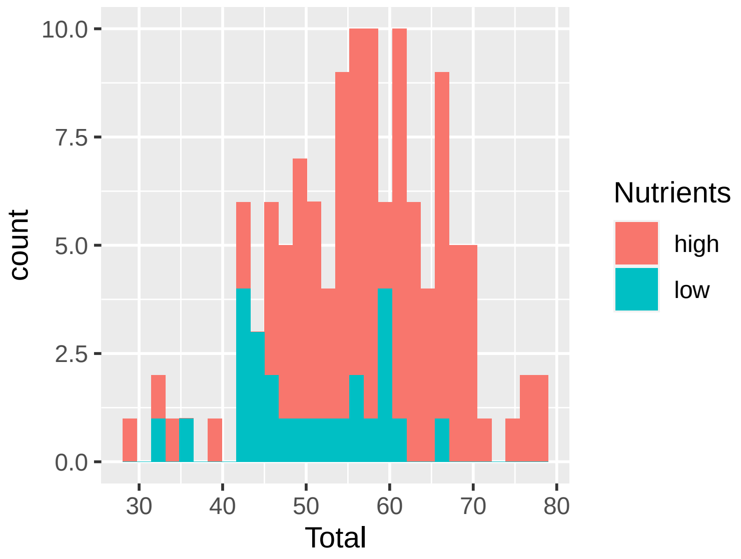
The coloured outlines might be useful but we usually will want the inside coloured.

4.5.4 `fill`

This parameter is used for boxes and other shapes that have a separate outline (`colour=`) and interior (`fill=`).

```
ggplot(aes(x=Total), data=MyData) +
  geom_histogram(aes(fill=Nutrients))
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```

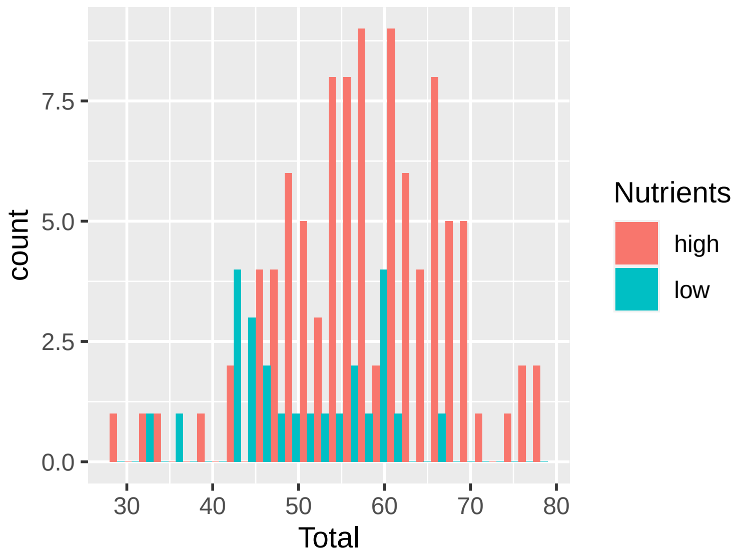


4.5.5 `position`

Use this to adjust the position, usually for histograms or bar graphs. For example, in the previous graph the bars are ‘stacked’ on top of each other. It can be hard to interpret a histogram with stacked bars, but we can shift the position using `dodge`.

```
ggplot(aes(x=Total), data=MyData) +
  geom_histogram(aes(fill=Nutrients), position="dodge")
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```

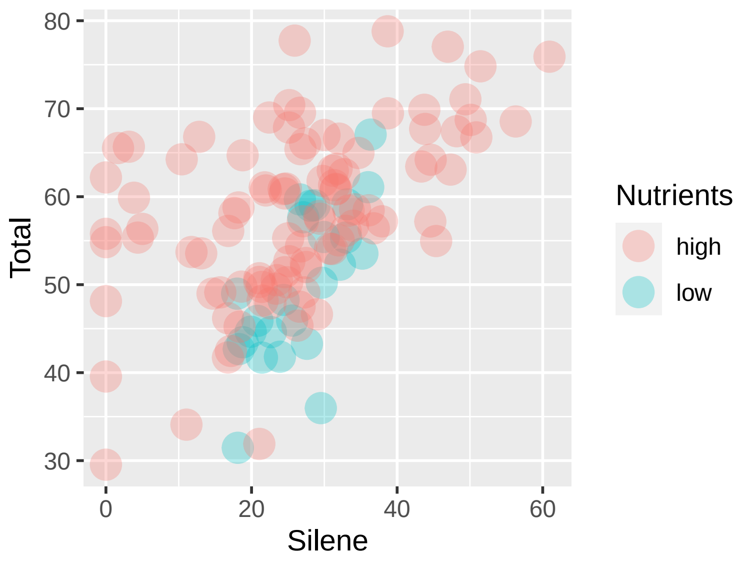


4.5.6 `alpha`

Think of `alpha` as a measure of opacity, ranging from 0 to 1 with 1 being the default – a solid point or line.

This is particularly useful for visualizing overlapping points.

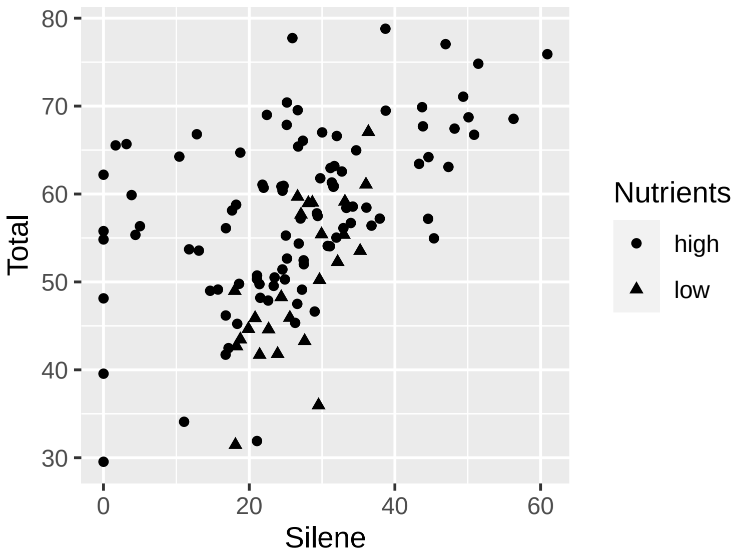
```
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point(aes(colour=Nutrients), size=5, alpha=0.3)
```



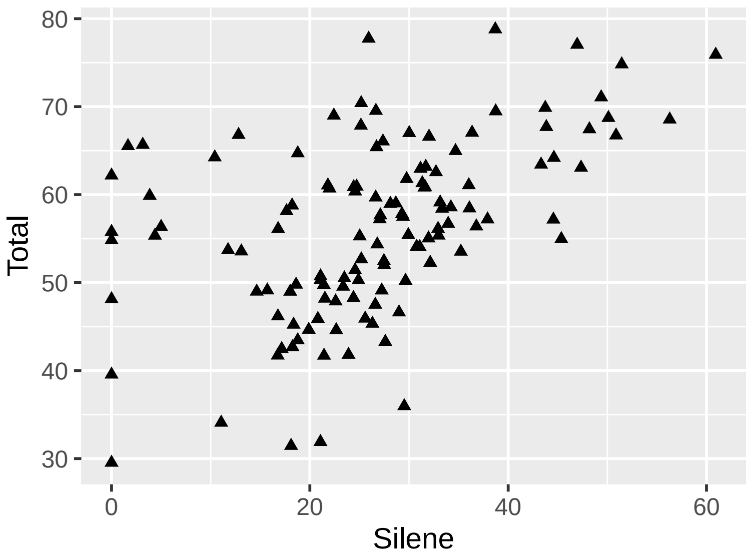
4.5.7 `shape`

You can also change the shape of your points, again using a column of data or a specific value.

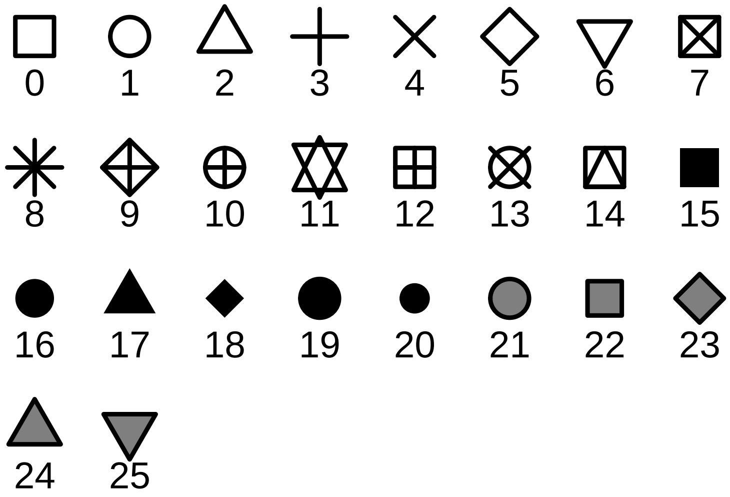
```
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point(aes(shape=Nutrients))
```



```
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point(shape=17)
```



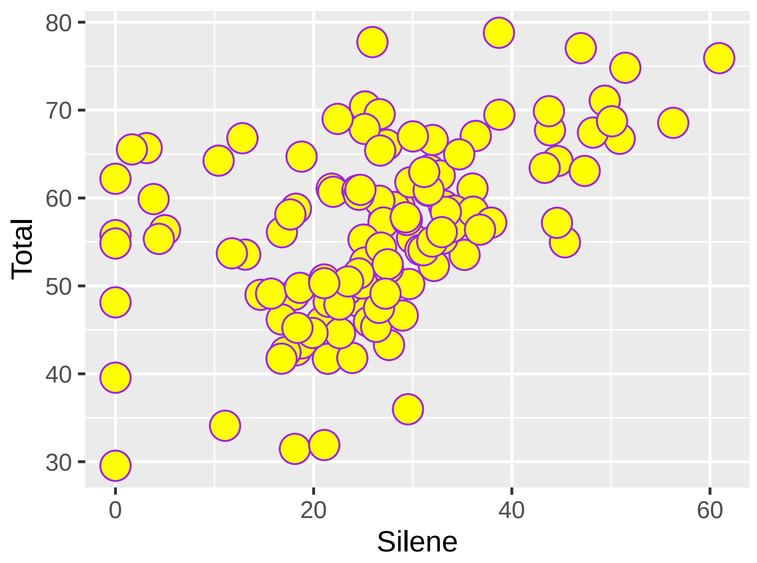
There are a number of different shapes available, by specifying a number from 0 through 25.



Note that the shapes with grey in the above figure can be coloured with `fill=` parameter, while all of the black parts (lines and fill) can be coloured with the `colour=` parameter.

You can use `fill` and `colour` to customize these separately.

```
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point(shape=21, size=5, colour="purple", fill="yellow")
```

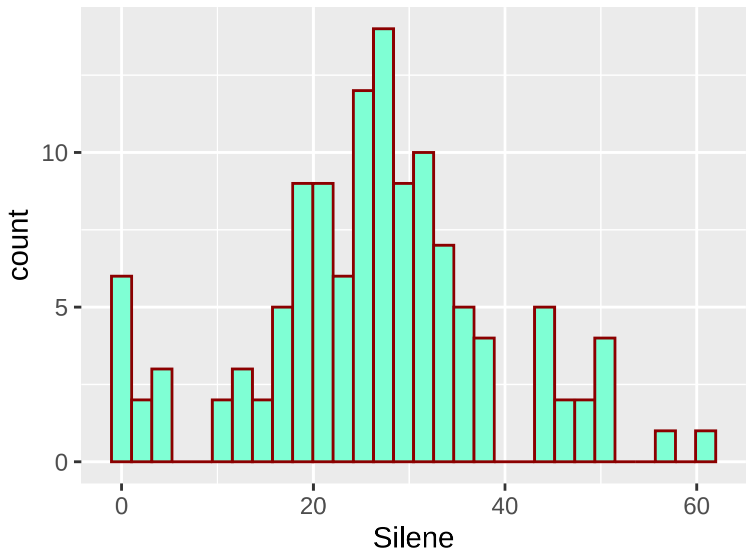


Note how a solid outline can help your points 'pop'.

Similarly, specifying a solid `colour` can also help to add a 'pop' to your histogram graphs

```r
ggplot(aes(x=Silene), data=MyData) +
  geom_histogram(colour="darkred",fill="aquamarine")
```

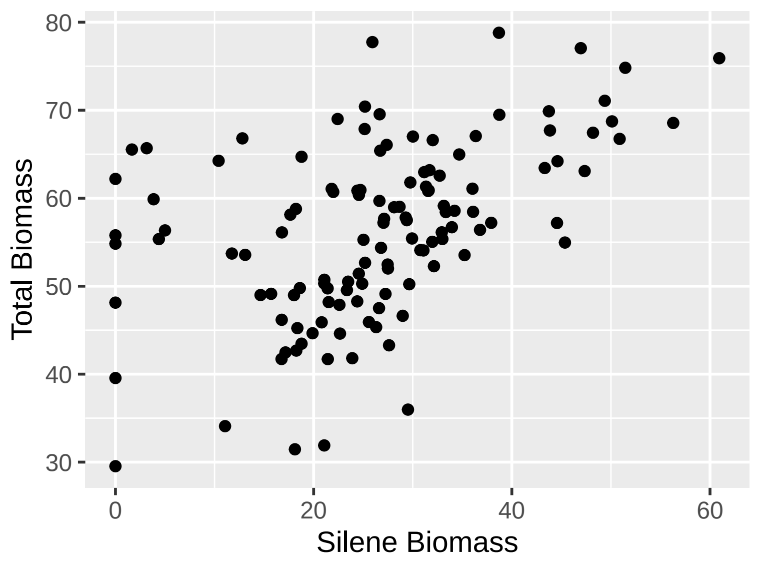
```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



4.5.8 `lab`, `xlab`, and `ylab`

Use these to customize your axis labels.

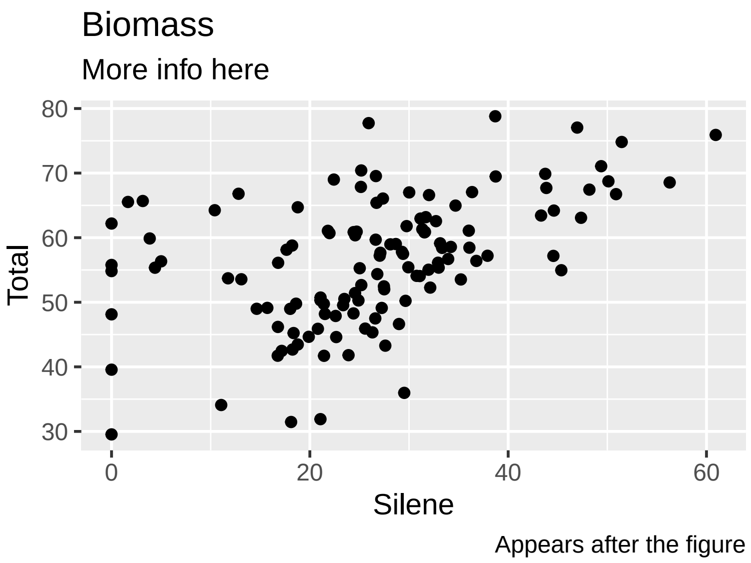
```
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point() +
  xlab("Silene Biomass") + ylab("Total Biomass")
```



4.5.9 `labs`

This will add other labels to your plot. Usually you wouldn't use this for a figure intended for publication – for this you would need a detailed caption, usually just a paragraph of text below the figure. However, these be useful for other things: reports, websites, presentations, supplementary material, appendices, etc.

```r
ggplot(aes(x=Silene, y=Total), data=MyData) +
  geom_point() + labs(title="Biomass", subtitle="More info here",
                      caption="Appears after the figure")
```



4.6 Themes and Geoms

We have already seen explored a few of the many **Geoms** available. These determine the *geometry* of your graph, which is how your data are mathematically mapped to the graphing space.

Themes define the look and 'feel' of your graphs.

In `ggplot()`, themes and geoms are added with a separate function linked to the graph by using the plus sign `+`.

4.6.1 `geom_<name>()`

We explored a few *geoms* above, but there are many more available on the `ggplot2` website, with examples:

https://ggplot2.tidyverse.org/reference/

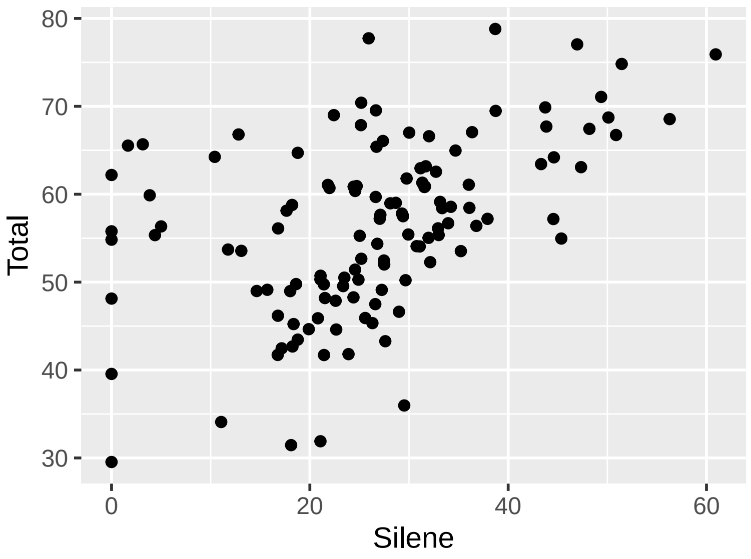
4.6.2 `+ theme_<name>()`

There are a number of available themes, defined by changing the part of `theme_<name>()`.

We are going to explore these diffent themes on the same graph, so rather than type out the same `ggplot` and `geom` functions every time, we can define an object to hold the data for the plot, and then just change the theme.

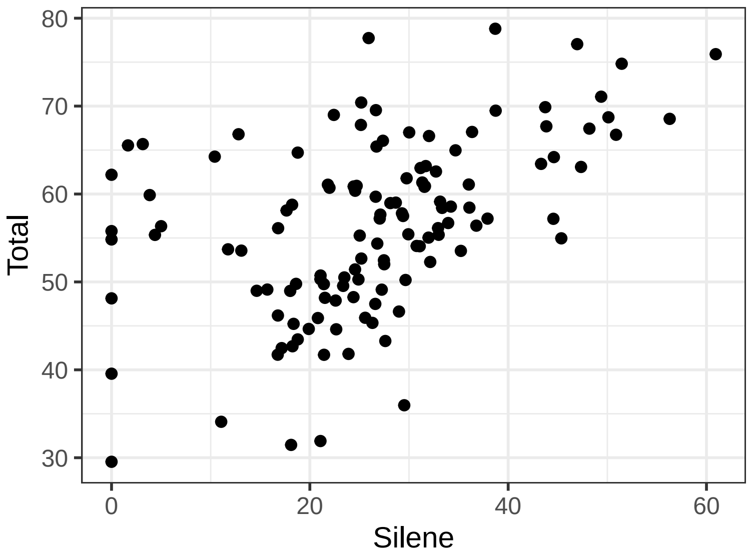
Default theme:

```
Plot1<-ggplot(aes(x=Silene, y=Total), data=MyData) + geom_point()
Plot1 + theme_grey()
```



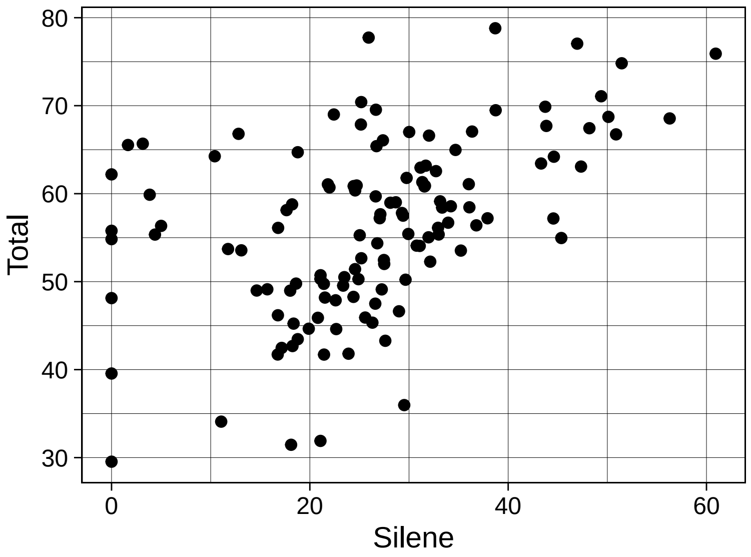
A cleaner theme with better contrast:

```
Plot1 + theme_bw()
```



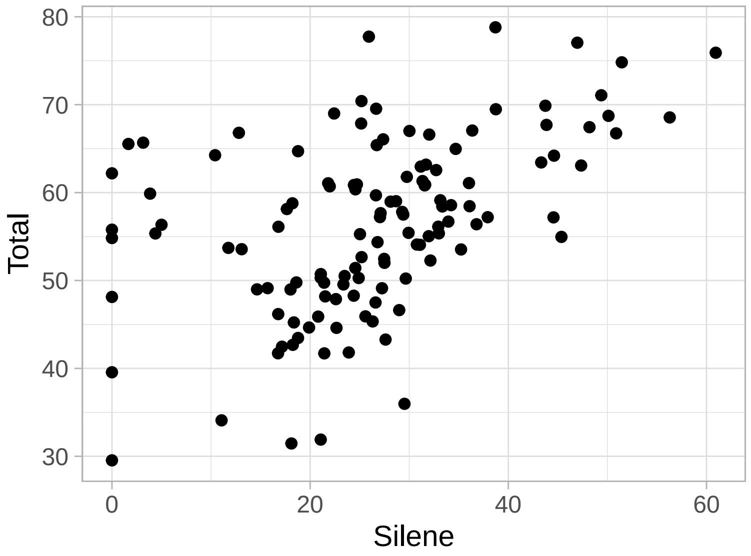
Thicker grid lines:

```
Plot1 + theme_linedraw()
```



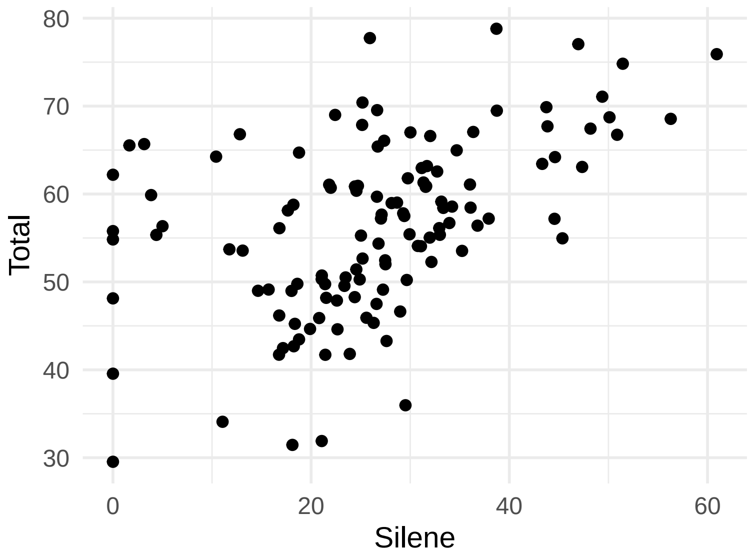
Fainter border and axis values

```
Plot1 + theme_light()
```



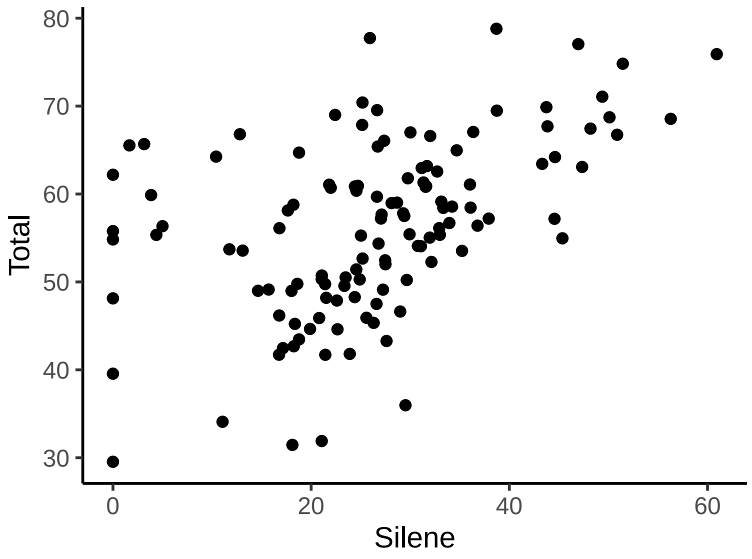
No borders at all

```
Plot1 + theme_minimal()
```



A minimal theme, closest to what you would see in a published paper, with x- and y-axis lines only

```
Plot1 + theme_classic()
```



These can be further customized. Or you can create a completely new theme.

4.6.3 Custom Theme

Here is a simplified and cleaner version of `theme_classic` but with bigger axis labels that are more suitable for figures in presentation or publication. The theme is a function, which can be customized. Custom functions are covered in the Advanced R Chapter. For now you can just copy the code block below.

```
# Clean theme for presentations & publications used in the Colautti Lab
theme_pub <- function (base_size = 12, base_family = "") {
  theme_classic(base_size = base_size, base_family = base_family) %+replace%
    theme(
      axis.text = element_text(colour = "black"),
      axis.title.x = element_text(size=18),
      axis.text.x = element_text(size=12),
      axis.title.y = element_text(size=18,angle=90),
      axis.text.y = element_text(size=12),
      axis.ticks = element_blank(),
      panel.background = element_rect(fill="white"),
      panel.border = element_blank(),
      plot.title=element_text(face="bold", size=24),
      legend.position="none"
    )
}
```

To use this theme, you have to make sure you run the entire function (e.g. highlight and press `Ctl + R`).

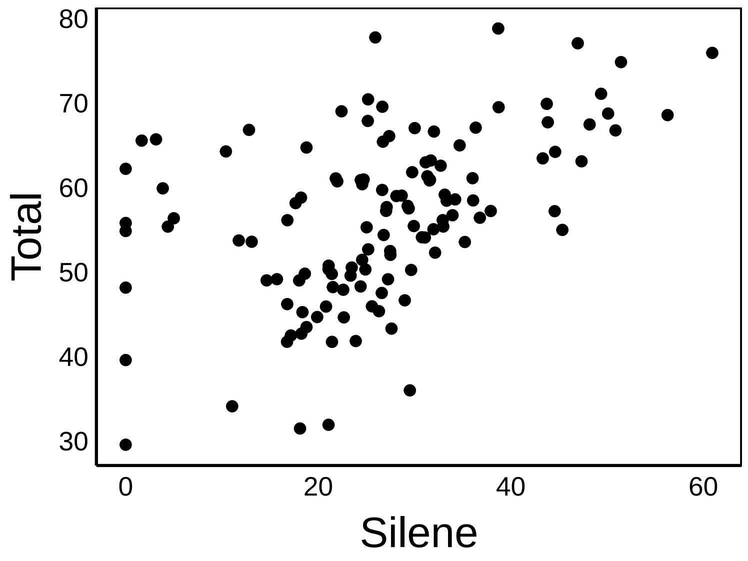
Alternatively, you could save it as a separate `.R` file and then load it with the `source()` function.

A third, even easier option, is to load the version of this code that is available online.

```
source("http://bit.ly/theme_pub")
```

The theme is called `theme_pub` (pub is short for publication). To use it, run the above line, and then add it to your graphing functions:

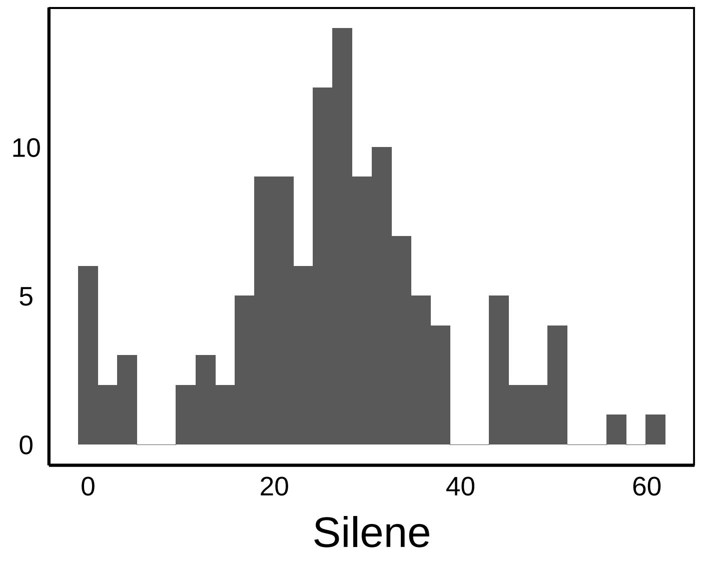
```
Plot1 + theme_pub()
```



```
qplot(x=Silene,data=MyData) + theme_pub()
```

```
## Warning: `qplot()` was deprecated in ggplot2 3.4.0.
```

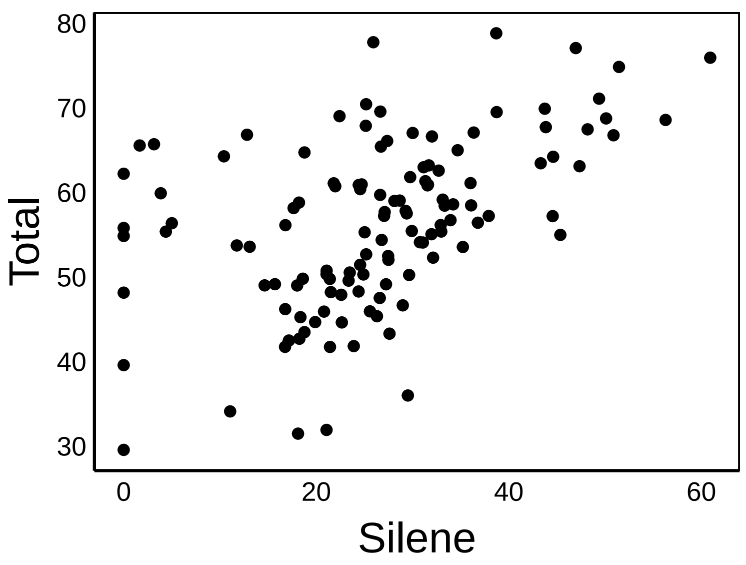
```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



4.6.4 `theme_set`

If you want to use the same theme throughout your code, you can use the `theme_set` function.

```
theme_set(theme_pub())
Plot1
```



Now that we have run the `source` and `theme_set` functions, all of the graphs we make in this session will use the improved formatting. No more ugly grey background and tiny axis labels!

4.7 Multiple graphs

It is often handy to plot separate graphs for different categories of a grouping variable. This can be done with `facets` in `qplot`.

4.7.1 `facets`

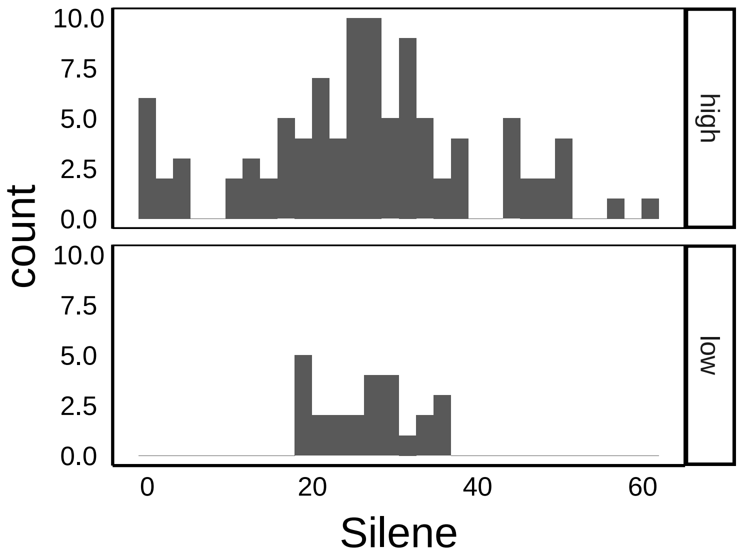
Facets have the general form `VERTICAL ~ HORIZONTAL`. Use the period `.` to indicate 'all data' or 'do not separate my data'.

Vertical stacking

```
Plot2<-ggplot(aes(x=Silene),data=MyData) +
  geom_histogram()

Plot2 + facet_grid(Nutrients~.)
```

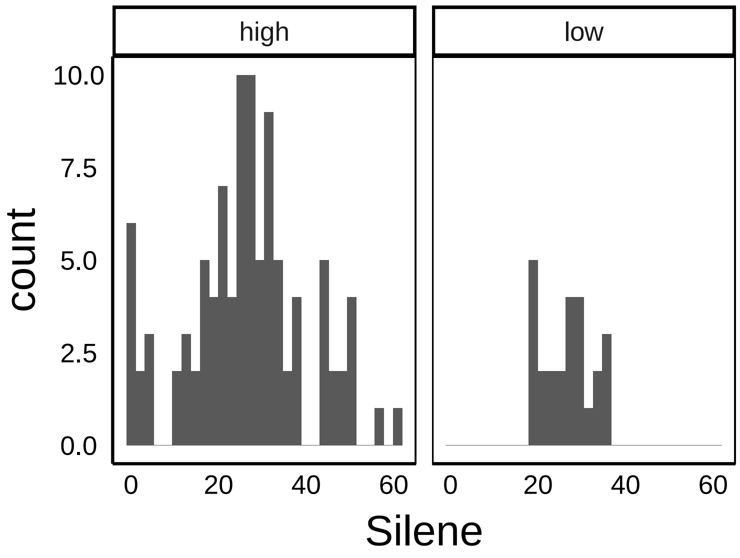
```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



Horizontal stacking

```
Plot2 + facet_wrap(.~Nutrients)
```

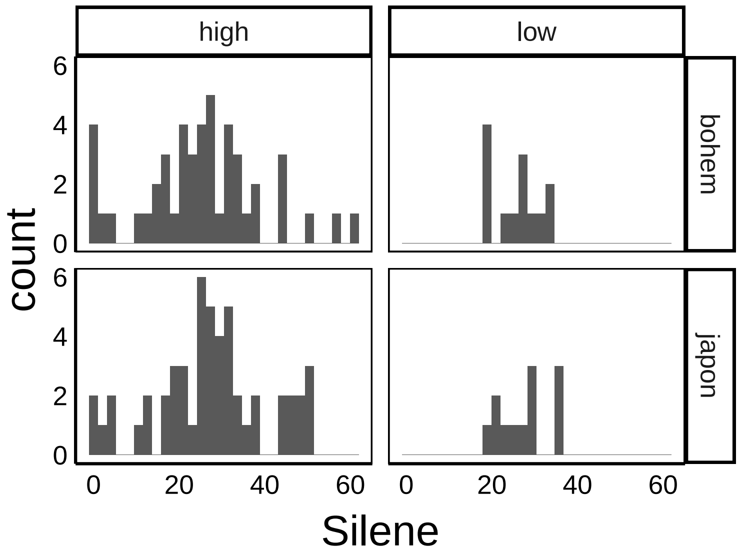
```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



Horizontal by Vertical

```
Plot2 + facet_grid(Taxon~Nutrients)
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



4.8 Graph output

Graphing in R studio is okay for exploration but eventually you are going to want to save those beautiful figures you made, and this can be part of a reproducible workflow.

Writing code in R to save your graphs to an external file requires three important steps:

1. Open a file using a function like `pdf` or `svg` for the **vector** format, or `png` for the **raster** format. Remember that you usually will want to stick with a vector format.
2. Run the code to produce the graph. Instead of seeing a graph in your R interface, you will not see anything because the graph is being sent to the file.
3. **IMPORTANT**: Close the file! Do this with the `dev.off()` function.

Failing to close the file is a common source of error when saving graphs. If you are having problems with graphing outputs, try running the `dev.off()` function a few times to make sure you close any files that are 'hanging' open.

Here's an example code for making a `pdf` output of a graph. When you run it you should see a file appear in your working folder (you may have to refresh).

```
pdf("SileneHist.pdf") # 1. Open
  Plot2 + facet_grid(Taxon~Nutrients) # 2. Write
dev.off() # 3. Close
```

Note how the plotting command on the second line does not open in the plots window when you run this. This is because the info is sent to *SileneHist.pdf* file instead of the graphing area in your R console (e.g. *plots* tab in R Studio)

4.9 Practice

Graphing may seem slow and tedious at first, but the more you practice, the faster you will be able to produce meaningful visualizations.

Don't be afraid to try new things. Try mixing up components and see what happens. At worst you will just get an error message.

Once you have a good understanding of these basics, you can see how to build more advanced plots with `ggplot()`.

5 Advanced Visualizations

5.1 Overview

Before continuing with this tutorial/chapter, you should be familiar with the qplot() tutorial/chapter, and you should have lots of practice making graphs with different formatting options using `qplot`.

In this self-tutorial, we look at some more advanced options for visualizations by using the `ggplot` function. If you have a good feel for `plot`, then this will be an easy transition, with `ggplot` adding even more flexibility to our visualizations. This includes everything you will need to make professional-grade figures.

The ggplot 'cheat sheet' is a downloadable pdf that provides a good summary and quick-reference guide for advanced graphics. Other useful cheat sheets are available here: https://www.rstudio.com/resources/cheatsheets/

5.2 Getting Started

First, we'll load the `ggplot2` library and set a custom theme as described in the `qplot` Tutorial

```
library(ggplot2)
source("http://bit.ly/theme_pub")
theme_set(theme_pub())
```

The `source` function loads an external file, in this case from the internet. The file is just a script saved as .R file with a custom function defining different aspects of the graph (e.g. text size, line width, etc.) You can open the link in a web browser or download and open in a text editor to see the script

The `theme_set()` command sets our custom theme (`theme_pub`) as the default plotting theme. Since the theme is a function in R, we need to include the brackets, even though there is nothing needed inside the function: `theme_pub()`

5.3 Rules of thumb

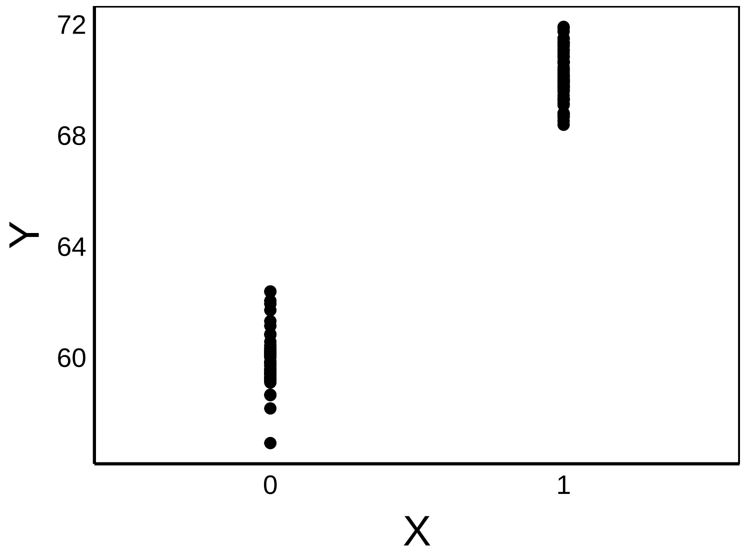
Before we dig into the code, it's worth reviewing some more general graphical concepts. Standards of practice for published graphs in professional journals can vary depending on format (e.g. print vs online), audience, and historical precedent. Nevertheless, there are a number of useful 'rules of thumb' to keep in mind. These are not hard and fast rules but helpful for new researchers who aren't sure how or where to start. In making decisions, always think of your audience and remember that the main goal is to communicate information as clearly and efficientl as possible.

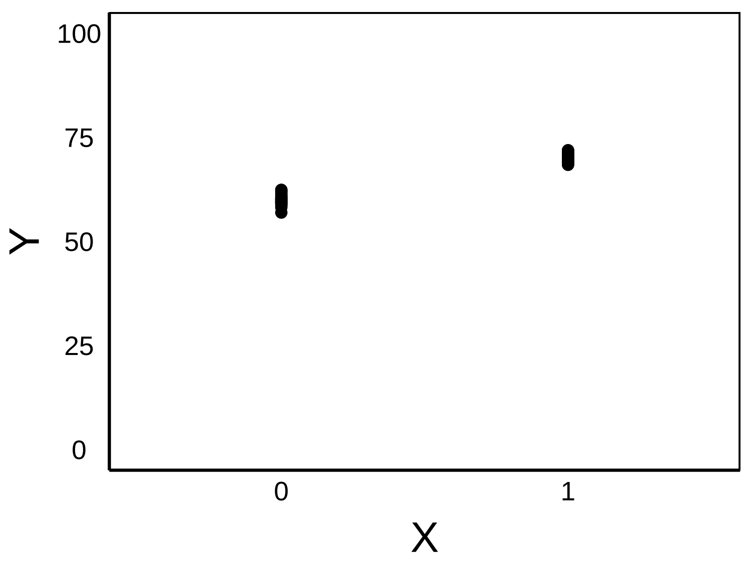
1. Minimize 'ink'

In the old days, when most papers were actually printed and mailed to journal subscribers, black ink was expensive and printing in colour was very expensive. Printing is still expensive but of course most research articles are available online where there is no additional cost to colour or extra ink. However, the concept of minimizing ink (or pixels) can go a long way toward keeping a graph free from clutter and unnecessary distraction.

2. Use space wisely

Empty space is not necessarily bad, but ask yourself if it is necessary and what you want the reader to take away. Consider the next two graphs:





In the first example, the Y-axis is scaled to the data. In the second case, Y-axis scaled between 0 and 100.

What are the benefits/drawbacks of scaling the axes? When might you choose to use one over the other?

3. Choose a colour palette

Colour has three basic components

a. **Hue** – the relative proportion of red vs green vs blue light
b. **Saturation** – how vivid the colour is
c. **Brightness** – the amount of white (vs black) in the colour

The abbreviation HSB is often used, or HSL (L = 'Lightness') or HSV (V = 'Value').

In R these can be easily defined with the `rgb()` function. For example:

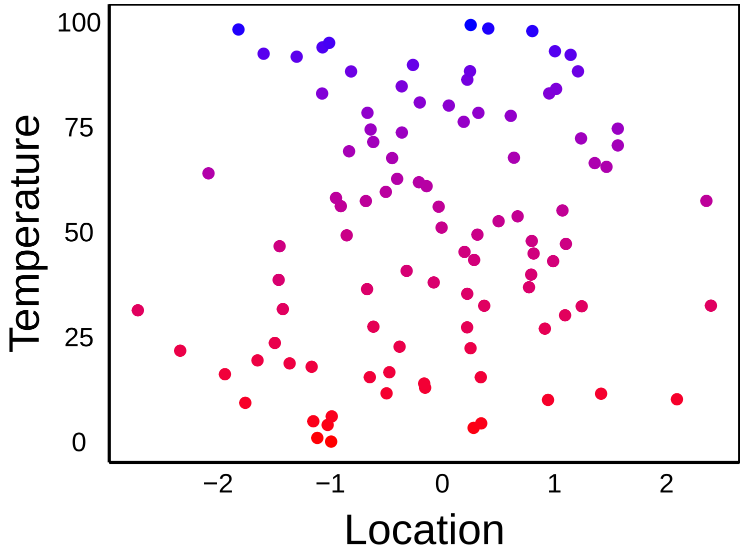
- `rgb(1,0,0)` – a saturated red
- `rgb(0.1,0,0)` – a dark red (low brightness, low saturation)
- `rgb(1,0.9,0.9)` – a light red (high brightness, low saturation)

Don't underestimate the impact of choosing a good colour palette, especially for presentations. Colour theory can get a bit overwhelming but here are a few good websites to help:

- Quickly generate your own palette using Coolors: https://coolors.co
- Use a colour wheel to find complementary colours using Adobe : https://color.adobe.com/create

4. Colours have meaning

What's wrong with this graph?

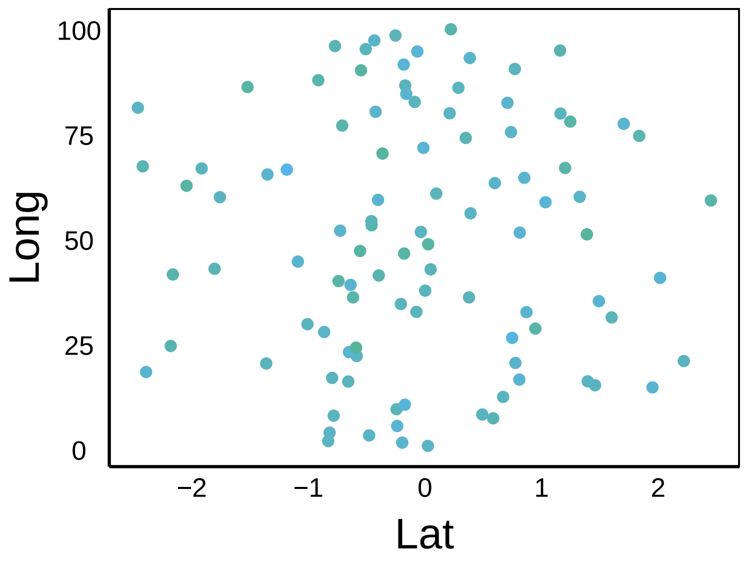


Technically, there is nothing wrong. But we naturally associate colours with particular feelings. In this case, intuitively we associate red with hot and blue with cold, which is the opposite of what is shown in this graph. Be mindful of these associations when choosing a colour palette

Another important consideration is that not everyone sees colour the same way. About 5% to 10% of the population has colour blindness. In order to make colour graphs readable to everyone, you should make sure to use colours that can still be interpreted when printed in greyscale.

5. Maximize contrast

Colours that are too similar will be hard to distinguish



Can you see the gradient of colours?

6. Keep relevant information

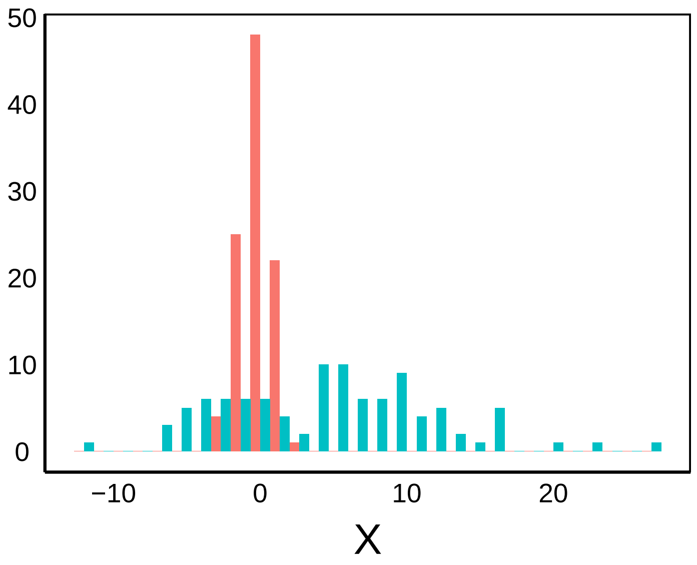
Make sure to include proper axis **labels** (i.e. names) and **tick marks** (i.e. numbers or categories showing the different values). These labels, along with the figure caption, should act as a stand-alone unit. The reader should be able to understand the figure without having to read through the rest of the paper.

7. Choose the right graph

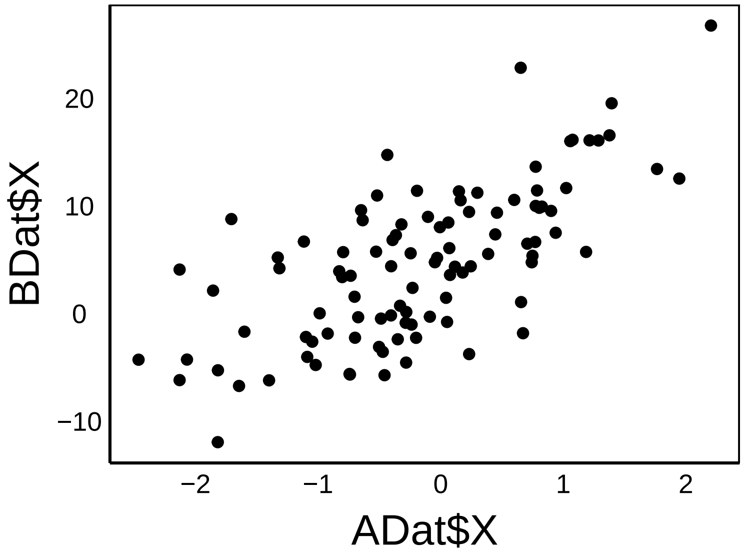
Often the same data can be presented in different ways but some are easier to interpret than others. Think carefully about the story you want to present and the main ideas you want your reader to get from your figures. Look at these two graphs that show the same data.

```r
ADat<-data.frame(X=rnorm(100), Trait="A")
BDat<-data.frame(X=5 + rnorm(100) *5 + ADat$X * 5, Trait="B")
PDat<-rbind(ADat,BDat)
qplot(X, fill=Trait, posit="dodge", data=PDat)
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



```
qplot(ADat$X, BDat$X)
```



The first graph tells a story about the distributions – the mean and variance of each trait. The second graph tells a story about the correlated relationship between trait A and trait B. One is not necessarily better than the other. It depends on the story you want to tell.

5.4 Example

Now that we have gone over some basic graphing concepts, let's look at how to build a professional-grade figure. In fact, we'll reconstruct a figure published in a paper by Colautti & Lau in the journal Molecular Ecology (2015).

5.4.1 Setup

5.4.1.1 Import data Download selection dataset from Colautti & Lau (2015), published in the journal **Molecular Ecology**: https://doi.org/10.1111/mec.13162

The paper is a meta-analysis and review of evolution occurring during biological invasions. We will recreate Figure 2, which shows the result of a meta-analysis of selection gradients (β) and selection differentials (s). First, we'll just recreate the top panel, and then we'll look at ways to make more advanced multi-panel graphs like this.

The data from the paper are archived on Dryad: https://datadryad.org/stash/dataset/doi:10.5061/dryad.gt678

You could download the zip file and look for the file called `Selection_Data.csv` and save it to your working directory.

Or you can just download directly from this website:

```
SelData<-read.csv(
  "https://colauttilab.github.io/RCrashCourse/Selection_Data.csv")
```

We are also going to change the names from the file to make them a bit more intuitive and easier to work with in R.

```
names(SelData)<-c("Collector", "Author", "Year", "Journal",
                  "Vol", "Species", "Native", "N",
                  "Fitness.measure", "Trait", "s",
                  "s.SE", "s.P", "B", "B.SE", "B.P")
```

5.4.2 Inspect

Let's take a quick look at the data

```
head(SelData)
```

```
##           Collector               Author Year           Journal
## 1 KingsolverDiamond Alatalo and Lundberg 1986          Evolution
## 2 KingsolverDiamond Alatalo and Lundberg 1986          Evolution
## 3 KingsolverDiamond Alatalo and Lundberg 1986          Evolution
## 4 KingsolverDiamond       Alatalo et al. 1990 American Naturalist
## 5 KingsolverDiamond       Alatalo et al. 1990 American Naturalist
## 6 KingsolverDiamond       Alatalo et al. 1990 American Naturalist
##              Vol             Species Native    N       Fitness.measure
## 1     40:574-583  Ficedula hypoleuca    yes  641   male mating success
## 2     40:574-583  Ficedula hypoleuca    yes  713 female mating success
## 3     40:574-583  Ficedula hypoleuca    yes 1705              survival
## 4 135(3):464-471 Ficedula albicollis    yes <NA>              survival
## 5 135(3):464-471 Ficedula albicollis    yes <NA>              survival
## 6 135(3):464-471 Ficedula albicollis    yes <NA>              survival
##           Trait     s s.SE s.P     B B.SE B.P
## 1 tarsus length -0.01       ns    NA
## 2 tarsus length  0.01      sig    NA
## 3 tarsus length  0.04       ns    NA
## 4  tarus length  0.02       ns -0.06
## 5  tarus length  0.08       ns -0.01
## 6  tarus length  0.19      sig  0.01
```

It's worth taking some time to look at this to understand how a meta-analysis works. The **collector** column indicates the paper that the data came from. The **Author** indicates the author(s) of the original paper that reported the data. The **Year**, **Journal**, and **Vol** give information about the publication that the data came from originally.

We can see above the collector `KingsolverDiamond`, which represents a paper from Kingsolver and Diamond that was itself a meta-analysis of natural selection. Most of the studies came from this meta-analysis, but a few of the more recent papers were added by grad students, denoted by initials:

```
unique(SelData$Collector)
```

```
## [1] "KingsolverDiamond" "JAL"               "DJW"
## [4] "CPT"
```

Species is the study species, and **Native** is its status as a binary yes/no variable. **N** is the sample size and **Fitness.measure** is the specific trait that defines fitness. **Trait** is the trait on which selection was measured. Finally, s is the **selection differential** and β is the **selection gradient**. Note that these are slopes in units of relative fitness per trait standard deviation. This is explained in more detail below.

5.4.3 Absolute Value

In this analysis, we are interested in the magnitude but not the direction of natural selection. In other words we would want to treat a slope of -4 the same as a slope of +4 because they have the same magnitude. Therefore, we can replace the s column with $|s|$

```
SelData$s<-abs(SelData$s)
```

We'll also add a couple of columns with random variables that we can use later to explore additional plotting options.

First, a column of values sampled from a z-distribution – this is a Gaussian (a.k.a. 'normal') distribution with mean = 0 and sd = 1.

```
SelData$Rpoint<-rnorm(nrow(SelData))
```

Second, a columnn of 1 and 0 sampled randomly with equal frequency ($p = 0.5$)

```
SelData$Rgroup<-sample(c(0,1), nrow(SelData), replace=T)
```

5.4.4 Missing values

Check for missing data (denoted NA)

```
print(SelData$s)
```

We can subset to remove missing data

```
SelData<-SelData[!is.na(SelData$s),]
```

Recall from the R Fundamentals Tutorial that `!` means 'not' or 'invert'

There is also has a convenient `drop_na` function in the `tidyr` package

```
library(tidyr)
SelData<-SelData %>%
  drop_na(s)
```

5.5 Measuring Selection

5.5.1 Don't Panic!

We're going to get a bit technical here. Don't worry if you don't completely understand all of the stuff below about measuring selection. Keep it for reference in case you decide you want to use it for your own research. For now, just try to understand it as well as you can and focus on the code used to producing the figures.

A simple analysis of phenotypic selection was proposed by Lande & Arnold (1983) and provides a simple but powerful tool for measuring natural selection. It is just a linear model with **relative fitness** on the y-axis and the **standardized trait value** on the x-axis.

5.5.2 Relative Fitness

Fitness can be measured in many ways, such as survival or lifetime seed or egg production. Check out the list of specific fitness measures used in these studies:

```
unique(SelData$Fitness.measure)
```

Absolute fitness is just the observed value (e.g. seed set or survival yes/no). **Relative fitness** is just the *absolute* fitness divided by the mean. **Absolute fitness** is usually denoted by the capital letter W and **relative fitness** is usually represented by a lower-case w or omega ω. Expressing this in mathematical terms:

$$\omega = W_i/\bar{W}$$

5.5.3 Trait Value

A **Trait Value** is literally just the measured trait. Use `unique(SelData$Trait)` to see the list of specific traits that were measured in these studies. The **Standardized Trait Value** is the traits z-score. See the Distributions Tutorial for more information about z-scores. To calculate the z-score, we take each value, subtract the mean, and then divide by the standard deviation.

$$\frac{x_i - \bar{X}}{s}$$

Since traits have different metrics, they are hard to compare: e.g. days to flower, egg biomass, foraging intensity, aggression. But standardizing traits to z-scores puts them all on the same scale for comparison. Specifically, the scale is in standard deviations from the mean.

5.5.4 s vs β

Selection differentials (s) and selection gradients (β) measure selection using linear models but represent slightly different measurements. Linear models are covered in the Linear Models Tutorial.

Both models use relative fitness (ω) as the response variable (Y).

Selection differentials (s) measure selection on only a single trait, ignoring all other traits. In theory, the response to selection is a simple function of the genetic correlation between a trait and fitness. Some of this theory, with examples in R, is covered in the Population Genetics Tutorials.

Fitness differences among individuals can depend on a lot of things – genetic variation for the trait itself, but also environmental effects on the trait as well as effects on other traits that are under selection and correlated with the trait of interest.

Selection gradients (β) measure selection on a trait of interest while also accounting for selection on other correlated traits. This is done via a **multiple regression** – a linear model with multiple predictors.

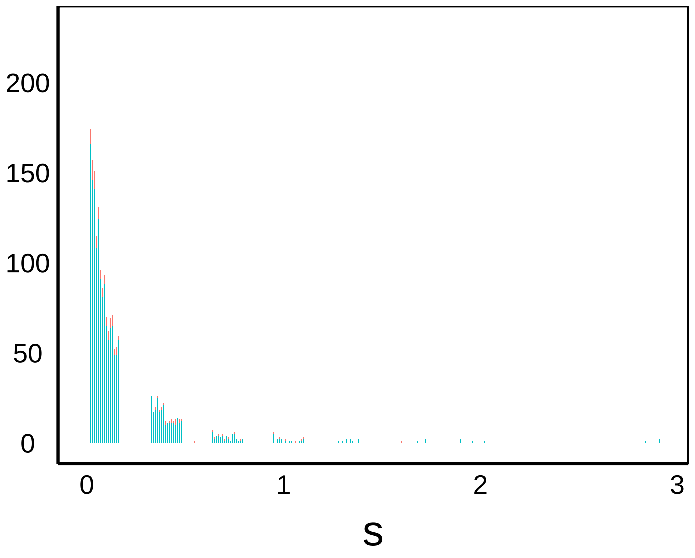
5.6 `ggplot` vs `qplot`

We can create similargraph using `qplot` and ggplot, but the syntax can be quite different.

5.6.1 Histogram

Let's start with a simple `qplot`

```
BarPlot<-qplot(s, data=SelData, fill=Native, geom="bar")
print(BarPlot)
```



Now let's try with `ggplot`. We'll make it into an object that we can work with.

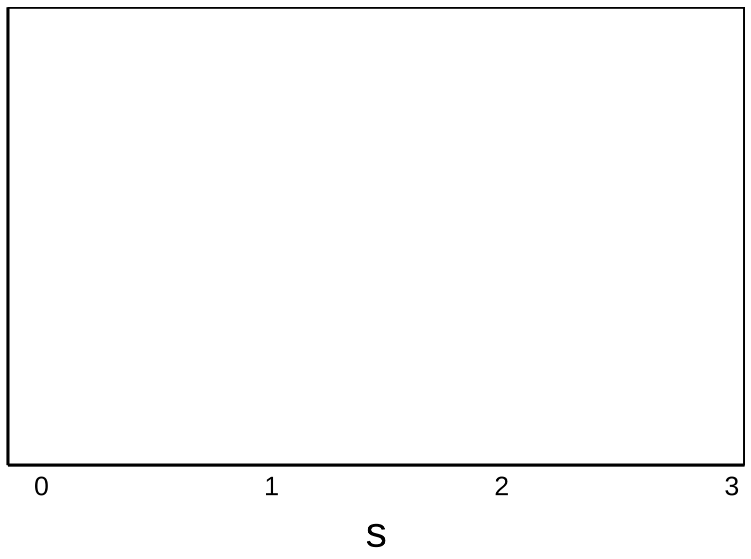
```
BarPlot<-ggplot(aes(s, fill=Native), data=SelData)
```

5.6.2 aes

Note the use of the aesthetic function `aes()`. This defines the data that we want to use for our `ggplot` graph. We will see how we do this by adding layers to our plot, similar to the way old-timey cartoons were made by layering multiple clear pages of cellphane with characters painted on them. The `aes` function inside of the `ggplot` function defines that data that will be shared among all of the layers. In addition, we can have separate `aes` functions inside different `geom_` layers that define and restrict the plotting data to that specific layer.

Let's look at the `ggplot` object so far:

```
print(BarPlot)
```



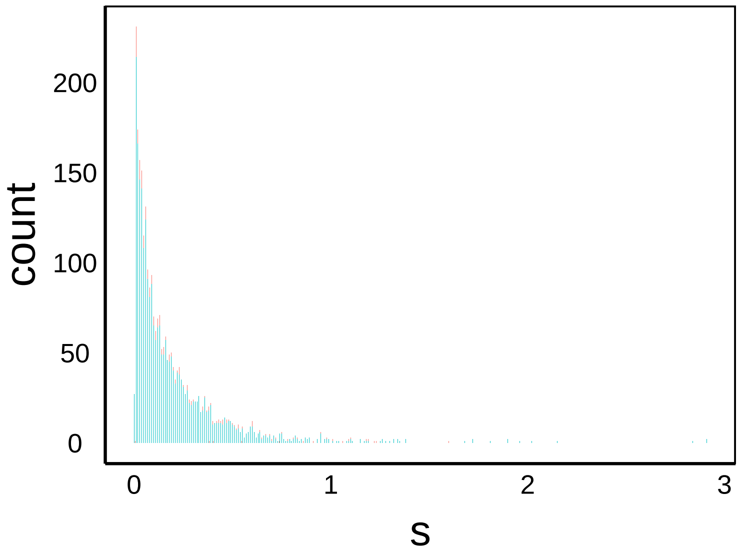
No data! This is one key difference between `qplot` and `ggplot`. The former has default `geoms` that it applies depending on the type of input data. We can modify geoms with the `geom = "NAME"` parameter in `qplot`, where 'NAME' is the specific name of the geom we want to use. In the above `qplot` example we used `geom = "bar"`.

In `ggplot` we have to explictly add geoms as overlapping layers using `+ geom_NAME`, where name is the specific name of the geom – the same text that would go in quotation marks for the geom in `qplot`. The advantage of using `ggplot` is that its easier to create multiple, overlapping layers with different geoms from types data sources.

5.6.3 Layers

So far, we have only loaded in the data info for plotting. We have to specify which geom(s) we want.

```
BarPlot<- BarPlot + geom_bar()
BarPlot
```



Compare this graph and code to the above `qplot` figure.

Let's explore the components of our BarPlot object:

```
summary(BarPlot)
```

```
## data: Collector, Author, Year, Journal, Vol, Species, Native, N,
##   Fitness.measure, Trait, s, s.SE, s.P, B, B.SE, B.P, Rpoint, Rgroup
##   [2766x18]
## mapping:  x = ~s, fill = ~Native
## faceting: <ggproto object: Class FacetNull, Facet, gg>
##     compute_layout: function
##     draw_back: function
##     draw_front: function
##     draw_labels: function
##     draw_panels: function
##     finish_data: function
##     init_scales: function
##     map_data: function
##     params: list
##     setup_data: function
##     setup_params: function
##     shrink: TRUE
##     train_scales: function
##     vars: function
##     super:  <ggproto object: Class FacetNull, Facet, gg>
## -----------------------------------
## geom_bar: just = 0.5, width = NULL, na.rm = FALSE, orientation = NA
## stat_count: width = NULL, na.rm = FALSE, orientation = NA
## position_stack
```

This shows us the columns of **data** available for plotting, the **mapping** for our x and y axes, and our **fill** colours. It also shows some of the functions and parameters used to generate the graph. At the bottom we see parameters for `geom_bar` and `stat_count`. Note that there are more parameters listed than what we explicitly put into the `ggplot()` function. These extra parameters are the **default parameters** for the function.

5.6.4 `geom_` and `stat_`

If *geoms* are the *geometry* of the shapes in the plot, *stats* are the *statistics* or mathematical functions that create the geoms. In the above case, the bars in `geom_bar` are created by counting the number of observations in each bin. The `stat_count` function is responsible for this calculation, and it is called by default when we use the `geom_bar` function.

Ws we can change the geometry of the plotted shapes with `geom_<NAME>`, and we can define different functions for generating the geometric shapes with `stat_<NAME>` (in both cases is a specific name like `bar` or `count`. To make things easier on us, there is a default *stat* for each *geom*, so in most cases we can just focus on which geometry we want for our graph, and use the ignore the *stat* (i.e. use the default).

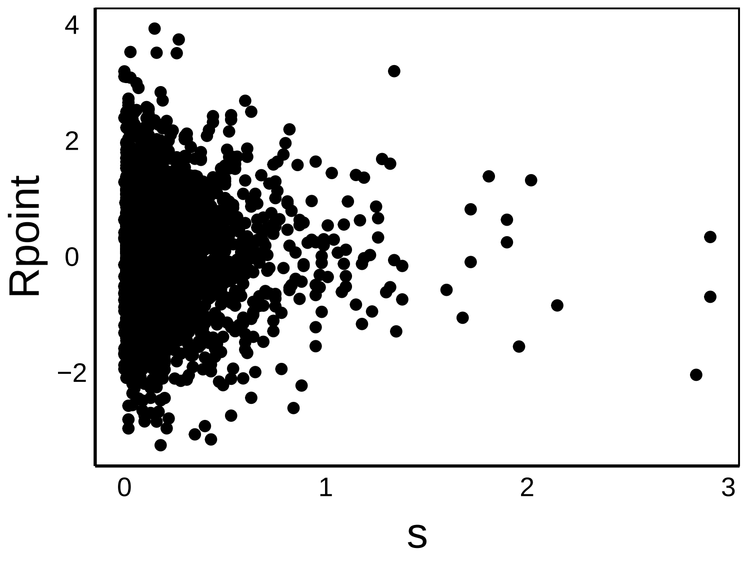
For more information on the parameters and stast of `geom_bar()` or any geom, use the R help function.

```
?geom_bar
```

5.6.5 Bivariate geom

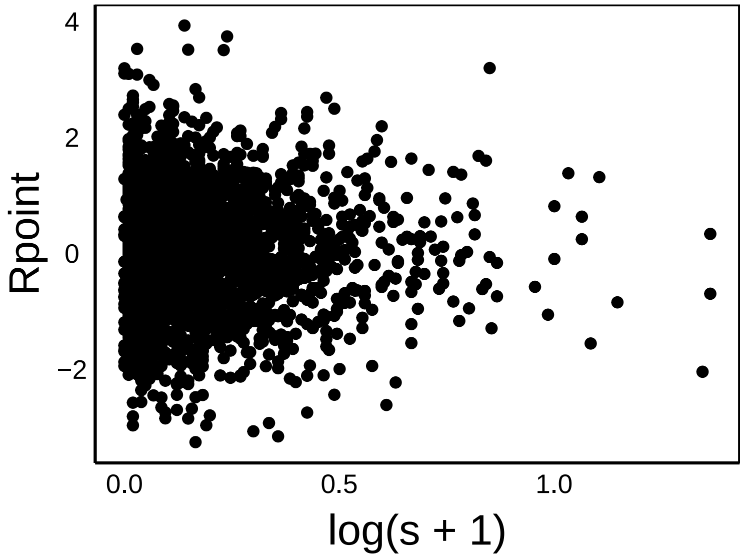
Let's explore a few more plotting options. Here we'll use the random normal values we generated above so that we can make a bivariate plot:

```
BivPlot<-ggplot(data=SelData, aes(x=s, y=Rpoint)) +
  geom_point()
print(BivPlot)
```



Notice how the points are all clustered to the left. This looks like a classic log-normal variable, so let's log-transform s (x-axis)

```
BivPlot<-ggplot(data=SelData, aes(x=log(s+1), y=Rpoint)) +
  geom_point()
print(BivPlot)
```



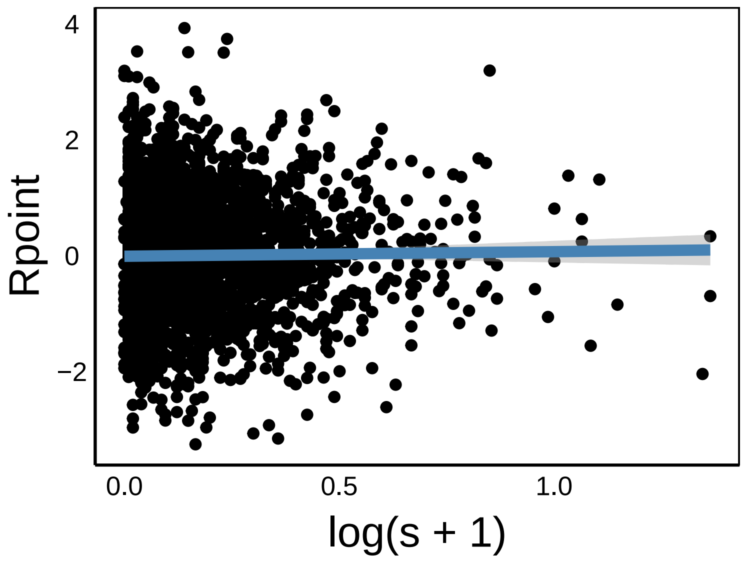
5.6.6 `geom_smooth`

A really handy feature of `ggplot` is the `geom_smooth` function, which has several options for calculating and plotting a statistical model to the observations.

Here's a simple linear regression slope (lm = linear model):

```
BivPlot +
  geom_smooth(method="lm", colour="steelblue", size=2)
```

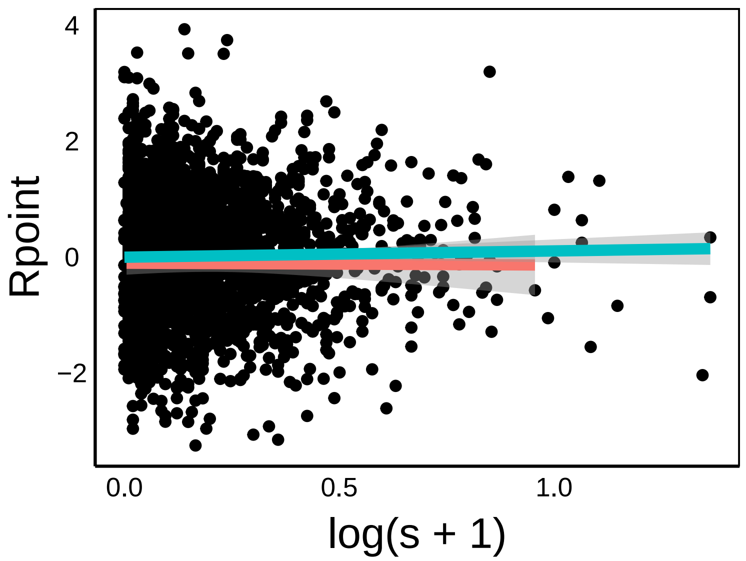
```
## Warning: Using `size` aesthetic for lines was deprecated in
## ggplot2 3.4.0.
## i Please use `linewidth` instead.
## `geom_smooth()` using formula = 'y ~ x'
```



We can use a grouping variable to add separate regression lines for each group

```
BivPlot +
  geom_smooth(method="lm" ,size=2, aes(group=Native, colour=Native))
```

```
## `geom_smooth()` using formula = 'y ~ x'
```



5.7 Full ggplot

Now that we've done a bit of exploration, let's try to recreate the selection histograms from Colautti & Lau:

1. Create separate data for native vs. introduced species
2. Use a bootstrap to estimate non-parametric mean and 95% confidence intervals
3. Plot all of the components on a single graph

5.7.1 Separate data

Since this is a relatively simple resampling model, we'll use two separate vectors to keep track of each interation: one for native and one for non-native.

```
NatSVals<-SelData$s[SelData$Native=="yes"]
IntSVals<-SelData$s[SelData$Native=="no"]
```

An alternative would be to set up a data frame and keep track of values as separate columns, with a different row for each iteration.

5.7.2 Bootstrap

The graph includes a bootstrap model to estimate the mean and variance for each group ($native = yes$ vs no). Bootstrapping is covered in the Bootstrapping and Randomization Tutorial. The example below is not the most efficient approach but it applies the flow control concepts covered in the R Fundamentals Tutorial

5.7.2.1 Data Setup

First we define the number of iterations and set up two objects to hold the data from our bootstrap loops.

```
IterN<-100 # Number of iterations
NatSims<-{} # Dummy objects to hold output
IntSims<-{}
```

5.7.2.2 `for` loop

Here we apply our `for` loop. in each round, we:

1. Sample, with replacement and calculate average
2. Store average in `NatSims` (native species) or `IntSims` (non-native species)

```
for (i in 1:IterN){
  NatSims[i]<-mean(sample(
    NatSVals, length(NatSVals), replace=T))
  IntSims[i]<-mean(sample(
    IntSVals, length(IntSVals), replace=T))
}
```

Note in the above code we use ‘nested’ functions. First we `sample`, then calculate the `mean`.

5.7.2.3 95% CI

Confidence Intervals (CI) are calculated from the bootstrap output.

First, sort the datea from low to high

```
NatSims<-sort(NatSims)
IntSims<-sort(IntSims)
```

Each of the objects contains a number of values equal to our `Iter` variable defined above. Now we identify the lower 2.5% and upper 97.5% values in each vector. For example, with 1000 iterations our 2.5% would be the 25th value in the sorted vector and the upper 97.5% would be the 975th value in the sorted vector.

We use this number to index the vector with square brackets. We make sure to round to a whole number since we can't have a fractional cell position.

```
CIs<-c(NatSims[round(IterN*0.025,0)], # Lower 2.5%
       NatSims[round(IterN*0.975,0)], # Upper 97.5%
       IntSims[round(IterN*0.025,0)], # Lower 2.5%
       IntSims[round(IterN*0.975,0)]) # Upper 97.5%
```

Note that the output is a vector of length 4:

```
print(CIs)
```

```
## [1] 0.1828555 0.2015692 0.2189243 0.3138703
```

Note: your numbers should be similar but won't be exact because each random sample will be slightly different.

> What line could we add above t ensure that these numbers were exactly the same for everyone who ran this code?

5.7.3 Plot data

We'll combine the separate bootstrap vectors into a single data.frame object to make it easier to incorporate into our `ggplot` functions.

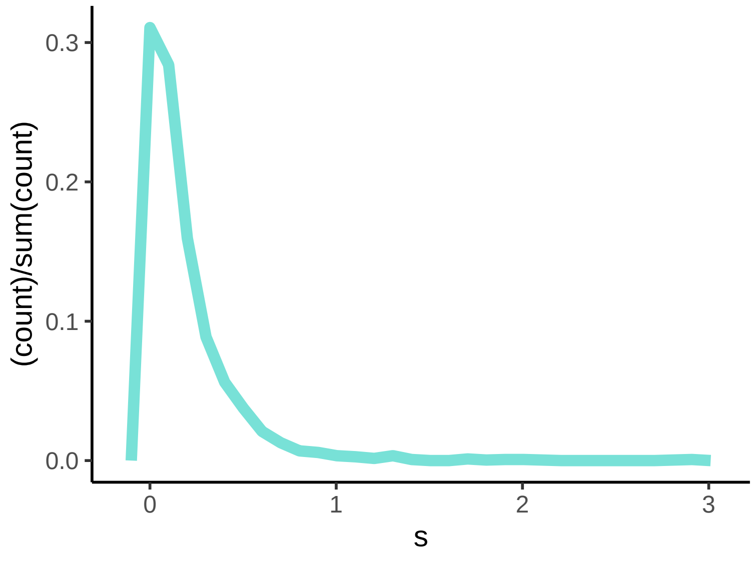
```r
HistData<-data.frame(s=SelData$s,Native=SelData$Native)
```

Now we can add layers to the plot. We'll print out each layer as we go, so that we can see what each layer adds to the overall graph. The coding is a bit complex here, so don't worry if it's hard to follow everything. The key thing to understand is how the different geoms contribute to the final plot.

```r
p <- ggplot() + theme_classic()
p <- p + geom_freqpoly(data=HistData[HistData$Native=="yes",],
                       aes(s,y=(..count..)/sum(..count..)),
                       alpha = 0.6,colour="#1fcebd",size=2)
print(p) # native species histogram
```

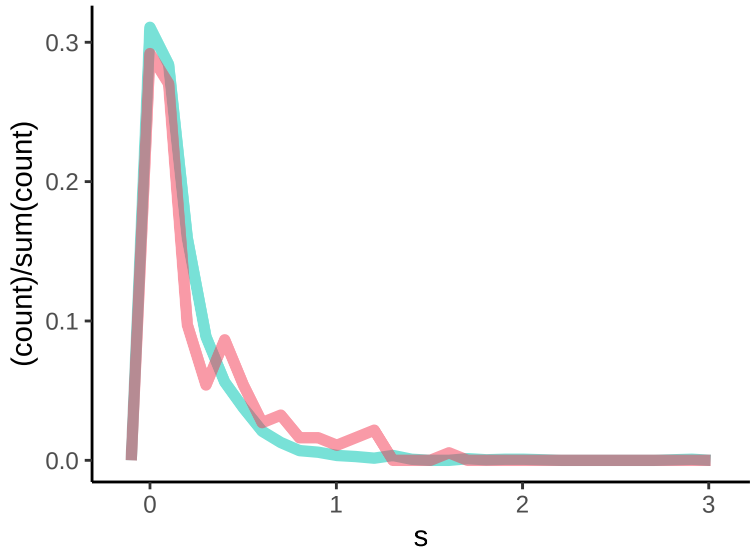
```
## Warning: The dot-dot notation (`..count..`) was deprecated in
## ggplot2 3.4.0.
## i Please use `after_stat(count)` instead.
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



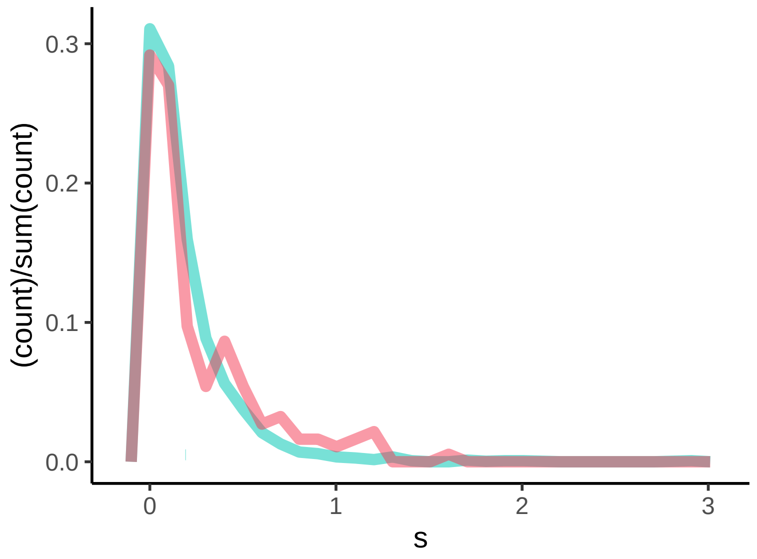
```
p <- p + geom_freqpoly(data=HistData[HistData$Native=="no",],
                       aes(s,y=(..count..)/sum(..count..)),
                       alpha = 0.5,colour="#f53751",size=2)
print(p) # introduced species histogram
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



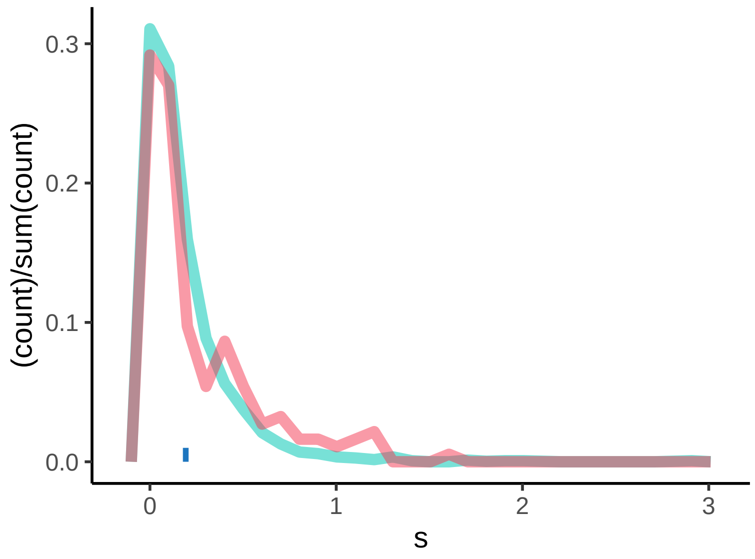
```
p <- p + geom_rect(aes(xmin=CIs[1],xmax=CIs[2],ymin=0,ymax=0.01),
                   colour="white",fill="#1fcebd88")
print(p) # native species 95% CI bar
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



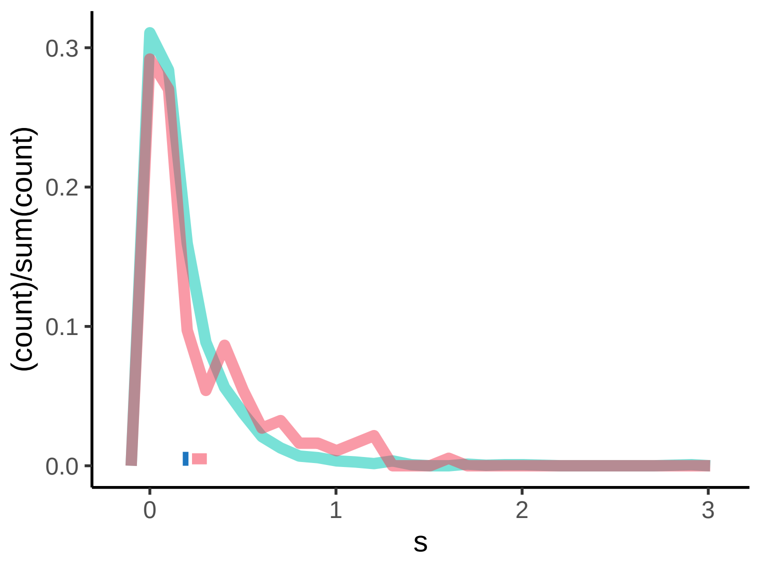
```r
p <- p + geom_line(aes(x=mean(NatSims),y=c(0,0.01)),
                   colour="#1d76bf",size=1)
print(p) # native species bootstrap mean
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



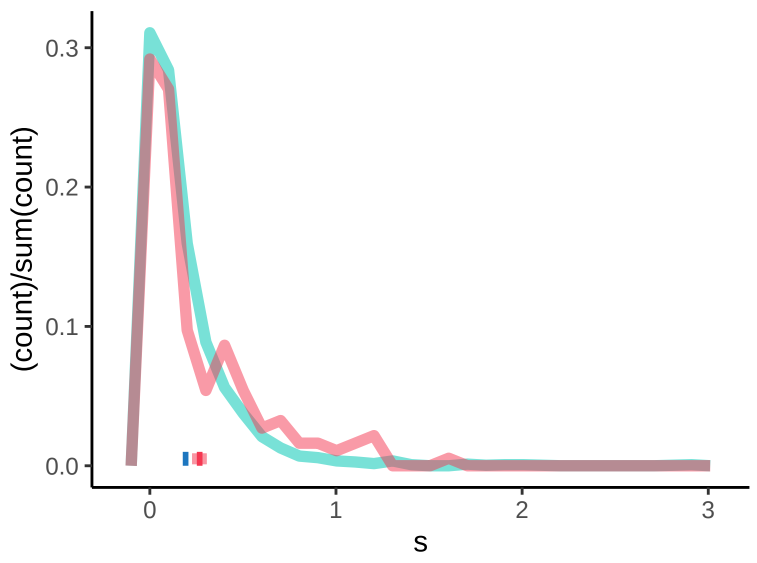
```
p <- p + geom_rect(aes(xmin=CIs[3],xmax=CIs[4],ymin=0,ymax=0.01),
                    colour="white",fill="#f5375188")
print(p) # introduced species 95% CI bar
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



```r
p <- p + geom_line(aes(x=mean(IntSims),y=c(0,0.01)),
                   colour="#f53751",size=1)
print(p) # introduced species bootstrap mean
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



```
p <- p + ylab("Frequency") +
  scale_x_continuous(limits = c(0, 1.5))
print(p) # labels added, truncated x-axis
```

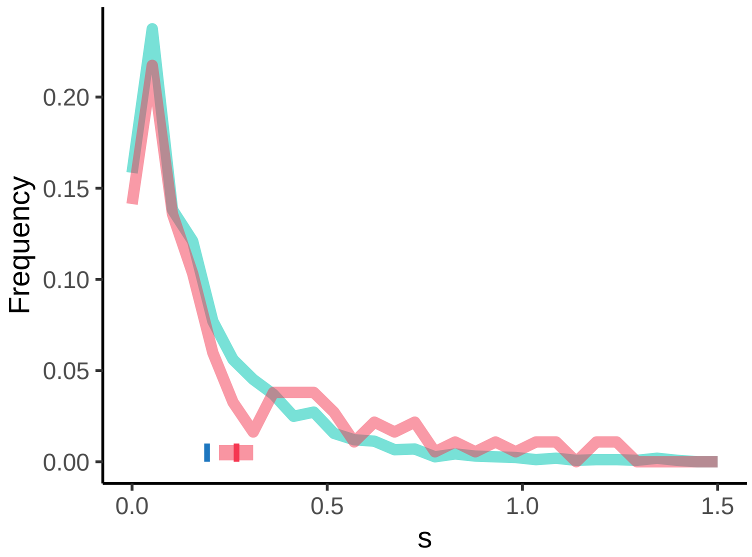
```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.

## Warning: Removed 12 rows containing non-finite values
## (`stat_bin()`).

## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.

## Warning: Removed 1 rows containing non-finite values
## (`stat_bin()`).

## Warning: Removed 2 rows containing missing values
## (`geom_path()`).
## Removed 2 rows containing missing values
## (`geom_path()`).
```



Another important point to note is that case we leave the `ggplot()` function empty because each geom uses different data. The data for each geom is defined by separate `aes` functions inside of each geom.

5.8 Multi-graph

In the qplot Tutorial we saw a quick and easy way to make multiple graphs for different groups using the `facets` parameter.

5.8.1 `facets`

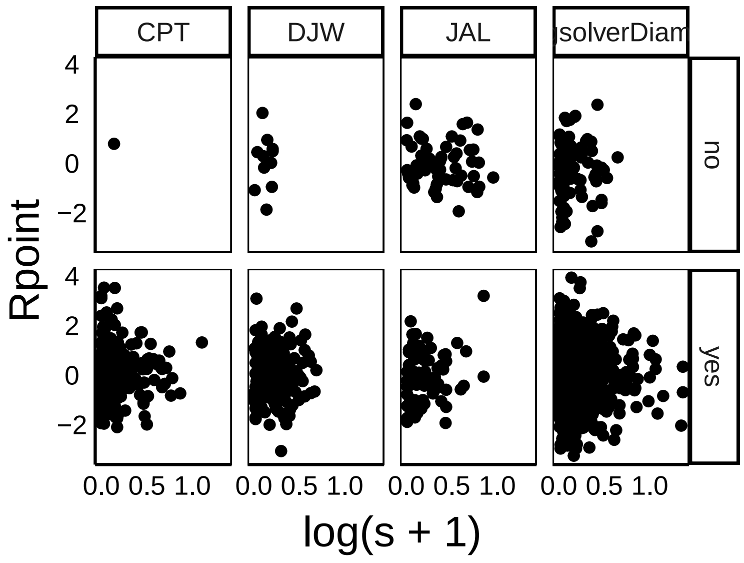
We can also use facets with `gpplot`, just using a slightly different syntax giving a couple of options:

1. `facet_grid` lets us define a grid and set the vertical and horizontal variables
2. `facet_wrap` is a convenient option if only have one categorical variable but many categories

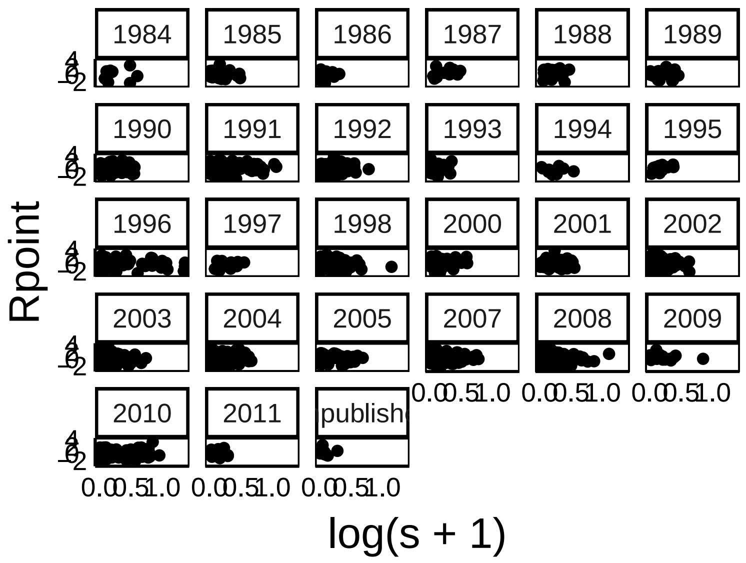
NOTE: one little tricky part of facets with `ggplot` is that it uses `vars` instead of the `aes` function to indicate which categorical variables from the original dataset should be used to subset the graphs.

Returning to the `BivPlot` example above:

```
BivPlot<-ggplot(data=SelData, aes(x=log(s+1), y=Rpoint)) +
  geom_point()
BivPlot + facet_grid(rows=vars(Native), cols=vars(Collector))
```



```
BivPlot<-ggplot(data=SelData, aes(x=log(s+1), y=Rpoint)) +
  geom_point()
BivPlot + facet_wrap(vars(Year))
```



5.8.2 `grid.extra` package

Facets produce graphs that all have the same dimension and the same x- and y-axes. We might call these 'homogeneous' plots because they use a homogeneous format. For publications though, we might want to includ 'heterogeneous' plots with different axes and different sizes. The `gridExtra` package provides options for this.

Install with `install.packages("gridExtra")` if you haven't installed it already, then load the library

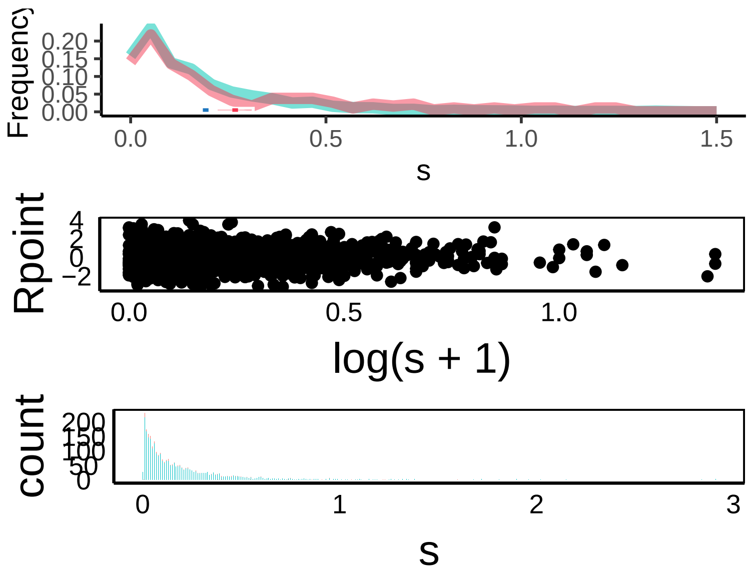
```
library(gridExtra)
```

5.8.2.1 `grid.arrange()`

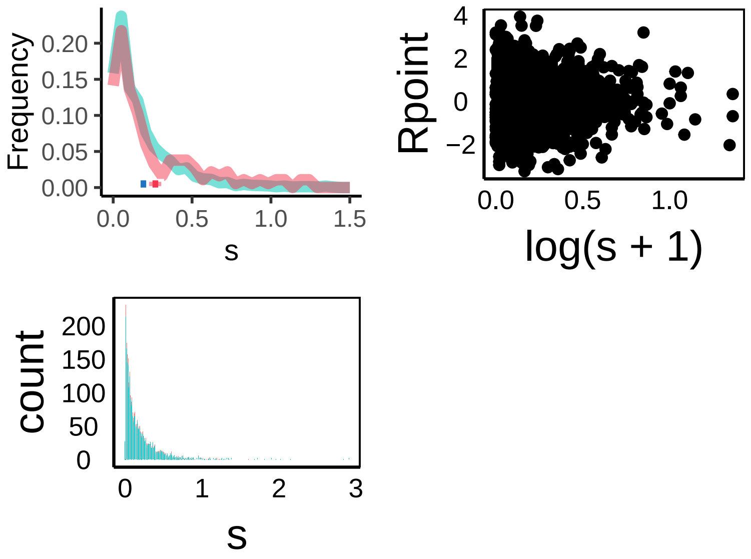
Use this to combine heterogeous ggplot objects into a single multi-panel plot.

Note that this will print graphs down rows, then across columns, from top left to bottom right. You can use `nrow` and `ncol` to control the layout in a grid format.

```
HistPlot<-p # Make a more meaningful name
grid.arrange(HistPlot,BivPlot,BarPlot,ncol=1)
```



```
grid.arrange(HistPlot,BivPlot,BarPlot,nrow=2)
```



Note: You might get some warnings based on missing values or wrong binwidth. You will also see some weird things with different text sizes in the graphs. Normally, you would want to fix these for a final published figure but here we are just focused on showing what is possible with the layouts.

5.8.3 `grid` package

What if we want to have graphs of different sizes? Or what if we want one figure to be inside another? We can make some even more advanced graphs using the `grid` package. This is part of the base installation of R so you don't need to use `install.packages()` this time.

```
library(grid)
```

First, we set up the plotting area with `grid.newpage`

```
grid.newpage() # Open a new page on grid device
```

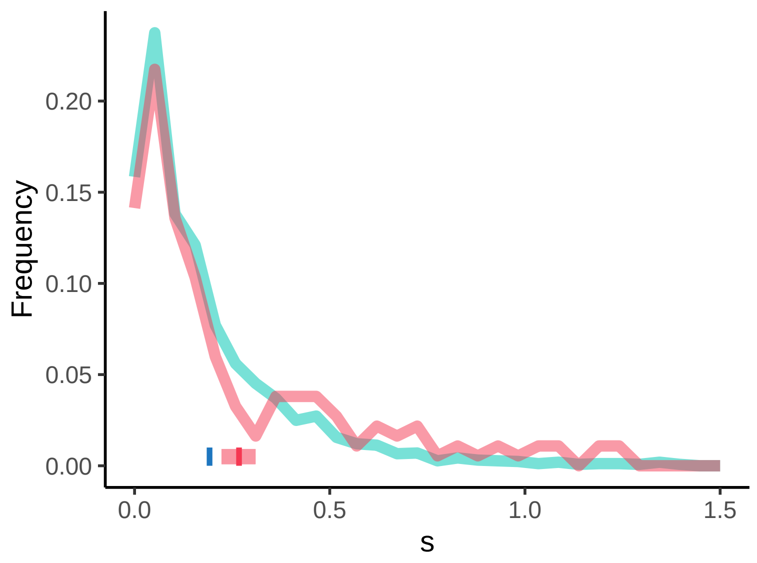
To insert a new graph on top (or inside) the current graph, we use `pushViewport` to set up an imaginary plotting grid. In this case, imagine breaking up the plotting space into 3 rows by 2 columns.

```
pushViewport(viewport(layout = grid.layout(3, 2)))
```

Finally, we print each `ggplot` object, specifying which grid(s) to plot in.

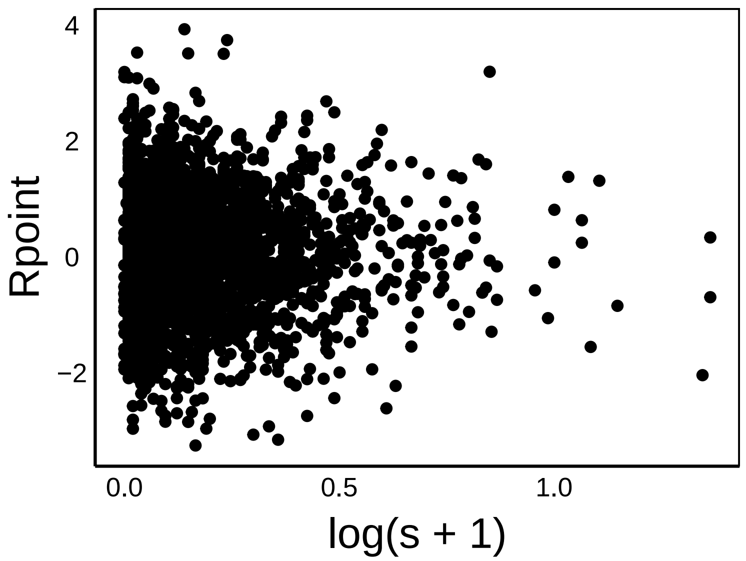
Add the first figure in row 3 and across columns 1:2

```
print(HistPlot, vp = viewport(layout.pos.row = 3,
                              layout.pos.col = 1:2))
```



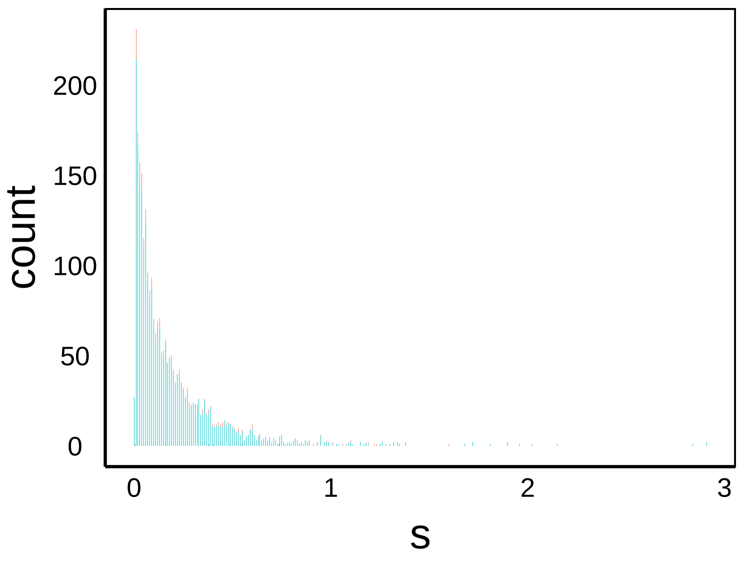
Add the next figure across rows 1 and 2 of column 1

```
print(BivPlot, vp = viewport(layout.pos.row = 1:2,
                             layout.pos.col = 1))
```



Add the final figure across rows 1 and 2 of column 2

```
print(BarPlot, vp = viewport(layout.pos.row = 1:2,
                             layout.pos.col = 2))
```



5.8.3.1 Inset We can also use `pushViewport` to set up a grid for plotting on top of an existing graph or image. This can be used to generate a figure with an inset.

First generate the 'background' plot. Note that you could alternatively load an image here to place in the background.

```
HistPlot
```

Next, overlay an invisible 4x4 grid layout (number of cells, will determine size/location of graph)

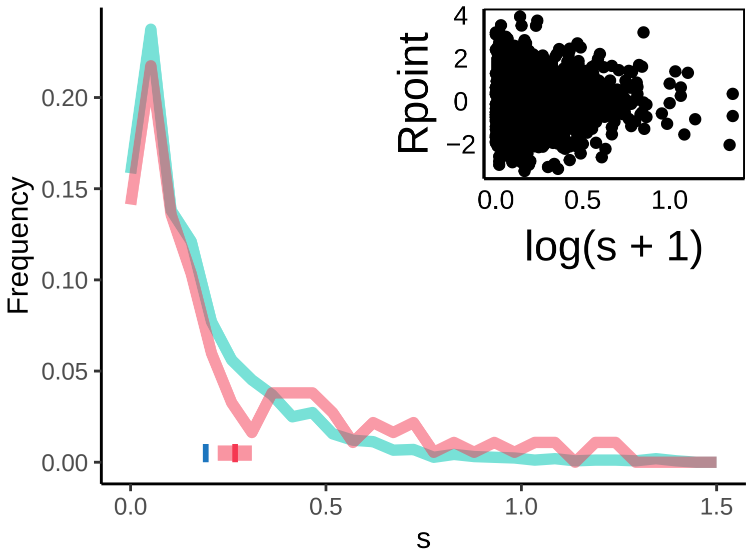
```
pushViewport(viewport(layout = grid.layout(4, 4)))
```

Finally, add the graph. In this case we want it only in the top two rows and the right-most two columns – i.e. the top-right corner.

```
print(BivPlot, vp = viewport(layout.pos.row = 1:2, layout.pos.col = 3:4))
```

The final product:

```
HistPlot
pushViewport(viewport(layout = grid.layout(4, 4)))
print(BivPlot, vp = viewport(layout.pos.row = 1:2, layout.pos.col = 3:4))
```



5.9 Further Reading

The 2009 book *ggplot2: Elegant Graphics for Data Analysis* by Hadly Wickham is the definitive guide to all things ggplot.

A physical copy is published by Springer http://link.springer.com/book/10.1007%2F978-0-387-98141-3

And there is a free ebook version: https://ggplot2-book.org/

6 Regular Expressions

6.1 Overview

Regular Expressions, also known as **regex** and **regexp** is a syntax that allows for coders to run complex find-and-replace functions. I didn't learn regular expressions until I was a postdoc working at Duke University, but I wish I had learned this a lot earlier! This remains one of the most useful programming tools I have ever used. It is absolutely essential for working with any kind of large text files or large datasets.

A lot of programming tools in biology use input text files that require very specific formatting (e.g. .txt, .csv, .fasta, .nex). Sometimes, you might need to reorganize or recode data in a large text file. This can be a big pain that can lead to errors if you try to do everything manually. But regular expressions can automate the process.

Here's one example. As a PhD student I co-founded a project called the **Global Garlic Mustard Field Survey (GGMFS)** with collaborator Dr. Oliver Bossdorf at the University of Tuebingen – yes the same Dr. Bossdorf mentioned in the qplot Tutorial. We were fortunate to have over 100 collaborators across Europe and North America who helped to collect samples for the project. Details of the project were published in the Journal **Neobiota**: https://neobiota.pensoft.net/article/1270/ but one BIG problem is the way that each of these 100+ collaborators entered their data online. For example, latitudes and longitudes were entered in a variety of different formats. Regular expressions allowed me to write a small program to automatically convert all of these different formats to a common, decimal format that we could use for the analysis. This saved a huge amount of time and prevented errors that could have been introduced if we tried to edit these values by hand.

Often when you work with large datasets, you will need to automate some of your error correction, and regular expressions can be a big help here. For example, imagine a simple field where people were simply asked a simple yes or no question. You might find a variety of inputs such as: "YES, Y, yes, and Yes". These all mean the same thing but if you try to analyze it, R will treat these as different categories. Here again, regular expressions can be used to quickly change all the different examples to a common "Y" or even a boolean variable `TRUE`.

One final example, is pattern searching. This is common for the analysis of DNA, proteins or other large strings of data. You may want to find a particular sequence of data, possibly with a few variable sites: e.g. TCTA or TCAA or TCGA. This is another area where regular expressions can help.

6.1.1 Universal

Regular expressions are a universal language that extends to many other programming languages, including **C/C#/C++**, **Python**, **Unix/Linux**, and **Perl**. We focus here on R but most of the syntax is mantained across programming languages.

> WARNING!

There is a very steep learning curve here, and the only way to really learn this is to drown yourself in examples. There are lots of exercises you can do for practice online. You should also try to apply these whenever you can.

6.2 Functions

There are four main functions that use regular expressions in R.

`grep()` and `grepl()` are equivalent to 'find' in your favorite word processor

They have the general form: `gsub("find this pattern", in.this.object)`

`grep()` outputs a vector with all the address locations (i.e. numbers) that match. Thus the output length is equal to the number of matches.

`grepl()` outputs a vector of `TRUE` (match) and `FALSE` (no match). Thus, the output length is equal to the length of the input object.

`sub()` and `gsub()` are equivalent to 'find and replace'

They have the general form: `grep("find this pattern", "and replace with this", in.this.object)`

`sub()` replaces only the first match, whereas `gsub()` replaces all of the matches.

Some specific examples are provided below to help you understand these similarities and differences.

There are two other more advanced functions in R. These aren't covered in this tutorial, but may be of use once you are more comortable with the above functions.

`regexpr()` provides more detailed info about the first match

`gregexpr()` provides more detailed results about all matches

> See ?regexpr and ?gregexpr for more info

6.2.1 Examples

Some examples can help to understand the differences among the four main functions. Let's start with a simple data frame of species names.

```
Species<-c("petiolata", "verticillatus", "salicaria", "minor")
print(Species)
```

```
## [1] "petiolata"     "verticillatus" "salicaria"
## [4] "minor"
```

6.2.2 `grep()`

This returns cell addresses matching query. Note the vector length compared to the input vector.

```
grep("a",Species)
```

```
## [1] 1 2 3
```

We can also see the specific values with the `value=T` parameter

```
grep("a",Species, value=T)
```

```
## [1] "petiolata"     "verticillatus" "salicaria"
```

6.2.3 `grepl()`

This returns a vector of `TRUE` (match) and `FALSE` (no match). Compare this output with `grep()`.

```
grepl("a",Species)
```

```
## [1]  TRUE  TRUE  TRUE FALSE
```

6.2.4 `sub()`

This replaces the first match (in each cell)

```
sub("l","L",Species)
```

```
## [1] "petioLata"     "verticiLlatus" "saLicaria"
## [4] "minor"
```

6.2.5 `gsub()`

This replaces all matches (in each cell). Compare this output to `sub()`.

```
gsub("l","L",Species)
```

```
## [1] "petioLata"     "verticiLLatus" "saLicaria"
## [4] "minor"
```

6.3 Wildcards

6.3.1 \ escape character

The backslash is a special character. It's called the 'escape' character because it is used to 'escapes' the interpretation of the next character that occurs after it. This is easier to understand by example, as shown below.

6.3.2 \\ in R

In the introduction, we discussed the universality of **regular expressions** in the sense that a similar syntax is used by many different programming langagues. But now here is one exception. In R, the double-escape is usually needed, whereas other programming languages typically use just one. The reason is a bit meta – it's because we are running regular expressions within R object. So the first \ is used to escape special characters in R, applying it to the second \, which is itself the special character that needs to be escaped to pass through the function. The second slash is followed by the ‘escaped’ character. Some examples are provided below.

If that isn’t clear. Just remember that you need two backslashes instead of one.

6.3.3 `\\w`

Instead of finding the letter `w`, the `\\w` is a **wildcard** character that represents any letter or digit. It also includes underscore _ for some reason.

```
gsub("w","X","...which 1-100 words get replaced?")
```

```
## [1] "...Xhich 1-100 Xords get replaced?"
```

```
gsub("\\w","X","...which 1-100 words get replaced?")
```

```
## [1] "...XXXXX X-XXX XXXXX XXX XXXXXXXX?"
```

6.3.4 `\\W`

This is the inverse of `\\w` find a character that is NOT a letter or number.

```
gsub("\\W","X","...which 1-100  words get replaced?")
```

```
## [1] "XXXwhichX1X100XXwordsXgetXreplacedX"
```

6.3.5 `\\s`

This represents a space

```
gsub("\\s","X","...which 1-100  words get replaced?")
```

```
## [1] "...whichX1-100XXwordsXgetXreplaced?"
```

6.3.6 `\\t`

This is a tab character. A lot of data files stored as text are tab-delimited (.tsv) as well as comma-delimited (.csv)

```
gsub("\\t","X","...which 1-100 \t words get replaced?")
```

```
## [1] "...which 1-100 X words get replaced?"
```

Remember is a tab character:

```
cat("A\t\t\tB C")
```

```
## A             B C
```

6.3.7 `\\d`

Digit characters

```
gsub("\\d","X","...which 1-100  words get replaced?")
```

```
## [1] "...which X-XXX  words get replaced?"
```

6.3.8 `\\D`

Non-digit characters

```
gsub("\\D","X","...which 1-100  words get replaced?")
```

```
## [1] "XXXXXXXXX1X100XXXXXXXXXXXXXXXXXXXXXX"
```

6.4 New Lines

There are two special characters that indicate new lines in a text file.

6.4.1 `\\r`

This is the ‘carriage return’ special character

6.4.2 `\\n`

This is the ‘newline’ special character

6.4.3 Big Problem

One or two of these is/are generated when you press the ‘enter’ key while writing a text file. These also add a source of headache and confusion when working with text files because:

> Macs/Unix and PC/Windows use different standards!

Unix/Mac files – lines usually end with `\\n` only

Windows/DOS files – lines usually end with `\\r\\n`

This can cause problems when moving text files between Windows/DOS and Mac/Unix machines, particularly with older operating systems or when working on remote computers that use very basic Linux software.

6.5 Special characters

In addition to special characters that use the escape `\\`, there are a number of other special characters that don’t use the escape, but have a special meaning.

Note that if you want to search for the characters below you would have to use the escape character. E.g. `\\.` if you wanted to search for a period `.`.

6.5.1 `|`

This is sometimes called the **pipe** character, and it simply means ‘or’. For example, we can search for `w or e`.

```
gsub("w|e","X","...which 1-100  words get replaced?")
```

```
## [1] "...Xhich 1-100  Xords gXt rXplacXd?"
```

6.5.2 .

The period is a wild card that means ‘anything’. This includes all of the `\\w` characters but also other characters like puncutation marks.

```
gsub(".","X","...which 1-100  words get replaced?")
```

```
## [1] "XXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXXX"
```

So how to search for a period `.`? As noted above, we have to use the escape character

```
gsub("\\.","X","...which 1-100  words get replaced?")
```

```
## [1] "XXXwhich 1-100  words get replaced?"
```

6.5.3 `*`, `?`, `+`, `{}`

These special characters refer to details about the kind of search that we are trying to conduct. Look at these examples carefully, and remember that `sub` replaces the first match while `gsub` replaces all of the matches.

```
sub("\\w","X","...which 1-100 words get replaced?")
```

```
## [1] "...Xhich 1-100 words get replaced?"
```

```
gsub("\\w","X","...which 1-100 words get replaced?")
```

```
## [1] "...XXXXX X-XXX XXXXX XXX XXXXXXXX?"
```

Now let’s apply some of these special characters to see how they work.

6.5.3.1 + Finds 'one or more' matches (i.e. at least one match)

```r
sub("\\w+","X","...which 1-100 words get replaced?")
```

```
## [1] "...X 1-100 words get replaced?"
```

```r
gsub("\\w+","X","...which 1-100 words get replaced?")
```

```
## [1] "...X X-X X X X?"
```

Compare this match to the one above. Notice how we have replaced groups of letters instead of single letters. The algorithm works like this:

1. Start at the left and move to the right, one character at a time
2. Check if the character is a letter or number (`\\w`).
3. If NO, move to the next character
4. If YES, check the next character. If it is also a `\\w` then go to the next character. Repeat until the next character is not `\\w`, and replace the entire string of characters.

When run in the `sub` command, it does the above and then stops. When run with the `gsub` command, it continues to the next character, and then starts over.

6.5.4 *

This is a 'greedy' search (match the largest possible)

```r
sub("\\w*","X","...which 1-100 words get replaced?")
```

```
## [1] "X...which 1-100 words get replaced?"
```

```r
gsub("\\w*","X","...which 1-100 words get replaced?")
```

```
## [1] "X.X.X.X X-X X X X?X"
```

In the `sub` command, it detects a `.` as the first character, indicating no match. It replaces the 'null' or `0` match at the beginning, which has the effect of adding a character. In the `gsub` command it repeats this before each `.` until it finds the letter `w`. Then it finds a group of `\\w` matches, replacing with a single `X`. Then a space, which is skipped, then a `-`, which is another null match, prompting another insert.

6.5.5 `?`

This means ‘match zero or one time’

```
sub("\\w?","X","...which 1-100 words get replaced?")
```

```
## [1] "X...which 1-100 words get replaced?"
```

```
gsub("\\w?","X","...which 1-100 words get replaced?")
```

```
## [1] "X.X.X.XXXXX X-XXX XXXXX XXX XXXXXXXX?X"
```

Compare this to the `*` above. It behaves in a similar way, except it is not ‘greedy’ – in the second example, each letter is replaced instead of entire words.

6.5.6 `+?`

This is the ‘lazy’ version of + – note in particular the difference in `sub` which replaces on the the first letter here but the whole word when + is used alone. In the `gsub` example we end up replacing every letter instead of whole words. Remember, `sub` runs the algorithm once and then stops, while `gsub` repeats until it reaches the end of the line.

```
sub("\\w+?","X","...which 1-100 words get replaced?")
```

```
## [1] "...Xhich 1-100 words get replaced?"
```

```
gsub("\\w+?","X","...which 1-100 words get replaced?")
```

```
## [1] "...XXXXX X-XXX XXXXX XXX XXXXXXXX?"
```

6.5.7 `*?`

Similarly, we can combine these characters for the ‘lazy’ version of `*`

```
sub("\\w*?","X","...which 1-100 words get replaced?")
```

```
## [1] "X...which 1-100 words get replaced?"
```

```
gsub("\\w*?","X","...which 1-100 words get replaced?")
```

```
## [1] "X.X.X.XwXhXiXcXhX X1X-X1X0X0X XwXoXrXdXsX XgXeXtX XrXeXpXlXaXcXeXdX?X"
```

Try using `+*`. Why do you get an error message?

6.5.8 `{}`

Curly brackets are used to specify a number of matches, expanding on the options even further.

6.5.9 `{n,m}`

Find between n to m matches

```
gsub("\\w{3,4}","X","...which 1-100 words get replaced?")
```

```
## [1] "...Xh 1-X Xs X XX?"
```

6.5.10 `{n}`

Find exactly n matches

```
gsub("\\w{3}","X","...which 1-100 words get replaced?")
```

```
## [1] "...Xch 1-X Xds X XXed?"
```

6.5.11 `{n,}`

Find n or more matches

```
gsub("\\w{4,}","X","...which 1-100 words get replaced?")
```

```
## [1] "...X 1-100 X get X?"
```

6.5.12 {}?

As above, we can use `?` for the 'lazy' versions of these searches

```
gsub("\\w{4,}?","X","...which 1-100 words get replaced?")
```

```
## [1] "...Xh 1-100 Xs get XX?"
```

6.6 `[]`

Square brackets allow us to find 'any' of the values listed within them. We can also use the dash `-` to specify a range of numbers or letters.

```
gsub("[aceihw-z]","X","...which 1-100 words get replaced?")
```

```
## [1] "...XXXXX 1-100 Xords gXt rXplXXXd?"
```

In the above example, we search for 1 of any of the listed letters: a, c, e, i h, w, x, y, z. Note that x and y are included in the `x-z` statement.

What if we want to find 1 or more of these characters in a row?

```
gsub("[aceihw-z]+","X","...which 1-100 words get replaced?")
```

```
## [1] "...X 1-100 Xords gXt rXplXd?"
```

6.7 `^` and `$`

Use these characters to specify searches at the start `^` or end `$` of the input string.

6.7.1 `^`

Find species starting with the letter *a*

```
grep("^a",Species)
```

```
## integer(0)
```

> IMPORTANT: ^ Also means 'negate' when used within `[]`

Find species containing any letter other than *a*

```
grep("[^a]",Species)
```

```
## [1] 1 2 3 4
```

Replace every letter except *a*

```
gsub("[^a]","X",Species)
```

```
## [1] "XXXXXXaXa"     "XXXXXXXXXaXXX" "XaXXXaXXa"
## [4] "XXXXX"
```

6.7.2 `$`

Find species ending with *a*

```
grep("a$",Species)
```

```
## [1] 1 3
```

6.8 `()`

Regular parentheses are used to 'capture' text, which can then be specified in the replacement string using `\\1`. Or you can capture multiple pieces of text and reorganize them by using the corresponding number – `\\1` for the first set of `()`, `\\2` for the second set of `()`, etc. Some examples should help.

Replace each word with its first letter

```
gsub("(\\w)\\w+","\\1",
     "...which 1-100 words get replaced?")
```

```
## [1] "...w 1-1 w g r?"
```

Pull out only the numbers and reverse their order

```
gsub(".*([0-9]+)-([0-9]+).*","\\2-\\1",
     "...which 1-100 words get replaced?")
```

```
## [1] "100-1"
```

Reverse first two letters of each word

```
gsub("(\\w)(\\w)(\\w+)","\\2\\1\\3",
     "...which 1-100 words get replaced?")
```

```
## [1] "...hwich 1-010 owrds egt erplaced?"
```

6.9 Scraping

Scraping is a method for collecting data from online sources. In R, we can use the functions `readLines` and `curl()`, both from the `curl` library, to 'scrape' data from websites. Websites with the `.html` extension are a special kind of text file.

We can use regular expressions to pull out text from the website. Here's an example where we will scrape a record for the Green Fluorescent Protein (GFP) from the Protein Data Bank (PDB). Note that this is a file with the extension `.pdb` but this is a human-readable text file that can be opened in any text editor

First, we'll import the text into an R object.

```
library(curl)
```

```
## Using libcurl 7.64.1 with Schannel
```

You will have to use `install.packages("curl")` to download this package to your computer. You only need to do this once but you will have to use `library(curl)` whenever you want to use the commands, as explained in the R Fundamentals Tutorial

Now we can download a file to play with.

```
Prot<-readLines(curl("http://www.rcsb.org/pdb/files/1ema.pdb"))
```

> HINT: Download this link to your computer and open with a text file.

This hint is a simple trick to understand what kind of file(s) you are working with.

This is a tab-delimited file, which we could import as a data frame using `read.delim` but we'll keep it this way to see how we can use regular expressions.

The `Prot` object we have made is a simple vector of strings, with each cell corresponding to a different row of text:

```
length(Prot)
```

```
## [1] 2363
```

```
Prot[grep("TITLE",Prot)]
```

```
## [1] "TITLE     GREEN FLUORESCENT PROTEIN FROM AEQUOREA VICTORIA
```

We can pull out the amino acid sequences, which are rows that start with the word 'ATOM'

```
AAseq<-Prot[grep("^ATOM",Prot)]
length(AAseq)
```

```
## [1] 1717
```

```
AAseq[1]
```

```
## [1] "ATOM      1  N   SER A   2      28.888   9.409  52.301  1.00 85.05
```

> Try to isolate the 3-letter amino acid code

There are lots of possibilities. Take the time to try a few.

Here's one good option, since we know it's a tab-delimited file with the amino acid in the 4th column:

```
gsub("ATOM\\t\\w+\\t\\w+\\t(\\w+).*","\\1",AAseq[1])
```

```
## [1] "ATOM      1  N   SER A   2      28.888   9.409  52.301  1.00 85.05
```

That didn't work. Sometimes the 'tabs' are actually just multiple 'spaces'

```
AAchain<-gsub("ATOM\\s+\\w+\\s+\\w+\\s+(\\w+).*","\\1",AAseq)
AAchain[1:100]
```

```
##   [1] "SER" "SER" "SER" "SER" "SER" "SER" "LYS" "LYS" "LYS"
##  [10] "LYS" "LYS" "LYS" "LYS" "LYS" "LYS" "GLY" "GLY" "GLY"
##  [19] "GLY" "GLU" "GLU" "GLU" "GLU" "GLU" "GLU" "GLU" "GLU"
##  [28] "GLU" "GLU" "GLU" "GLU" "GLU" "GLU" "GLU" "LEU" "LEU"
##  [37] "LEU" "LEU" "LEU" "LEU" "LEU" "LEU" "PHE" "PHE" "PHE"
##  [46] "PHE" "PHE" "PHE" "PHE" "PHE" "PHE" "PHE" "PHE" "THR"
##  [55] "THR" "THR" "THR" "THR" "THR" "THR" "GLY" "GLY" "GLY"
##  [64] "GLY" "VAL" "VAL" "VAL" "VAL" "VAL" "VAL" "VAL" "VAL"
##  [73] "VAL" "VAL" "VAL" "VAL" "VAL" "VAL" "PRO" "PRO" "PRO"
##  [82] "PRO" "PRO" "PRO" "PRO" "ILE" "ILE" "ILE" "ILE" "ILE"
##  [91] "ILE" "ILE" "ILE" "LEU" "LEU" "LEU" "LEU" "LEU" "LEU"
## [100] "LEU"
```

6.10 Examples

Let's try practicing with a couple of examples

6.11 Transect Data

Regular expressions are also useful with data objects

Imagine you have a repeated measures design. 3 transects (A-C) and 3 positions along each transect (1-3)

```
Transect<-data.frame(Species=letters[1:20],
                     A1=rnorm(20), A2=rnorm(20), A3=rnorm(20),
                     B1=rnorm(20), B2=rnorm(20) ,B3=rnorm(20),
                     C1=rnorm(20), C2=rnorm(20), C3=rnorm(20))
head(Transect)
```

```
##   Species         A1         A2         A3          B1
## 1       a  0.5547274 -0.2933032 -1.8640889 -0.04285598
## 2       b -0.6095312 -1.4151213 -1.1402859 -1.52193318
## 3       c -0.9280047 -1.4229605 -0.2768315  1.25626690
## 4       d  0.8363974  0.9556493  1.8036944  0.50032420
## 5       e  0.4275708 -1.1593840  0.3202867  0.53156430
## 6       f  0.5727893  2.0820319  0.1950647 -0.90458168
##            B2         B3          C1         C2         C3
## 1  0.70904146  1.2014545  0.03805626 -1.5173462 -2.1907316
## 2 -1.04186494 -1.5966388  0.50545743  0.9140523 -0.3635619
## 3 -0.72679199 -0.5933103  0.90281923  1.2363348 -0.5279240
## 4 -0.66987884  0.7615593 -1.56320911 -1.3979829 -1.2292463
## 5 -0.32402919  0.5994643  0.59707710 -0.9129076 -0.5840427
## 6  0.07432932  0.3569005  0.73976615 -0.5949824  0.2035260
```

> TIP: the object `letters` contains lower-case letter, while `LETTERS` contains upper case.

6.11.1 Challenge

Use your knowledged gained above with substting data outlined in the R Fundamentals Tutorial to do the following:

1. Subset only the columns that have an “A” in their name
2. Subset the data for species “D”

Take the time to do this on your own. It will take you a while and you will make a lot of mistakes. That's all part of the learning process. The longer you struggle, the faster you will learn.

Now here is a more challenging example:

6.12 Genbank

Here is a line of code to import DNA from genbank. (The one line is broken up into three physical lines to make it easier to read)

```
Lythrum_18S<-scan(
  "https://colauttilab.github.io/RCrashCourse/sequence.gb",
  what="character",sep="\n")
```

This is the sequence of the 18S subunit from the ribosome gene of *Lythrum salicaria* (from Genbank)

```
print(Lythrum_18S)
```

```
##  [1] "LOCUS       AF206955                1740 bp    DNA
##  [2] "DEFINITION  Lythrum salicaria 18S ribosomal RNA gene, complete sequence."
##  [3] "ACCESSION   AF206955"
##  [4] "VERSION     AF206955.1"
##  [5] "KEYWORDS    ."
##  [6] "SOURCE      Lythrum salicaria"
##  [7] "  ORGANISM  Lythrum salicaria"
##  [8] "            Eukaryota; Viridiplantae; Streptophyta; Embryophyta;
##  [9] "            Spermatophyta; Magnoliopsida; eudicotyledons; Gunneridae;"
## [10] "            Pentapetalae; rosids; malvids; Myrtales; Lythraceae;
## [11] "REFERENCE   1  (bases 1 to 1740)"
## [12] "  AUTHORS   Soltis,P.S., Soltis,D.E. and Chase,M.W."
## [13] "  TITLE     Direct Submission"
## [14] "  JOURNAL   Submitted (19-NOV-1999) School of Biological Sciences,
## [15] "            State University, Pullman, WA 99164-4236, USA"
## [16] "FEATURES             Location/Qualifiers"
## [17] "     source          1..1740"
## [18] "                     /organism=\"Lythrum salicaria\""
## [19] "                     /mol_type=\"genomic DNA\""
## [20] "                     /db_xref=\"taxon:13129\""
## [21] "                     /note=\"Lythrum salicaria L.\""
## [22] "     rRNA            1..1740"
## [23] "                     /product=\"18S ribosomal RNA\""
## [24] "ORIGIN      "
## [25] "        1 gtcatatgct tgtctcaaag attaagccat gcatgtgtaa gtatgaacaa attcagactg"
## [26] "       61 tgaaactgcg aatggctcat taaatcagtt atagtttgtt tgatggtatc tgctactcgg"
## [27] "      121 ataaccgtag taattctaga gctaatacgt gcaacaaacc ccgacttctg gaagggacgc"
## [28] "      181 atttattaga taaaaggtcg acgcgggctt tgcccgatgc tctgatgatt catgataact"
## [29] "      241 tgacggatcg cacggccatc gtgccggcga cgcatcattc aaatttctgc cctatcaact"
## [30] "      301 ttcgatggta ggatagtggc ctaccatggt gtttacgggt aacggagaat tagggttcga"
## [31] "      361 ttccggagag ggagcctgag aaacggctac cacatccaag gaaggcagca ggcgcgcaaa"
## [32] "      421 ttacccaatc ctgacacggg gaggtagtga caataaataa caatactggg ctctttgagt"
## [33] "      481 ctggtaattg gaatgagtac aatctaaatc ccttaacgag gatccattgg agggcaagtc"
## [34] "      541 tggtgccagc agccgcggta attccagctc caatagcgta tatttaagtt gttgcagtta"
## [35] "      601 aaaagctcgt agttggacct tgggttgggt cgaccggtcc gcctttggtg tgcaccgatc"
## [36] "      661 ggctcgtccc ttctaccggc gatgcgcgcc tggccttaat tggccgggtc gttcctccgg"
## [37] "      721 tgctgttact ttgaagaaat tagagtgctc aaagcaagca ttagctatga atacattagc"
## [38] "      781 atgggataac attataggat tccgatccta ttatgttggc cttcgggatc ggagtaatga"
## [39] "      841 ttaacaggga cagtcggggg cattcgtatt tcatagtcag aggtgaaatt cttggattta"
## [40] "      901 tgaaagacga acaactgcga aagcatttgc caaggatgtt ttcattaatc aagaacgaaa"
## [41] "      961 gttgggggct cgaagacgat cagataccgt cctagtctca accataaacg atgccgacca"
## [42] "     1021 gggatcagcg aatgttactt ttaggacttc gctggcacct tatgagaaat caaagttttt"
## [43] "     1081 gggttccggg gggagtatgg tcgcaaggct gaaacttaaa ggaattgacg gaagggcacc"
## [44] "     1141 accaggagtg gagcctgcgg cttaatttga ctcaacacgg ggaaacttac caggtccaga"
## [45] "     1201 catagtaagg attgacagac tgagagctct ttcttgattc tatgggtggt ggtgcatggc"
## [46] "     1261 cgttcttagt tggtggagcg atttgtctgg ttaattccgt taacgaacga gacctcagcc"
## [47] "     1321 tgctaactag ctatgtggag gtacacctcc acggccagct tcttagaggg actatggccg"
## [48] "     1381 cttaggccaa ggaagtttga ggcaataaca ggtctgtgat gcccttagat gttctgggcc"
## [49] "     1441 gcacgcgcgc tacactgatg tattcaacga gtctatagcc ttggccgaca ggcccgggta"
## [50] "     1501 atctttgaaa tttcatcgtg atggggatag atcattgcaa ttgttggtct tcaacgagga"
## [51] "     1561 attcctagta agcgcgagtc atcagctcgc gttgactacg tccctgccct ttgtacacac"
## [52] "     1621 cgcccgtcgc tcctaccgat tgaatggtcc ggtgaaatgt tcggatcgcg gcgacgtggg"
## [53] "     1681 cgcttcgtcg ccgacgacgt cgcgagaagt ccattgaacc ttatcattta gaggaaggag"
## [54] "//"
```

Notice that each line is read in as a separate cell in a vector, with sequences beginning with a number ending with 1. We can take advantage of this to extract just the sequence data

6.12.1 Challenge

Before proceeding try to do the following:

1. Isolate only the rows containing DNA sequences. This should include a. Removing all of the characters that are not a, t, g, or c. b. Combining separate cells/lines into a single string. You can do this with using the `paste()` function with the `collapse=""` parameter
2. Convert lower-case to upper-case. To do this, you can use:

```
gsub("([actg])","\\U\\1",Seq,perl=T)
```

The `\\U\\\1` means ’paste brackets as upper-case, and is only available as a **Perl** command, which is accessible in gsub with the `perl=T` parameter. 3. Replace start codons (ATG) with "–>START–>ATG" 4. Replace stop codons (TAA or TAG or TGA) with TAA or TAG or TGA followed by ">–STOP–|"

Take the time to stuggle with this and try different combinations until you find a way through. The more you struggle, the faster you will learn.

A cool thing about regular expressions is that there is rarely a single right answer, especially for complicated problems. When you are ready, Continue on to see one possible solution.

6.13 Solutions

6.14 Transects

You want to look at only transect A for the first 3 species:

```
Transect[1:3,grep("A",names(Transect))]
```

```
##           A1         A2         A3
## 1  0.5547274 -0.2933032 -1.8640889
## 2 -0.6095312 -1.4151213 -1.1402859
## 3 -0.9280047 -1.4229605 -0.2768315
```

Subset the data for the first plot of each transect:

```
Transect[grep("1",names(Transect)),]
```

```
##   Species         A1          A2         A3         B1
## 2       b -0.6095312 -1.41512135 -1.1402859 -1.5219332
## 5       e  0.4275708 -1.15938397  0.3202867  0.5315643
## 8       h -0.9738583 -0.07433424 -1.3899374 -2.9097919
##           B2         B3         C1         C2         C3
## 2 -1.0418649 -1.5966388  0.5054574  0.9140523 -0.3635619
## 5 -0.3240292  0.5994643  0.5970771 -0.9129076 -0.5840427
## 8 -1.3064418  0.7259242 -0.4339716  0.6932336  0.2425620
```

6.15 Genbank

Use `.*` with `()` to delete everything before the DNA sequence

Use the `.*` and space with + to eliminate all text before the sequence :

Elimminate spaces and the two `//` at the end

Capital letters look nicer, but requires a PERL qualifier `\\U` that is not standard in R

Look for start codons?

Look for stop codons?

6.16 More Exercises

Here are some more exercises to practice your skils. No solutions are given for these, you will have to solve them on your own. Note that they may find their way onto a test, assignment or quiz.

6.16.1 1. Consider a vector of email addresses scraped from the internet:

- robert ‘dot’ colautti ‘at’ queensu ‘dot’ ca
- chris.eckert[at]queensu.ca
- lonnie.aarssen at queensu.ca

Use regular expressions to convert all email addresses to the standard format: name@queensu.ca

6.16.2 2. Create a random sequence of DNA:

```
My.Seq<-sample(c("A","T","G","C"),1000,replace=T)
```

- Replace T with U
- Find all start codons (AUG) and stop codons (UAA, UAG, UGA)
- Find all open reading frames (hint: consider each sequence beginning with AUG and ending with a stop codon; how do you know if both sequences are in the same reading frame?)
- Count the length of bp for all open reading frames

6.16.3 3. More online examples

http://regex.sketchengine.co.uk/extra_regexps.html

6.16.4 4. Regex Golf

Have fun! LINK

7 Data Science

7.1 Setup

If you don't have it installed, then run `install.packages("tidyverse")` – it can take a while to download and install.

The **tidyverse** library is a set of packages created by the same developers responsible for R Studio. There are a number of packages and functions that improve on base R. The name is based on the idea of living in a data universe that is neat and *tidy*.

The book R for Data Science by Hadley Wickham & Garrett Grolemund is an excellent resource for learning about the tidyverse. In this chapter we'll touch on a few of the main packages and functions.

> **Protip** In general, any book by Hadley Wickham that you come across is worth reading if you want to be proficient in R.

While we wait for the `tidyverse` to install, let's consider a few general principles of data science.

7.2 Introduction to Data Science

Data Science is a relatively new field of study that merges **computer science** and **statistics** to answer questions in other domains (e.g. business, medicine, biology, psychology). Data Science as a discipline has grown in popularity in response to the rapid rate of increase in data collection and publication.

Data Science often involves 'Big Data', which doesn't have a strict quantitative definition but will usually have one or more of the following characteristics:

1. High **Volume** – large file sizes with lots of observations.
2. Wide **Variety** – lots of different types
3. High **Velocity** – accumulating at a high rate
4. Compromised **Veracity** – variable quality that must be dealt otherwise downstream analyses will be compromised.

> What are some examples of 'big data' in Biology?

Medical records, remote sensing data (e.g. climate stations, satellite images), and ‘omics data are good examples of ’big data’ in biology.

In biology, it can be helpful to think of Data Science as a continuous life-cycle with multiple stages:

7.2.1 Data Science Life-Cycle

1. **Hypothesize** – Make initial observations of about the natural world, or insights from other data, that lead to testable hypotheses. Your core biology training is crucial here.
2. **Collect** – This may involve taking measurements yourself, manually entering data that is not yet in electronic format, requesting data from authors of published studies, or importing data from online sources. Collecting data is a crucial step that is often done poorly. Some tips on this are provided in a paper by Wu et al
3. **Correct** – Investigate the data for quality assurance, to identify and fix potential errors. Start to visualize the data to look for outliers or nonsensical relationships (or lack thereof).
4. **Explore** – Try to understand the data, where they come from, and potential limitations on their use. Continue visualizing data; this may cause you to modify your hypotheses slightly.
5. **Model** – Now that hypotheses are clearly defined, apply statistical tests of their validity.
6. **Report** – Use visualizations along with the results of your statistical tests to summarize your findings.
7. **Repeat** – Return to step 1.

In this tutorial, we focus mainly on coding in R for steps 2, 3, and 6. Step 5 requires a firm understanding of statistics. Step 4 is covered in the tutorials on qplot and ggplot. Step 1 is everything covered in a typical degree in the biological sciences.

Data collection and management are crucial steps in the Data Science Life-Cycle. Read the `baRcodeR` paper by Wu et al. called *baRcodeR with PyTrackDat: Open-source labelling and tracking of biological samples for repeatable science.* Pay particular attention to the ‘*Data Standards*’ section. The *baRcodeR* and *PyTrackDat* programs and their application to current projects may also be of interest.

7.3 2D Data Wrangling

The `dplyr` library in R has many useful features for importing and reorganizing your data for steps 2, 3 and 4 in the Data Science Life-Cycle outlined above. Don't forget to install the `dplyr` library and load it into memory.

```
library(dplyr)
```

```
##
## Attaching package: 'dplyr'

## The following object is masked from 'package:gridExtra':
##
##     combine

## The following objects are masked from 'package:stats':
##
##     filter, lag

## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

```
library(tidyr)
```

> Note: This error message just informs you that `dplyr` uses function or parameter names that are the same as other base or stats packages in R. These base/stats functions are 'masked' meaning that when you run one (e.g. `filter`) then R will run the `dplyr` version rather than the stats version.

We'll work with our FallopiaData.csv dataset, and remind ourselves of the structure of the data

7.3.1 `tibbles` and `readr()`

We looked at `data.frame` objects in the first chapter as an expansion of *matrices* with a few additional features like column and row names. A `tibble` is the `tidyverse` version of the `data.frame` object and includes a few more useful features. To import a dataset to a `tibble` instead of a `data.frame` object, we use `read_csv` instead of `read.csv`.

```
library(tidyverse)
```

```
## -- Attaching packages ---------------- tidyverse 1.3.2 --
## v tibble  3.1.8     v stringr 1.4.1
## v readr   2.1.3     v forcats 0.5.2
## v purrr   0.3.5
## -- Conflicts ------------------- tidyverse_conflicts() --
## x dplyr::combine()    masks gridExtra::combine()
## x dplyr::filter()     masks stats::filter()
## x dplyr::lag()        masks stats::lag()
## x readr::parse_date() masks curl::parse_date()
```

```
Fallo<-read_csv(
  "https://colauttilab.github.io/RCrashCourse/FallopiaData.csv")
```

```
## Rows: 123 Columns: 13
## -- Column specification ---------------------------------
## Delimiter: ","
## chr  (3): Scenario, Nutrients, Taxon
## dbl (10): PotNum, Symphytum, Silene, Urtica, Geranium, G...
##
## i Use `spec()` to retrieve the full column specification for this data.
## i Specify the column types or set `show_col_types = FALSE` to quiet this
```

```
str(Fallo)
```

```
## spc_tbl_ [123 x 13] (S3: spec_tbl_df/tbl_df/tbl/data.frame)
##  $ PotNum      : num [1:123] 1 2 3 5 6 7 8 9 10 11 ...
##  $ Scenario    : chr [1:123] "low" "low" "low" "low" ...
##  $ Nutrients   : chr [1:123] "low" "low" "low" "low" ...
##  $ Taxon       : chr [1:123] "japon" "japon" "japon" "japon" ...
##  $ Symphytum   : num [1:123] 9.81 8.64 2.65 1.44 9.15 ...
##  $ Silene      : num [1:123] 36.4 29.6 36 21.4 23.9 ...
##  $ Urtica      : num [1:123] 16.08 5.59 17.09 12.39 5.19 ...
##  $ Geranium    : num [1:123] 4.68 5.75 5.13 5.37 0 9.05 3.51 9.64 7.3 6.36 ...
##  $ Geum        : num [1:123] 0.12 0.55 0.09 0.31 0.17 0.97 0.4 0.01 0.47 0.33 ...
##  $ All_Natives : num [1:123] 67 50.2 61 40.9 38.4 ...
##  $ Fallopia    : num [1:123] 0.01 0.04 0.09 0.77 3.4 0.54 2.05 0.26 0 0 ...
##  $ Total       : num [1:123] 67.1 50.2 61.1 41.7 41.8 ...
##  $ Pct_Fallopia: num [1:123] 0.01 0.08 0.15 1.85 8.13 1.12 3.7 0.61 0 0 ...
##  - attr(*, "spec")=
##   .. cols(
##   ..   PotNum = col_double(),
##   ..   Scenario = col_character(),
##   ..   Nutrients = col_character(),
##   ..   Taxon = col_character(),
##   ..   Symphytum = col_double(),
##   ..   Silene = col_double(),
##   ..   Urtica = col_double(),
##   ..   Geranium = col_double(),
##   ..   Geum = col_double(),
##   ..   All_Natives = col_double(),
##   ..   Fallopia = col_double(),
##   ..   Total = col_double(),
##   ..   Pct_Fallopia = col_double()
##   .. )
##  - attr(*, "problems")=<externalptr>
```

This file is an example of a 2-dimensional data set, which is common in biology. 2D datasets have the familiar row x column layout used by spreadsheet programs like Microsoft Excel or Google Sheets. There are some exceptions, but data in this format should typically follows 3 rules:

1. Each cell contains a single value
2. Each variable must have its own column
3. Each observation must have its own row

Making sure your data are arranged this way will usually make it much easier to work with.

7.3.2 `filter()`

Let’s subset observations based on value

```
Pot1<-filter(Fallo,PotNum==1)
head(Pot1)
```

```
## # A tibble: 1 x 13
##   PotNum Scena~1 Nutri~2 Taxon Symph~3 Silene Urtica Geran~4
##    <dbl> <chr>   <chr>   <chr>   <dbl>  <dbl>  <dbl>   <dbl>
## 1      1 low     low     japon    9.81   36.4   16.1    4.68
## # ... with 5 more variables: Geum <dbl>, All_Natives <dbl>,
## #   Fallopia <dbl>, Total <dbl>, Pct_Fallopia <dbl>, and
## #   abbreviated variable names 1: Scenario, 2: Nutrients,
## #   3: Symphytum, 4: Geranium
```

7.3.3 `rename()`

It's possible to change the names of columns in your data. In base R you can use the `names()` function with the square bracket index `[]`:

```
X<-Fallo
names(X)
```

```
##  [1] "PotNum"       "Scenario"     "Nutrients"
##  [4] "Taxon"        "Symphytum"    "Silene"
##  [7] "Urtica"       "Geranium"     "Geum"
## [10] "All_Natives"  "Fallopia"     "Total"
## [13] "Pct_Fallopia"
```

```
names(X)[12]<-"Total_Biomass"
names(X)
```

```
##  [1] "PotNum"        "Scenario"       "Nutrients"
##  [4] "Taxon"         "Symphytum"      "Silene"
##  [7] "Urtica"        "Geranium"       "Geum"
## [10] "All_Natives"   "Fallopia"       "Total_Biomass"
## [13] "Pct_Fallopia"
```

There is also a simple `dplyr` function to do this:

7.3.4 `rename()`

```
X<-rename(Fallo, Total_Biomass = Total)
names(X)
```

```
##  [1] "PotNum"        "Scenario"      "Nutrients"
##  [4] "Taxon"         "Symphytum"     "Silene"
##  [7] "Urtica"        "Geranium"      "Geum"
## [10] "All_Natives"   "Fallopia"      "Total_Biomass"
## [13] "Pct_Fallopia"
```

7.3.5 `arrange()`

Use the `arrange()` function to sort the *rows* of your data based on the *columns* of your data. For example, let's re-arrange our FallopiaData.csv dataset based on Taxon (a string denoting the species of Fallopia used) and Total (a float denoting the total biomass in each pot).

```
X<-arrange(Fallo, Taxon, Total)
head(X)
```

```
## # A tibble: 6 x 13
##   PotNum Scena~1 Nutri~2 Taxon Symph~3 Silene Urtica Geran~4
##    <dbl> <chr>   <chr>   <chr>   <dbl>  <dbl>  <dbl>   <dbl>
## 1     26 low     low     bohem   13.2    18.1   0       0
## 2     17 low     low     bohem    4.9    29.5   1.36    0
## 3     80 gradual high    bohem   11.9    17.2   8.92    0.94
## 4     18 low     low     bohem    3.51   27.6   8.14    3.81
## 5     28 low     low     bohem   10.6    18.8   7.19    6.73
## 6     22 low     low     bohem    0.76   22.7   9.85   10.6
## # ... with 5 more variables: Geum <dbl>, All_Natives <dbl>,
## #   Fallopia <dbl>, Total <dbl>, Pct_Fallopia <dbl>, and
## #   abbreviated variable names 1: Scenario, 2: Nutrients,
## #   3: Symphytum, 4: Geranium
```

use the `desc()` function with `arrange()` to change reverse alphabetical order, or use - to sort from low to high

```
X<-arrange(Fallo, desc(Fallo), Taxon, -Total)
head(X)
```

```
## # A tibble: 6 x 13
##   PotNum Scena~1 Nutri~2 Taxon Symph~3 Silene Urtica Geran~4
##    <dbl> <chr>   <chr>   <chr>   <dbl>  <dbl>  <dbl>   <dbl>
## 1    149 fluctu~ high    bohem    1.72   10.4  23.5     8.51
## 2    148 fluctu~ high    bohem    4.15   38.7  23.6     5.11
## 3    147 fluctu~ high    bohem    7.84   31.2  13.6     6.58
## 4    145 fluctu~ high    bohem    4.89   32.9   6.3     9.64
## 5    144 fluctu~ high    bohem   19.9    21.1   6.08    2.8
## 6    143 fluctu~ high    bohem    5.06   12.8  23.8     3.64
## # ... with 5 more variables: Geum <dbl>, All_Natives <dbl>,
## #   Fallopia <dbl>, Total <dbl>, Pct_Fallopia <dbl>, and
## #   abbreviated variable names 1: Scenario, 2: Nutrients,
## #   3: Symphytum, 4: Geranium
```

7.3.6 `select()`

The `select()` function can be used to select a subset of columns (i.e. variables) from your data.

Suppose we only want to look at total biomass, but keep all the treatment columns:

```
X<-select(Fallo, PotNum, Scenario, Nutrients, Taxon, Total)
head(X)
```

```
## # A tibble: 6 x 5
##   PotNum Scenario Nutrients Taxon Total
##    <dbl> <chr>    <chr>     <chr> <dbl>
## 1      1 low      low       japon  67.1
## 2      2 low      low       japon  50.2
## 3      3 low      low       japon  61.1
## 4      5 low      low       japon  41.7
## 5      6 low      low       japon  41.8
## 6      7 low      low       japon  48.3
```

You can also use the colon `:` to select a range of columns:

```
X<-select(Fallo, PotNum:Taxon, Total)
head(X)
```

```
## # A tibble: 6 x 5
##   PotNum Scenario Nutrients Taxon Total
##    <dbl> <chr>    <chr>     <chr> <dbl>
## 1      1 low      low       japon  67.1
## 2      2 low      low       japon  50.2
## 3      3 low      low       japon  61.1
## 4      5 low      low       japon  41.7
## 5      6 low      low       japon  41.8
## 6      7 low      low       japon  48.3
```

Exclude columns with -

```
X<-select(Fallo, -PotNum:Taxon, -Total)
```

```
## Warning in x:y: numerical expression has 12 elements: only
## the first used
```

> Oops, what generated that error? Take a careful look at the error message and see if you can figure it out.

The problem is we are using the range of columns between PotNum and Taxon, but in one case we are excluding and the other we are including. We need to keep both the same:

```
X<-select(Fallo, -PotNum:-Taxon, Total)
head(X)
```

```
## # A tibble: 6 x 9
##   Symphy~1 Silene Urtica Geran~2  Geum All_N~3 Fallo~4 Total
##      <dbl>  <dbl>  <dbl>   <dbl> <dbl>   <dbl>   <dbl> <dbl>
## 1     9.81   36.4  16.1     4.68  0.12    67.0    0.01  67.1
## 2     8.64   29.6   5.59    5.75  0.55    50.2    0.04  50.2
## 3     2.65   36.0  17.1     5.13  0.09    61.0    0.09  61.1
## 4     1.44   21.4  12.4     5.37  0.31    40.9    0.77  41.7
## 5     9.15   23.9   5.19    0     0.17    38.4    3.4   41.8
## 6     6.31   24.4   7        9.05  0.97    47.7    0.54  48.3
## # ... with 1 more variable: Pct_Fallopia <dbl>, and
## #   abbreviated variable names 1: Symphytum, 2: Geranium,
## #   3: All_Natives, 4: Fallopia
```

Or a bit more clear:

```
X<-select(Fallo, -(PotNum:Taxon), Scenario)
head(X)
```

```
## # A tibble: 6 x 10
##   Symphy~1 Silene Urtica Geran~2  Geum All_N~3 Fallo~4 Total
##      <dbl>  <dbl>  <dbl>   <dbl> <dbl>   <dbl>   <dbl> <dbl>
## 1     9.81   36.4  16.1     4.68  0.12    67.0    0.01  67.1
## 2     8.64   29.6   5.59    5.75  0.55    50.2    0.04  50.2
## 3     2.65   36.0  17.1     5.13  0.09    61.0    0.09  61.1
## 4     1.44   21.4  12.4     5.37  0.31    40.9    0.77  41.7
## 5     9.15   23.9   5.19    0     0.17    38.4    3.4   41.8
## 6     6.31   24.4   7       9.05  0.97    47.7    0.54  48.3
## # ... with 2 more variables: Pct_Fallopia <dbl>,
## #   Scenario <chr>, and abbreviated variable names
## #   1: Symphytum, 2: Geranium, 3: All_Natives, 4: Fallopia
```

7.3.7 `everything()`

Use the `everything()` function with `select()` to rearrange your columns without losing any:

```
X<-select(Fallo, Taxon, Scenario, Nutrients, PotNum,
          Pct_Fallopia, everything())
head(X)
```

```
## # A tibble: 6 x 13
##   Taxon Scena~1 Nutri~2 PotNum Pct_F~3 Symph~4 Silene Urtica
##   <chr> <chr>   <chr>    <dbl>   <dbl>   <dbl>  <dbl>  <dbl>
## 1 japon low     low          1    0.01    9.81   36.4  16.1
## 2 japon low     low          2    0.08    8.64   29.6   5.59
## 3 japon low     low          3    0.15    2.65   36.0  17.1
## 4 japon low     low          5    1.85    1.44   21.4  12.4
## 5 japon low     low          6    8.13    9.15   23.9   5.19
## 6 japon low     low          7    1.12    6.31   24.4   7
## # ... with 5 more variables: Geranium <dbl>, Geum <dbl>,
## #   All_Natives <dbl>, Fallopia <dbl>, Total <dbl>, and
## #   abbreviated variable names 1: Scenario, 2: Nutrients,
## #   3: Pct_Fallopia, 4: Symphytum
```

7.3.8 `mutate()`

Suppose we want to make a new column (variable) to our data.frame object (dataset) that is the sum of biomass of Urtica and Geranium only. In base R you would use $:

```
X<-Fallo
X$UrtSil<-X$Urtica+X$Silene
```

In the dplyr package you can use mutate

```
X<-mutate(Fallo, UrtSil = Urtica + Silene)
head(X)
```

```
## # A tibble: 6 x 14
##   PotNum Scena~1 Nutri~2 Taxon Symph~3 Silene Urtica Geran~4
##    <dbl> <chr>   <chr>   <chr>   <dbl>  <dbl>  <dbl>   <dbl>
## 1      1 low     low     japon    9.81   36.4  16.1     4.68
## 2      2 low     low     japon    8.64   29.6   5.59    5.75
## 3      3 low     low     japon    2.65   36.0  17.1     5.13
## 4      5 low     low     japon    1.44   21.4  12.4     5.37
## 5      6 low     low     japon    9.15   23.9   5.19    0
## 6      7 low     low     japon    6.31   24.4   7       9.05
## # ... with 6 more variables: Geum <dbl>, All_Natives <dbl>,
## #   Fallopia <dbl>, Total <dbl>, Pct_Fallopia <dbl>,
## #   UrtSil <dbl>, and abbreviated variable names
## #   1: Scenario, 2: Nutrients, 3: Symphytum, 4: Geranium
```

This is a lot more readable, especially when you have complicated equations or you want to add lots of new columns.

> What if you only wanted to retain the new columns and delete everything else? Try it.

Which functions did you use?

7.3.9 `transmute()`

You can also use `transmute()` instead of `mutate()` + `select()`

```
X<-transmute(Fallo, UrtSil = Urtica + Silene)
head(X)
```

```
## # A tibble: 6 x 1
##   UrtSil
##    <dbl>
## 1   52.4
## 2   35.2
## 3   53.1
## 4   33.8
## 5   29.1
## 6   31.4
```

7.3.10 `summarize()` + `group_by()`

This can be useful for quickly summarizing your data, for example to find the mean or standard deviation based on a particular treatment or group.

```
TrtGrp<-group_by(Fallo,Taxon,Scenario,Nutrients)
summarize(TrtGrp, Mean=mean(Total), SD=sd(Total))
```

```
## `summarise()` has grouped output by 'Taxon', 'Scenario'.
## You can override using the `.groups` argument.
```

```
## # A tibble: 10 x 5
## # Groups:   Taxon, Scenario [10]
##    Taxon Scenario     Nutrients  Mean    SD
##    <chr> <chr>        <chr>     <dbl> <dbl>
##  1 bohem extreme      high       58.3  7.34
##  2 bohem fluctuations high       58.4  9.20
##  3 bohem gradual      high       57.5  9.34
##  4 bohem high         high       60.3  8.68
##  5 bohem low          low        48.0  8.86
##  6 japon extreme      high       57.2 10.9
##  7 japon fluctuations high       56.4 13.7
##  8 japon gradual      high       59.7  9.57
##  9 japon high         high       56.4  8.20
## 10 japon low          low        52.0  8.29
```

7.3.11 Weighted Mean

In our dataset, the **Taxon** column shows which of two species of *Fallopia* were used in the competition experiments. We might want to take the mean total biomass for each of the two *Fallopia* species:

```
X<-group_by(Fallo,Taxon)
summarize(X, Mean=mean(Total), SD=sd(Total))
```

```
## # A tibble: 2 x 3
##   Taxon  Mean    SD
##   <chr> <dbl> <dbl>
## 1 bohem  56.3  9.54
## 2 japon  56.4 10.4
```

However, there are other factors in our experiment that may affect biomass. The *Nutrients* column tells us whether pots received high or low nutrients, and this also affects biomass:

```
X<-group_by(Fallo,Nutrients)
summarize(X, Mean=mean(Total), SD=sd(Total))
```

```
## # A tibble: 2 x 3
##   Nutrients  Mean    SD
##   <chr>     <dbl> <dbl>
## 1 high       58.0  9.61
## 2 low        49.9  8.66
```

Now imagine if our sampling design is 'unbalanced'. For example, maybe we had some plant mortality or lost some plants to a tornado. If one of the two species in the *Taxon* column had more high-nutrient pots, then it would have a higher mean. BUT, the higher mean is not an effect of the Taxon, but is simply due to the unbalanced nature of the design. We can simulate this effect by re-shuffling the species names:

```
RFallo<-Fallo
set.seed(256)
RFallo$Taxon<-rbinom(nrow(RFallo),size=1,prob=0.7)

X<-group_by(RFallo,Taxon)
summarize(X, Mean=mean(Total))
```

```
## # A tibble: 2 x 2
##   Taxon  Mean
##   <int> <dbl>
## 1     0  56.1
## 2     1  56.5
```

To fix this problem, we may want to take a *weighted mean*:

```
X1<-group_by(RFallo,Taxon,Scenario,Nutrients)
Y1<-summarize(X1,Mean=mean(Total))
```

```
## `summarise()` has grouped output by 'Taxon', 'Scenario'.
## You can override using the `.groups` argument.
```

```
X2<-group_by(Y1,Taxon,Scenario)
Y2<-summarize(X2,Mean=mean(Mean))
```

```
## `summarise()` has grouped output by 'Taxon'. You can
## override using the `.groups` argument.
```

```
X3<-group_by(Y2,Taxon)
Y3<-summarize(X3, Mean=mean(Mean))
arrange(Y3,desc(Mean))
```

```
## # A tibble: 2 x 2
##   Taxon  Mean
##   <int> <dbl>
## 1     1  56.6
## 2     0  55.8
```

7.3.12 %>% (pipe)

The combination %>% is called ‘pipe’ for short. Be careful though – in Unix, ‘pipe’ is slightly different and uses the vertical line (often shift-backslash): |

The pipe is useful to combine operations without creating a whole bunch of new objects. This can save on memory use.

> Use `Ctl` + `Shift` + `m` to add a pipe quickly

For example, we can re-write the weighted mean example using pipes:

```
RFallo %>%
  group_by(Taxon,Scenario,Nutrients) %>%
  summarize(Mean=mean(Total)) %>%
  group_by(Taxon,Scenario) %>%
  summarize(Mean=mean(Mean)) %>%
  group_by(Taxon) %>%
  summarize(Mean=mean(Mean)) %>%
  arrange(desc(Mean))
```

```
## `summarise()` has grouped output by 'Taxon', 'Scenario'.
## You can override using the `.groups` argument.
## `summarise()` has grouped output by 'Taxon'. You can
## override using the `.groups` argument.
```

```
## # A tibble: 2 x 2
##   Taxon  Mean
##   <int> <dbl>
## 1     1  56.6
## 2     0  55.8
```

This also avoids potential for bugs in our program. Imagine if we mis-spelled ‘Taxon’ in our second line by accidentally pressing ‘s’ along with ‘x’. Compare the output:

```
X<-group_by(Fallo,Taxon,Scenario,Nutrients)
X<-group_by(X,Tasxon,Scenario)
```

```
## Error in `group_by()`:
## ! Must group by variables found in `.data`.
## x Column `Tasxon` is not found.
```

```
X<-group_by(X,Taxon)
X<-summarize(X, Mean=mean(Total), SD=sd(Total))
arrange(X,desc(Mean))
```

```
## # A tibble: 2 x 3
##   Taxon  Mean    SD
##   <chr> <dbl> <dbl>
## 1 japon  56.4 10.4
## 2 bohem  56.3  9.54
```

```
Fallo %>%
  group_by(Taxon,Scenario,Nutrients) %>%
  group_by(Tasxon,Scenario) %>%
  group_by(Taxon) %>%
  summarize(Mean=mean(Total), SD=sd(Total)) %>%
  arrange(desc(Mean))
```

```
## Error in `group_by()`:
## ! Must group by variables found in `.data`.
## x Column `Tasxon` is not found.
```

In both cases we get an error, but in one case we still calculate the means and sd of the two species.

> A bug that produces no output is much less dangerous than an error that gives an output. Why?

7.4 Join datasets

The `dplyr` package has some handy tools for joining datasets. There are four main ways to join datasets, similar to a Venn diagram. You can get more information on these with the help command `?join` after loading the dplyr library, but here is a quick overview. For each of these, imagine a Venn diagram with two datasets: X as a circle on the left side and Y as a circle on the right side. The rows we choose to combine from the two datasets depend on one or more identifying columns that we can define (e.g. sample ID, date, time).

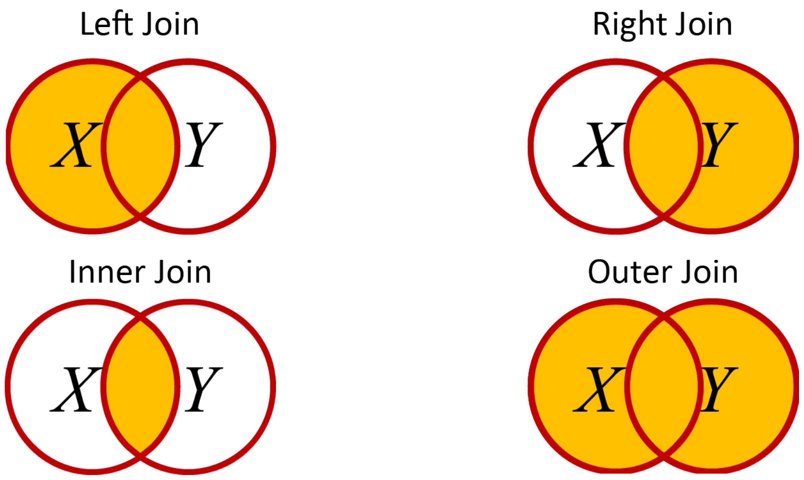


Figure 3: Venn diagram of datasets

`left_join()` - Keep all rows of X and add matching rows from Y. Any rows in Y that don't match X are excluded.

`right_join()` - The reverse of `left_join()`

`inner_join()` - Only keep rows that are common to **both** X **AND** Y. Remove any rows that don't match.

`full_join()` - Keep **any** columns that are in **either** X **OR** Y.

To try these out, we can create a couple of quick datasets and compare the output. For each case, note the addition of NA for missing data.

```r
X<-data.frame(ID=c("A","C"),Xdat=c(1,3))
Y<-data.frame(ID=c("B","C"),Ydat=c(2,3))
X
```

```
##   ID Xdat
## 1  A    1
## 2  C    3
```

```r
Y
```

```
##   ID Ydat
## 1  B    2
## 2  C    3
```

```r
left_join(X,Y,by="ID")
```

```
##   ID Xdat Ydat
## 1  A    1   NA
## 2  C    3    3
```

```r
right_join(X,Y,by="ID")
```

```
##   ID Xdat Ydat
## 1  C    3    3
## 2  B   NA    2
```

```r
inner_join(X,Y,by="ID")
```

```
##   ID Xdat Ydat
## 1  C    3    3
```

```r
full_join(X,Y,by="ID")
```

```
##   ID Xdat Ydat
## 1  A    1   NA
## 2  C    3    3
## 3  B   NA    2
```

7.5 Wide vs Long data

Most of the data examples we've looked at are in the 'wide' format, where we have a single individual as a row, and multiple measurements as separate columns.

However, there are many cases where we may want to reorganize our data into the 'long' format, where each row is an individual observation. Many statistical models use this format, and it's also useful for visualizations. For example, if we have a bunch of columns of data and we want to generate histograms quickly, we can use `facet_` functions from ggplot2 if our data is in the long format.

7.5.1 `pivot_longer`

The `pivot_longer()` function in the `tidyr` library does this. We use the `cols=` parameter to specify the data columns, then `names_to=` specifies the column name containing the parameter, and the `cols_to=` specifies the column name of the values.

This is a bit confusing to read, but it's easier to understand if you compare the output with the `full_join` function above.

```
LongData<-full_join(X,Y,by="ID") %>%
  pivot_longer(cols=c("Xdat","Ydat"),
               names_to="Measurement",
               values_to="Value")
LongData
```

```
## # A tibble: 6 x 3
##   ID    Measurement Value
##   <chr> <chr>       <dbl>
## 1 A     Xdat            1
## 2 A     Ydat           NA
## 3 C     Xdat            3
## 4 C     Ydat            3
## 5 B     Xdat           NA
## 6 B     Ydat            2
```

Note how there is only 1 column of data values, with the `Measurement` column indicating which measurement the value belongs to, and the `ID` column is repeated for each measurement.

This is why the *long* data format is sometimes called the *repeated measures* data format.

7.5.2 `pivot_wider`

The `pivot_wider()` function does the reverse, but this time we specify the column that contains the values with `values_from=` and the corresponding column names with `names_from=`. This should recover the original dataset:

```
WideData<-LongData %>%
  pivot_wider(values_from=Value,
              names_from=Measurement)
WideData
```

```
## # A tibble: 3 x 3
##   ID     Xdat  Ydat
##   <chr> <dbl> <dbl>
## 1 A         1    NA
## 2 C         3     3
## 3 B        NA     2
```

7.6 Missing Data

So far we have worked on a pristine data set that has already been edited for errors. More often datasets will contain missing values.

7.6.1 `NA` and `na.rm()`

The R language uses a special object `NA` to denote missing data.

```
Vec<-c(1,2,3,NA,5,6,7)
Vec
```

```
## [1]  1  2  3 NA  5  6  7
```

When a function is run on a vector or other object containing NA, the function will often return NA or give an error message:

```
mean(Vec)
```

```
## [1] NA
```

This is by design, because it is not always clear what NA means. Many functions in R include an na.rm parameter that is set to FALSE by default. Setting it to true tells the function to ignore the NA

```
mean(Vec, na.rm=T)
```

```
## [1] 4
```

7.6.2 `NA` vs `0`

A common mistake students make is to put 0 for missing data. This can be a big problem when analyzing the data since the calculations are very different.

```
Vec1<-c(1,2,3,NA,5,6,7)
mean(Vec1, na.rm=T)
```

```
## [1] 4
```

```
Vec2<-c(1,2,3,0,5,6,7)
mean(Vec2, na.rm=T)
```

```
## [1] 3.428571
```

7.6.3 `is.na()`

In large datasets you might want to check for missing values. Let's simulate this in our *FallopiaData.csv* dataset.

To set up a test dataset, randomly select 10 rows and replace the value for 'Total' with NA. The `sample` function is a

```
X<-round(runif(10,min=1,max=nrow(Fallo)),0)
Fallo$Total[X]<-NA
Fallo$Total
```

```
##   [1] 67.06 50.22 61.08 41.71 41.81 48.27 55.42 42.68    NA
##  [10] 45.89 59.02 57.66 48.98 35.97 43.28 52.27 45.92 44.61
##  [19] 59.13 58.97 55.36 31.46 43.46 44.65 59.69 60.82 57.21
##  [28] 34.09 58.57 66.74 63.18    NA 54.09 55.27 61.31 53.56
##  [37] 52.66 64.71 61.06 45.34 64.20 57.50 68.55 49.55 56.70
##  [46] 54.06 66.60 74.82 53.71 49.75 58.45 66.06 67.01 70.41
##  [55]    NA 63.43 77.05 47.50 61.79 54.96 48.99 52.01    NA
##  [64] 57.18 42.47 46.18 62.56 54.36 69.54 75.91 56.34 64.97
##  [73] 60.71 57.80 41.72 67.44 58.78    NA    NA 58.42 55.35
##  [82]    NA 55.04 39.56 71.07 45.23 57.20 67.70 52.46 60.86
##  [91]    NA 65.53 48.19 60.89 48.13 60.37 67.86 56.40 49.13
## [100] 56.11 49.78 69.00 65.40 50.73 63.08 60.93    NA 49.12
## [109] 68.73 31.90 69.88 69.48 47.88 51.42 58.13 50.51 54.83
## [118] 66.80 50.31 56.12 62.96 78.80 64.25
```

Use `is.na()` to check for missing values:

```
is.na(Fallo$Total)
```

```
##   [1] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
##  [10] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [19] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [28] FALSE FALSE FALSE FALSE  TRUE FALSE FALSE FALSE FALSE
##  [37] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [46] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [55]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE
##  [64] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [73] FALSE FALSE FALSE FALSE FALSE  TRUE  TRUE FALSE FALSE
##  [82]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
##  [91]  TRUE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [100] FALSE FALSE FALSE FALSE FALSE FALSE FALSE  TRUE FALSE
## [109] FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE FALSE
## [118] FALSE FALSE FALSE FALSE FALSE FALSE
```

Note that the output is a vector of True/False. Each cell corresponds to a value of ‘Total’ with TRUE indicating missing values. This is an example of a boolean variable, which has some handy properties in R.

First, we can use it as an index. For example, let’s see which pots have missing ‘Total’ values:

```
Missing<-is.na(Fallo$Total)
Fallo$PotNum[Missing]
```

```
## [1]  10  39  68  78  95  96 100 111 129
```

Another handy trick to count missing values is:

```
sum(is.na(Fallo$Total))
```

```
## [1] 9
```

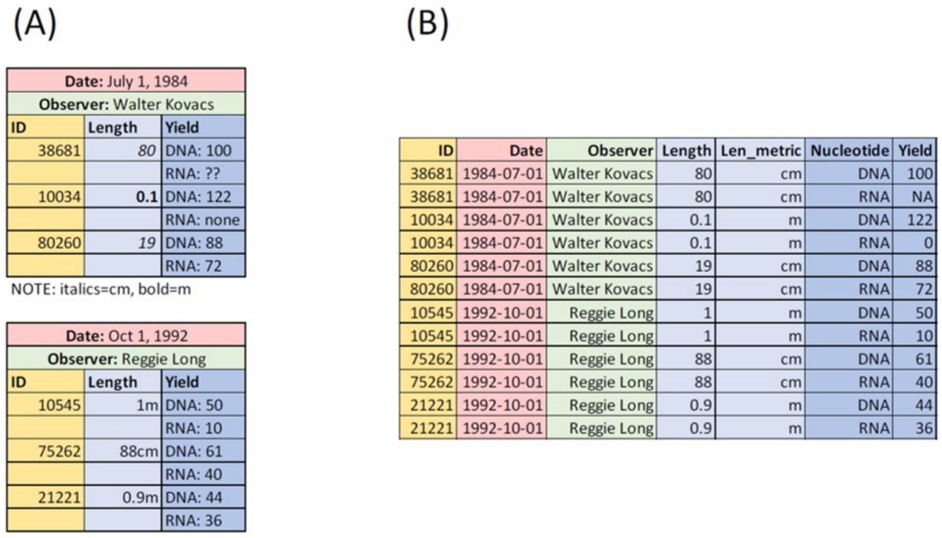
This takes advantage of the fact that the boolean TRUE/FALSE variable is equivalent to the binary 1/0 values.

7.7 Naughty Data

Naughty data contain the same information as a standard row x column (i.e. 2-dimensional) dataset but break the rules outlined above:

1. Each cell contains a single value
2. Each variable must have its own column
3. Each observation must have its own row

Examples of Naughty Data are shown in Figure 2A of the Wu et al. manuscript.



(A)

Date: July 1, 1984		
Observer: Walter Kovacs		
ID	**Length**	**Yield**
38681	*80*	DNA: 100
		RNA: ??
10034	**0.1**	DNA: 122
		RNA: none
80260	*19*	DNA: 88
		RNA: 72

NOTE: italics=cm, bold=m

Date: Oct 1, 1992		
Observer: Reggie Long		
ID	**Length**	**Yield**
10545	1m	DNA: 50
		RNA: 10
75262	88cm	DNA: 61
		RNA: 40
21221	0.9m	DNA: 44
		RNA: 36

(B)

ID	Date	Observer	Length	Len_metric	Nucleotide	Yield
38681	1984-07-01	Walter Kovacs	80	cm	DNA	100
38681	1984-07-01	Walter Kovacs	80	cm	RNA	NA
10034	1984-07-01	Walter Kovacs	0.1	m	DNA	122
10034	1984-07-01	Walter Kovacs	0.1	m	RNA	0
80260	1984-07-01	Walter Kovacs	19	cm	DNA	88
80260	1984-07-01	Walter Kovacs	19	cm	RNA	72
10545	1992-10-01	Reggie Long	1	m	DNA	50
10545	1992-10-01	Reggie Long	1	m	RNA	10
75262	1992-10-01	Reggie Long	88	cm	DNA	61
75262	1992-10-01	Reggie Long	88	cm	RNA	40
21221	1992-10-01	Reggie Long	0.9	m	DNA	44
21221	1992-10-01	Reggie Long	0.9	m	RNA	36

Figure 2. Example of (A) common errors in data management and (B) corresponding rearrangement of the same data to simplify reproducible data wrangling and analysis. Note that colours are added to show link between data in A and B and do not appear in the final text-based file (e.g. TXT, CSV, TSV).

Naughty data can be very time consuming to fix, but regular expressions can make this a bit easier (see the Regex tutorial).

7.8 Dates

As biologists, we often work with dates. We may want to analyze the date a sample was collected, or a measurement was taken. But dates are often encoded in formats that can't be analyzed directly. The `lubridate` package provides a convenient framework for switching between human-readable dates and mathematical relationships among them – for example, the number of days, minutes, or seconds between two time points.

```
library(lubridate)
```

```
## Loading required package: timechange

##
## Attaching package: 'lubridate'
## The following objects are masked from 'package:base':
##
##     date, intersect, setdiff, union
```

It can be convenient to automatically include the current date or time, especially when you are producing reports.

We can get the date, which we will call a `date` object

```
today()
```

```
## [1] "2022-11-23"
```

And we can get the date and time, which we will call a `datetime` object

```
now()
```

```
## [1] "2022-11-23 20:44:39 EST"
```

This is an important distinction, because the `datetime` object extends on the `date` object to include hours, minutes, seconds, etc.

We can use a `datetime` object to track how long it takes to run a particular program. We first create an object to store the computer clock before the program runs, then we subtract that object from the compter clock afterthe program finishes:

```
Before<-now()

for(i in 1:1000){
  rpois(10,lambda=10)^rnorm(10)
}

now()-Before
```

```
## Time difference of 0.008574963 secs
```

> **Protip**: Try adding a `print()` function to print out the result in each iteration of the for loop. How much does this slow down the run time?

7.8.1 `date` Objects

Human-readable dates come in many different forms, which we can encode as strings. Here are some examples that we might see for encoding the end-date of the most recent 5,126-year-long Mesoamerican calendar used by the ancient Maya:

```
Date2<-"2012-12-21"
Date3<-"21.12.2012"
Date4<-"Dec 21, 2012"
Date5<-"21 December, 2012"
```

The `lubridate` package has a number of related functions that correspond to the order of entry – `d` for day, `m` for month, and `y` for year:

```
ymd(Date2)
```

```
## [1] "2012-12-21"
```

```
dmy(Date3)
```

```
## [1] "2012-12-21"
```

```
mdy(Date4)
```

```
## [1] "2012-12-21"
```

```
dmy(Date5)
```

```
## [1] "2012-12-21"
```

Notice the flexibility here! Some dates have dashes, dots, spaces, and commas! But all are converted to a common object type. On the surface, these objects look like simple strings, but let's investigate:

```
str(Date2)
```

```
##  chr "2012-12-21"
```

```
str(ymd(Date2))
```

```
##  Date[1:1], format: "2012-12-21"
```

Notice how the first is a simple `chr` character object, whereas the second is a `Date` object. The date object can be treated as a numeric variable, that outputs as a readable date. For example, what if we want to know what the date 90 days before or after?

```
c(ymd(Date2)-90,ymd(Date2)+90)
```

```
## [1] "2012-09-22" "2013-03-21"
```

The above examples are single strings, but we can just as easily work with a column in a data frame or any other vector of strings:

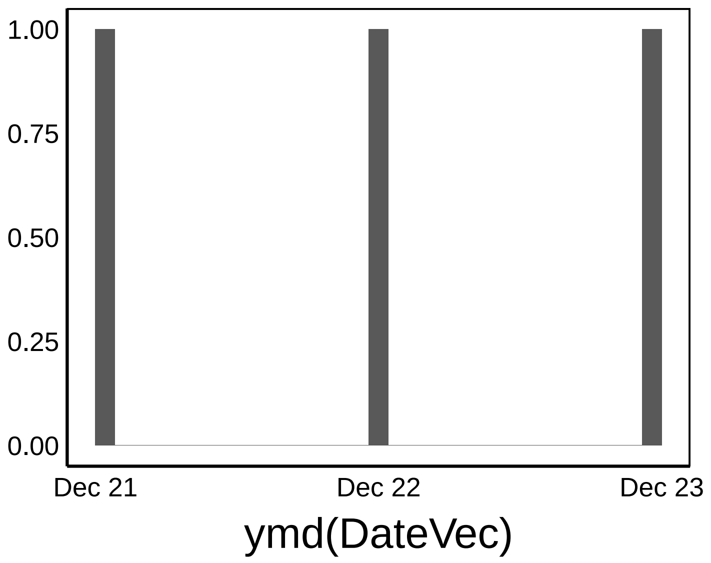
```
DateVec<-c("2012-12-21","2012-12-22","2012-12-23")
ymd(DateVec)
```

```
## [1] "2012-12-21" "2012-12-22" "2012-12-23"
```

Because these objects are numeric, we can also use them for plotting:

```
qplot(ymd(DateVec))
```

```
## `stat_bin()` using `bins = 30`. Pick better value with
## `binwidth`.
```



7.8.2 `datetime`

The `datetime` object adds a time element to the date with an underscore _ separating the time elements from the day, encoding . Here are a couple of examples

```
mdy_h("Dec 21, 2012 -- 10am")
```

```
## [1] "2012-12-21 10:00:00 UTC"
```

```
ymd_hm("2012-12-21, 08:30")
```

```
## [1] "2012-12-21 08:30:00 UTC"
```

```
dmy_hms("21 December, 2012; 11:59:59")
```

```
## [1] "2012-12-21 11:59:59 UTC"
```

7.8.3 Extracting Components

We can extract components from date objects

```
year(Date2)
```

```
## [1] 2012
```

```
month(Date2)
```

```
## [1] 12
```

We have several options for days.
First, we can get the day of the year, also known as the Julian day:

```
yday(Date2)
```

```
## [1] 356
```

Or the day of the month

```
mday(Date2)
```

```
## [1] 21
```

or the day of the week (rather than month) using `wday()`

```
wday(Date2)
```

```
## [1] 6
```

We can use the `label=T`parameter with the above, to get the specific month or day

```
month(Date2, label=T)
```

```
## [1] Dec
## 12 Levels: Jan < Feb < Mar < Apr < May < Jun < ... < Dec
```

```
wday(Date2, label=T)
```

```
## [1] Fri
## Levels: Sun < Mon < Tue < Wed < Thu < Fri < Sat
```

7.8.4 Categorical dates

We've seen above how dates are more like `numeric` rather than `strings`, but we can also treat dates as categorical data.

One example that is becoming more and more common in biology is the analysis of data from data loggers, which automatically save observations over time. Think of climate stations that measure temperature and precipitation as a common example. Another example might be location information of a study organism using image analysis or PIT tags (i.e. Passive Integrated Transponders).

In many cases, the timescale of collection is much shorter than what we need. Luckily, `dplyr` with `lubridate` are great tools for summarizing these data!

> Example: imagine we have observations taken every minute, and we just want to calculate the average for each hour in R. We can generate a toy dataset in R using the tibble function, and then assigning column names: DayTime for the day-time object and Obs for the observation (i.e. measurement):

First, we create the imaginary dataset, using the replicate function and the a random number generator:

```
TestData<-tibble(
  DayTime=now()+minutes(rep(c(0:359),100)),
  Obs=rnorm(36000))
```

We can calculate the hourly average by piping our TestData tibble (above) through a group_by and then a summarize function.

```
TestData %>%
  group_by(yday(DayTime),hour(DayTime)) %>%
  summarize(Mean=mean(Obs))
```

```
## `summarise()` has grouped output by 'yday(DayTime)'. You
## can override using the `.groups` argument.
```

```
## # A tibble: 7 x 3
## # Groups:   yday(DayTime) [2]
##   `yday(DayTime)` `hour(DayTime)`     Mean
##             <dbl>           <int>    <dbl>
## 1             327              20  0.0108
## 2             327              21 -0.0125
## 3             327              22  0.00744
## 4             327              23 -0.00957
## 5             328               0 -0.0204
## 6             328               1 -0.0281
## 7             328               2  0.00422
```

Question Why do we include `yday` in the group_by function.

HINT: Try removing `yday(DayTime)` and compare the output

8 Advanced R

8.1 Introduction

By now you have mastered the fundamentals of base R, visualizations, and data science!

In this tutorial, we will cover some a few of the more advanced but extremely useful topics.

8.2 Getting Started

Before beginning this tutorial, make sure you have installed these packages:

```
install.packages('rmarkdown')
install.packages('dplyr')
install.packages('knitr')
```

8.3 R Markdown

R Markdown is a powerful format for quickly making high-quality reports of your analysis. You can embed code and all kinds of output, including graphs, and output them to a Word Document, PDF or website. In fact, all of our tutorial webpages are written in R Markdown, including this one!

Here we'll cover just the basics, but a complete guide to R Markdown is available online from Yihui Xie, J. J. Allaire and Garrett Grolemund. You can also check out the R Markdown documents that we use to make our tutorial websites on our GitHub Pages (the website files have .html extension and the R Markdown files have the same name with .Rmd extensions):

- Main Colautti Lab Resources Website and GitHub Repository
- R Tutorials and GitHub Repository

8.3.1 Cheat Sheet

There is a very handy 2-page 'cheat sheet' that you can print out to help you remember some of the main commands. I use R Markdown for all kinds of documents

– including course tutorials like this one – so I have the 2-page cheat sheet printed out and taped to my wall next to my computer.

You can also access cheat sheets for R Markdown and several others R Studio also includes a number of cheat sheets under the *Help* menu: `Help -> Cheatsheets`

8.3.2 Create

In RStudio: `File-> New-> R Markdown`

Choose `Document` from the left-hand side menu

Make sure `html` is selected

Then click `OK`

Very few elements are needed for a basic markdown file, and these are provided when you create a new file.

8.3.3 YAML Header

This is generated automatically when you make a new .Rmd file in RStudio. Depending on what options you choose, it might look something like this:

```
---
title: "Untitled"
author: "Robert I. Colautti"
date: "January 20, 2019"
output: html_document
---
```

There are other options available for YAML, and you can includes a separate `_output.yml` to set other aspects of the layoug.

8.3.4 Markdown

R Markdown is based on the markdown language, which was created as a quick and easy way to encode formatted websites in a simple text document.

R Markdown has a few additions, including the ability to easily incorporate R code, graphs, and equations.

8.3.5 Basic elements:

8.3.5.1 Plain text

Plain text is converted into paragraph format.

To start a new paragraph, press *enter* twice, so to skip a line in the .Rmd file.

8.3.5.2 Formatted text

You can format text with `*` or `_`

`*italics*` or `_italics_`: *italics*

`**bold**` or `__bold__`: **bold**

Use greater-than sign for block quotes, eg. `> TIP: quote`

> TIP: quote

8.3.6 Headers

Add headers with up to 6x `#` – more headers = subheadings:

```
# Header 1
## Sub-Header = Header 2
### Sub-Sub Header = Header 3
#### Sub-Sub-Sub Header = Header 4
```

8.3.7 Other Elements

`--` for short–dash (a.k.a. 'n-dash'): –

`---` for long — dash (a.k.a. m-dash: —

8.3.8 Links

Links have a special format. The text you want the user to see goes in square brackets, followed immediately by the file or html link in regular brackets, with no space in between:

`[Colautti Lab Website](https://colauttilab.github.io/)`:

Colautti Lab Website

You can also use this with relative path names, for example to link a file in a folder called `images` inside of the project folder:

`[Linked .png file](./images/ColauttiLabLogo.png):`

Linked .png file

8.3.9 Images

Or you can embed the image directly by adding an exclamation point. You can leave the linked text blank or keep it to use as a caption.

`![Linked .png file](./images/ColauttiLabLogo.png):`

Figure 4: Linked .png file

8.3.10 Lists and tables

Lists are easy to create, simply start a line with ∗ or + for *unordered* lists or a number for *ordered* lists. Add tab characters for sub-lists:

```
+ Unordered list item 1
* Item 2
    + sub item 2.1
    * sub item 2.2
* Item 3
```

- Unordered list item 1
- Item 2

    - sub item 2.1
    - sub item 2.2

- Item 3

```
1. Ordered list item 1
2. Item 2
    + sub item 2.1
    * sub item 2.2
3. Item 3
```

1. Ordered list item 1

2. Item 2

    - sub item 2.1

    - sub item 2.2

3. Item 3

The fun thing about ordered lists is the numbers you use don't really matter – R Markdown will automatically start at 1 and increase for each item.

```
1. Ordered list item 1
1. Item 2
    + sub item 2.1
    * sub item 2.2
1. Item 3
```

1. Ordered list item 1

2. Item 2

    - sub item 2.1

    - sub item 2.2

3. Item 3

Tables are added using vertical pipe | to denote columns, and a line of horizontal dashes to separate the title of the table, and dashes with pipes to separate the header row from the rest of the table. For example, this code:

```
Tables
-----------------------


Date   | Length   | Width
------|---------|------
09/09/09 | 14 | 27
10/09/09 | 15 | 29
11/09/09 | 16 | 31
```

Produces this output:

8.4 Tables

Date	Length	Width
09/09/09	14	27
10/09/09	15	29
11/09/09	16	31

8.4.1 Embed R Code

Embed R code inline using the back-tick ‘ character: `embedded code`

Note that the back-tick is not the single quotation mark. It’s often on the same key as ~ on North American keyboards.

You can add larger blocks of code (multiple lines) using three back ticks ‘ and r in curly brackets. Then add three more tick marks after the code chunk:

```
#      ```{r}
#       <<your code goes here>>
#      ```
```

`Ctl-Alt-i` is a nice shortcut in R Studio for adding code chunks quickly

8.4.1.1 Code Chunk Names

You can name your code chunks, which becomes useful when making custom packages or other knitr uses. The name is added after the `r` separated only by spaces. The name cannot contain spaces. E.g. “‘`{r code-chunk-name, eval=F}`

8.4.1.2 Suppress code

You can use different options for your R code chunks, as shown on the cheatsheet. Three main ones are:

- `eval=F` – show the code but don’t run it.
- `include=F` – run the code but don’t show it and and don’t produce any output, plots, messages or warnings.
- `echo=F` – don’t show the code but run it and include any output, plots, messages and warnings.

8.4.2 Dynamic tables

Making tables from data is a bit more complicated. For example, if we wanted to summarize the `FallopiaData.csv` data, we could read in the file and then summarize with dplyr as we did in the Data Science Tutorial:

```
library(dplyr)

Fallo<-read.csv(
  "https://colauttilab.github.io/RCrashCourse/FallopiaData.csv")

SumTable<-Fallo %>%
  group_by(Taxon,Scenario,Nutrients) %>%
  summarize(Mean=mean(Total), SD=sd(Total)) %>%
  arrange(desc(Mean))

print(SumTable)
```

```
## # A tibble: 10 x 5
## # Groups:   Taxon, Scenario [10]
##    Taxon Scenario     Nutrients  Mean    SD
##    <chr> <chr>        <chr>     <dbl> <dbl>
##  1 bohem high         high       60.3  8.68
##  2 japon gradual      high       59.7  9.57
```

Table 7: Summary Table

Taxon	Scenario	Nutrients	Mean	SD
bohem	high	high	60.28091	8.677075
japon	gradual	high	59.72917	9.565376
bohem	fluctuations	high	58.36455	9.202334
bohem	extreme	high	58.30917	7.337015
bohem	gradual	high	57.46154	9.338311
japon	extreme	high	57.23643	10.903133
japon	high	high	56.44833	8.204091
japon	fluctuations	high	56.43692	13.724906
japon	low	low	52.02917	8.287938
bohem	low	low	47.98077	8.862164

```
##  3 bohem fluctuations high       58.4  9.20
##  4 bohem extreme      high       58.3  7.34
##  5 bohem gradual      high       57.5  9.34
##  6 japon extreme      high       57.2 10.9
##  7 japon high         high       56.4  8.20
##  8 japon fluctuations high       56.4 13.7
##  9 japon low          low        52.0  8.29
## 10 bohem low          low        48.0  8.86
```

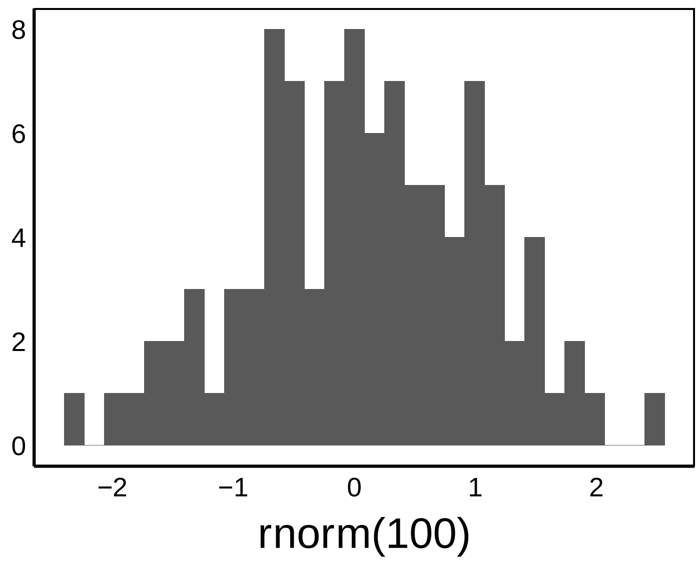
The output is legible but not very attractive for a final report. To make it look better, we can use the `kable` function from the `knitr` package:

```
library(knitr)
kable(SumTable, caption = "Summary Table")
```

8.4.3 Embed Graphs

Use R code to embed graphs.

```
qplot(rnorm(100))
```



8.4.4 Options for header

```
output:
  html_document: # Add options for html output
    toc: true # Add table of contents (TOC)
    number_sections: true # Add section numbers
    toc_float: # Have TOC floating at the side
      collapsed: false # Expand subsections
```

8.4.5 Content as tabs

```
## Quarterly Results {.tabset}

### By Product

(Product tab content)
```

```
### By Region

(Region tab content)
```

Looks like this:

8.4.6 Quarterly Results

8.4.6.1 By Product (Product tab content)

8.4.6.2 By Region (Region tab content)

8.4.7 Equations

Insert equations using LaTeX equations, which come in two forms:

1. Use single dollar signs for in-line equations, like `$Y = X$`, which will print as $Y = X$
2. Use double dollar signs on a new line for full-line equations, like `$$Y = X$$`:

$$Y = X$$

You can use a variety of Greek letters by using the backslash character `\`. For upper-case Greek letters, just use an upper-case letter in the spelling. For example:

- `\lambda`: λ OR `\Lambda` : Λ
- `\gamma`: γ OR `\Gamma`: Γ
- `\delta`: δ OR `\Delta`: Δ
- etc.

  Omicron is an odd exception; simply the letter o, with no backslash `o`: o

There are numerous other options but below is a quick rundown of some of the commonly used scripts. Create an R Markdown document and type each of these with either the inline `$` or new-line `$$`. Compare the rendered document with the input code:

Script	Description	Code	Example
`_`	Subscript	`X_i`	X_i
`^`	Superscript	`X^2`	X^2
`\sim`	Predict	`Y \sim X`	$Y \sim X$
`\times`	Multiply	`X \times Y`	$X \times Y$
`\pm`	Plus or minus	`X \pm Y`	$X \pm Y$
`\neq`	Note equal	`X \neq Y`	$X \neq Y$
`\leq`	Less than or equal	`X \leq Y`	$X \leq Y$
`\geq`	Greater than or equal	`X \geq Y`	$X \geq Y$
`{}`	Group together	`X_{subscript}`	$X_{subscript}$
`\frac`	Fraction	`\frac{X+1}{X-1}`	$\frac{X+1}{X-1}$
`\sum`	Sum	`\sum_{x=1}^{K}`	$\sum_{x=1}^{K}$
`\prod`	Product	`\prod_{x=1}^{K}`	$\prod_{x=1}^{K}$

To see how curly brackets `{}` work, try removing them from the code above, and then re-create your R markdown output.

Here are some more sophisticated examples. Again, try reproducing these in R markdown. If you don't get the same output, then check to see what is different with your code.

```
$$\idotsint_V \mu(u_1,\dots,u_k) \,du_1 \dots du_k$$
```

will produce:

$$\idotsint_V \mu(u_1,\dots,u_k) \,du_1 \dots du_k$$

and

```
$$sum_{n=1}^{\infty} 2^{-n} = 1$$
```

will produce:

$$\sum_{n=1}^{\infty} 2^{-n} = 1$$

Notice the use of special characters with the backslash \, along with subscripts _ and superscripts _ with the super/subscripted text in curly brackets {}

8.5 Custom Functions

8.5.1 General form:

Don't type this out, but read through it. This is called pseudocode. The purpose is to give you a general sense of how to create functions. We have variables (var1 and var2) and we can assign default values (Default1 and Default2), then we put in a bunch of lines of code (Meat and potatoes script) and return an output.

```
functionName<-function(var1=Default1,var2=Default2){
  ## Meat and potatoes script
  return(output)
}
```

You should already have a good sense of how functions work from all of the other tutorials/chapters. Now let's work through an example.

8.5.2 Example function

User inputs two objects; the function outputs a list of functions applied to the inputs

```r
my.function<-function(var1=0,var2=0){
  # You can make new variables within a function
  add<-var1+var2
  subt<-var1-var2
  mult<-var1*var2
  div<-var1/var2
  outlist<-list(input1=var1, input2=var2,
                addition=add, subtraction=subt,
                multiplication=mult, division=div)
  # So far, everything is contained within the function.
  # Use return() to generate output
  return(outlist)
}
```

Note: Nothing output when the funciton is run. This just loads the function into memory.

8.5.2.1 Run the function

Try running the function on its own, with default values:

```r
my.function()
```

```
## $input1
## [1] 0
##
## $input2
## [1] 0
##
## $addition
## [1] 0
##
## $subtraction
## [1] 0
##
## $multiplication
## [1] 0
##
## $division
## [1] NaN
```

Now try specifying the input parameters and compare the output.

```r
my.function(var1=10,var2=0.1)
```

```
## $input1
## [1] 10
##
## $input2
## [1] 0.1
##
## $addition
## [1] 10.1
##
## $subtraction
## [1] 9.9
##
## $multiplication
## [1] 1
##
## $division
## [1] 100
```

```r
my.function(var1=c(1:10),var2=c(10:1))
```

```
## $input1
##  [1]  1  2  3  4  5  6  7  8  9 10
##
## $input2
##  [1] 10  9  8  7  6  5  4  3  2  1
##
## $addition
##  [1] 11 11 11 11 11 11 11 11 11 11
##
## $subtraction
##  [1] -9 -7 -5 -3 -1  1  3  5  7  9
##
## $multiplication
##  [1] 10 18 24 28 30 30 28 24 18 10
##
```

```
## $division
##  [1]  0.1000000  0.2222222  0.3750000  0.5714286  0.8333333
##  [6]  1.2000000  1.7500000  2.6666667  4.5000000 10.0000000
```

Protip #1:

Consider annotating long or complex script with `cat()` to help with troubleshooting. The `cat` function is similar to `print` but lets you print directly to screen rather than passing through a data object. Note that `\n` is a ’new line‘ character; try removing them and compare the output.

```
my.function<-function(var1=0,var2=0){
  cat("\nInput variables:\nvar1 =", var1,"\nvar2 =", var2,"\n")
  cat("\nCalculating functions...\n")
  cat("\nAdding...\n")

  add<-var1+var2

  cat("\nSubtracting...\n")

  subt<-var1-var2

  cat("\nMultiplying...\n")

  mult<-var1*var2

  cat("\nDividing...\n")

  div<-var1/var2

  cat("\nGenerating output...\n\n")

  outlist<-list(input1=var1, input2=var2,
                addition=add, subtraction=subt,
                multiplication=mult, division=div)

  return(outlist)
}
```

```r
## Run
my.function(var1=10,var2=0.1)
```

```
##
## Input variables:
## var1 = 10
## var2 = 0.1
##
## Calculating functions...
##
## Adding...
##
## Subtracting...
##
## Multiplying...
##
## Dividing...
##
## Generating output...

## $input1
## [1] 10
##
## $input2
## [1] 0.1
##
## $addition
## [1] 10.1
##
## $subtraction
## [1] 9.9
##
## $multiplication
## [1] 1
##
## $division
## [1] 100
```

Printing text to the screen can slow down your function considerably. A good practice is to provide output as a user-defined option by adding a ‘verbose’ parameter and an if() statement.

```r
my.function<-function(var1=0,var2=0,verbose=FALSE){
  if(verbose==T){
    cat("\nInput variables:\nvar1 =", var1,"\nvar2 =", var2,"\n")
    cat("\nCalculating functions...\n")
    cat("\nAdding...\n")
  }

  add<-var1+var2

  if(verbose==T){
    cat("\nSubtracting...\n")
  }

  subt<-var1-var2

  if(verbose==T){
    cat("\nMultiplying...\n")
  }

  mult<-var1*var2

  if(verbose==T){
    cat("\nDividing...\n")
  }

  div<-var1/var2

  if(verbose==T){
    cat("\nGenerating output...\n")
  }

  outlist<-list(input1=var1, input2=var2,
                addition=add, subtraction=subt,
                multiplication=mult, division=div)

  return(outlist)
}
```

```r
# Run
my.function(var1=10,var2=0.1,verbose=FALSE)
```

```
## $input1
## [1] 10
##
## $input2
## [1] 0.1
##
## $addition
## [1] 10.1
##
## $subtraction
## [1] 9.9
##
## $multiplication
## [1] 1
##
## $division
## [1] 100
```

```r
my.function(var1=10,var2=0.1,verbose=TRUE)
```

```
##
## Input variables:
## var1 = 10
## var2 = 0.1
##
## Calculating functions...
##
## Adding...
##
## Subtracting...
##
## Multiplying...
##
## Dividing...
##
## Generating output...
## $input1
## [1] 10
##
## $input2
## [1] 0.1
##
## $addition
## [1] 10.1
##
## $subtraction
## [1] 9.9
##
## $multiplication
## [1] 1
##
## $division
## [1] 100
```

> Protip #2:

If you have a custom function, theme, script, etc., that you use repeatedly:

1. Save in a separate file

```
* e.g. make new "myfunction.R" file containing just my.function
```

2. Load using `source("PathName.FileName.R")`

```
* e.g. `source("C:/Users/ColauttiLab/myfunction.R")` if save
```

> Protip #3:

We have already been using functions that somebody else wrote in R.

To see 'under the hood' type a function without the brackets.

> Note: First run `install.packages("ggplot2")` if you don't already have it installed.

```
my.function
```

```
## function(var1=0,var2=0,verbose=FALSE){
##   if(verbose==T){
##     cat("\nInput variables:\nvar1 =", var1,"\nvar2 =", var2,"\n")
##     cat("\nCalculating functions...\n")
##     cat("\nAdding...\n")
##   }
##
##   add<-var1+var2
##
##   if(verbose==T){
##     cat("\nSubtracting...\n")
##   }
##
##   subt<-var1-var2
##
##   if(verbose==T){
##     cat("\nMultiplying...\n")
##   }
##
##   mult<-var1*var2
##
##   if(verbose==T){
##     cat("\nDividing...\n")
##   }
##
##   div<-var1/var2
##
##   if(verbose==T){
##     cat("\nGenerating output...\n")
##   }
##
##   outlist<-list(input1=var1, input2=var2,
##                 addition=add, subtraction=subt,
##                 multiplication=mult, division=div)
##
##   return(outlist)
## }
## <bytecode: 0x0000028dfd416610>
```

```
library(ggplot2)
qplot
```

```
## function (x, y, ..., data, facets = NULL, margins = FALSE, geom = "auto",
##     xlim = c(NA, NA), ylim = c(NA, NA), log = "", main = NULL,
##     xlab = NULL, ylab = NULL, asp = NA, stat = deprecated(),
##     position = deprecated())
## {
##     deprecate_soft0("3.4.0", "qplot()")
##     caller_env <- parent.frame()
##     if (lifecycle::is_present(stat))
##         lifecycle::deprecate_stop("2.0.0", "qplot(stat)")
##     if (lifecycle::is_present(position))
##         lifecycle::deprecate_stop("2.0.0", "qplot(position)")
##     if (!is.character(geom)) {
##         cli::cli_abort("{.arg geom} must be a character vector")
##     }
##     exprs <- enquos(x = x, y = y, ...)
##     is_missing <- vapply(exprs, quo_is_missing, logical(1))
##     is_constant <- (!names(exprs) %in% ggplot_global$all_aesthetics) |
##         vapply(exprs, quo_is_call, logical(1), name = "I")
##     mapping <- new_aes(exprs[!is_missing & !is_constant], env = parent.frame())
##     consts <- exprs[is_constant]
##     aes_names <- names(mapping)
##     mapping <- rename_aes(mapping)
##     if (is.null(xlab)) {
##         if (quo_is_missing(exprs$x)) {
##             xlab <- ""
##         }
##         else {
##             xlab <- as_label(exprs$x)
##         }
##     }
##     if (is.null(ylab)) {
##         if (quo_is_missing(exprs$y)) {
##             ylab <- ""
##         }
##         else {
##             ylab <- as_label(exprs$y)
##         }
##     }
##     if (missing(data)) {
##         data <- data_frame0()
##         facetvars <- all.vars(facets)
##         facetvars <- facetvars[facetvars != "."]
##         names(facetvars) <- facetvars
##         facetsdf <- as.data.frame(mget(facetvars, envir = caller_env))
##         if (nrow(facetsdf))
##             data <- facetsdf
##     }
##     if ("auto" %in% geom) {
##         if ("sample" %in% aes_names) {
##             geom[geom == "auto"] <- "qq"
##         }
##         else if (missing(y)) {
##             x <- eval_tidy(mapping$x, data, caller_env)
##             if (is.discrete(x)) {
##                 geom[geom == "auto"] <- "bar"
##             }
##             else {
##                 geom[geom == "auto"] <- "histogram"
##             }
##             if (is.null(ylab))
##                 ylab <- "count"
##         }
##         else {
##             if (missing(x)) {
##                 mapping$x <- quo(seq_along(!!mapping$y))
##             }
##             geom[geom == "auto"] <- "point"
##         }
##     }
##     p <- ggplot(data, mapping, environment = caller_env)
##     if (is.null(facets)) {
##         p <- p + facet_null()
##     }
##     else if (is.formula(facets) && length(facets) == 2) {
##         p <- p + facet_wrap(facets)
##     }
##     else {
```

```
##         p <- p + facet_grid(facets = deparse(facets), margins = margins)
##     }
##     if (!is.null(main))
##         p <- p + ggtitle(main)
##     for (g in geom) {
##         params <- lapply(consts, eval_tidy)
##         p <- p + do.call(paste0("geom_", g), params)
##     }
##     logv <- function(var) var %in% strsplit(log, "")[[1]]
##     if (logv("x"))
##         p <- p + scale_x_log10()
##     if (logv("y"))
##         p <- p + scale_y_log10()
##     if (!is.na(asp))
##         p <- p + theme(aspect.ratio = asp)
##     if (!missing(xlab))
##         p <- p + xlab(xlab)
##     if (!missing(ylab))
##         p <- p + ylab(ylab)
##     if (!missing(xlim) && !all(is.na(xlim)))
##         p <- p + xlim(xlim)
##     if (!missing(ylim) && !all(is.na(ylim)))
##         p <- p + ylim(ylim)
##     p
## }
## <bytecode: 0x0000028dfc215c60>
## <environment: namespace:ggplot2>
```

8.6 Custom R Package

Most of the general content can be found in Hadley Wickham's R Packages book. It goes into detail on almost everything you would need to know to make a package.

For a quick tutorial, see Hilary Parker's post on a "cat" function.

Install packages first and then read on.

```
install.packages(c("devtools", "roxygen2", "testthat", "knitr"))
```

Tutorial objectives:

1) Make a basic package in RStudio and make 1 function.
2) Make documentation for the function.
3) Installing the package and input checking.

8.6.1 Introduction

When should you use a function vs write a package?

Start with a piece of code, and be sure to add a comment to explain what the code does.

```
# take x, square it and add one to it
y <- x^2 + 1
```

If you are going to use that piece of code multiple times, it's easier to make it into a function and call it, rather than copying and pasting the same cod multiple times. (See functions tutorial LINK)

```
square_plus<-function(x){
  # take x, square it and add one to it
  y <-x^2 + 1
  return(y)
}
square_plus(2)
```

```
## [1] 5
```

```
square_plus(4)
```

```
## [1] 17
```

```
square_plus(1:10)
```

```
##  [1]   2   5  10  17  26  37  50  65  82 101
```

If you want to use the function across many scripts, you can save the function in its own .R file, and then load it into each script

```
source("/Path/To/CustomScript/Script.R")
```

When you have many functions that you use frequently, you might want to make your own R package so that you can load all the functions easily and quickly. This also makes it easy to share the functions.

```
square_plus<-function(x){
  # take x, square it and add one to it
  y <- x^2 + 1
  return(y)
}

cube_plus<-function(x){
  # take x, cube it and add one to it
  y <-x^3 + 1
  return(y)
}

quartic_plus<-function(x){
  # raise x to the power of 4 and add one to it
  y <-x^4 + 1
  return(y)
}
```

8.6.2 Getting started

R Studio makes it easy to create your own packages for R. Once you have installed devtools (see above), create a new R package in R Studio

```
File -> New Project -> New Directory -> R Package
```

You can also use the “R Package” option but delete the NAMESPACE file as it will be automatically generated later. Give the package a name and then click create.

RStudio should load and there will be a file structure with several files and two folders, “R” and “man”.

The “R” folder is for code, and there is a hello.R file in it. Save all of your custom functions here.

The “man” folder is for manual pages, the documents that show up when you use the ? for help `?some_function`.

8.6.3 Add functions

We are going to make a function to get public references from the Crossref API. Crossref is one of the organizations for Digital Object Identifiers and is frequently the one used for scientific journals. Crossref has “metadata” on digital objects such as type of object, author, dates etc etc.

We can access this information through the Crossref page.

For example, the link below shows the result of a search for the title of a paper by Primack and Miller-Rushing (2011).

https://search.crossref.org/?q=Broadening+the+study+of+phenology+and+climate+change

The DOI for the first paper (by Primack & Miller-Rushing) is “10.1111/j.1469-8137.2011.03773.x”

Clicking on the “Actions” button for this paper, and then “Metadata as JSON”, brings up a json file including citation information, and also citations for the papers referenced in the paper.

There’s been times where we read a paper and then go through the references of the paper, especially for literature reviews/meta-analyses. Automating the extraction of references from a paper of interest might be useful.

We can access the json file in R using the doi and using the Crossref api (documentation LINK).

Doing this will give us a list of the citations:

```r
# download jsonlite to parse json files
library(jsonlite)
```

```
##
## Attaching package: 'jsonlite'
## The following object is masked from 'package:purrr':
##
##     flatten
```

```r
url<-"https://api.crossref.org/works/10.1111/j.1469-8137.2011.03773.x"
result<-fromJSON(url)
```

`result` is a list containing a variety of information

```r
names(result)
```

```
## [1] "status"          "message-type"    "message-version"
## [4] "message"
```

`result$message$reference` is a data frame of citations containing 17 references that we can extract this.

```r
references<-as.data.frame(result$message$reference)
```

This can be easily writen to csv or other formats.

But we can also make this a function for any DOI of interest.

```
get_work_references<-function(DOI){
  url<-paste0("https://api.crossref.org/works/",DOI)
  result<-fromJSON(url)
  return(as.data.frame(result$message$reference))
}
```

We can save the script above in the R folder to make it part of the package.

Of course, we would want to add more functions in order to make this a useful package.

If we want to run the function, we can use the `source()` function as described above. But as a package this still lack two important pieces:

1. Documentation for this function (and any other functions we add)
2. A library that would let us load all functions using the `library()` function

8.6.4 Adding documentation

The first piece of documentation is the DESCRIPTION file. There are several fields to fill in for this.

1. The **package name** is already filled automatically.
2. We should add a **title** (ie. This Package Gets References).
3. Change the `Author` to `Authors@R` and add yourself as the author and creator.

```
Authors@R: person("First Name", "Last Name",
        email="email@email.com", role=c("aut", cre))

# Two authors
Authors@R: c(person("First Name", "Last Name",
        email="email@email.com", role=c("aut", cre)),
             person("Second person name", "second person last name",
             email="email@email.com", role="aut"))
```

4. Write a description:

   Interfacing with Crossref's API to get citation information using DOI. This package uses jsonlite and contains only one function. etc…

5. Choose one of the public licenses such as GPL-3, MIT etc. (see Wikipedia)

Save the DESCRIPTION file.

8.6.5 Add a Manual

The `roxygen2` package can be used to make manuals for R packages. This greatly simplifies the writing process, which otherwise would be written in LaTeX. The `roxygen2` package allows us to make comments directly in the script, and then `roxygen2` automatically generates the manual pages from these comments.

First, take out any library(*) commands and use packagename::function() for any functions from other libraries. Read R Packages - R code for more details on why.

When writing your comments, follow this logic:

- Roxygen2 commands start with `#'`.

- The first line is automatically the title field and should cover only one line.
- The next text paragraph goes into the description. The usage field is automatically generated.
- Use `@param` tags for arguments. (Only 1 in this case).
- Use the next line to write a longer description.
- Use `@return` to write what is expected output and `@example` to write example code that will be run when creating the man page.
- We also want to use a `@export` tag so that the function will be available for use when the library is loaded.
- We need to add details such as description, useage, arguments.
- The script would look something like this:

```
#' Takes a DOI and returns references for the object.
#'
#' This function queries the Crossref API to obtain a data frame
of references for the DOI. We use the paste0 function from base
and the fromJSON function from jsonlite.
#'
#' @param DOI String. Digital object identifier.
#'
#' @return data frame of references.
#' @example
#' get_work_references("10.1111/j.1469-8137.2011.03773.x")
#' @export

get_work_references<-function(DOI){
  url<-paste0("https://api.crossref.org/works/",DOI)
  result<-jsonlite::fromJSON(url)
  return(as.data.frame(result$message$reference))
}
```

Save the file and use `devtools::document()`.

We will now have a NAMESPACE file, and a new file within the man folder. The NAMESPACE file shows the function we have which will be available in the environment when the library is loaded.

Open `get_work_references.Rd` and then click preview to see how it looks.

However, our man page is a bit dull, and lacks the links most pages have. We have to add the links using code. For example, linking the paste0 function will be `\code{\link[base]{paste0}}`.

Use `document()` again. Now the functions are in monospace font. The actual links only appear when the package is built.

We can use the “CHECK” button on the “Build Pane” to check for any issues in the package.

We did not import the jsonlite package. To do this, go back to the DESCRIPTION file and add:

```
      jsonlite
```

Another CHECK will tell you that the package `curl` is required. Add this to the imports as well.

8.6.6 Installing the package

Once you pass the check, click “Install and Restart” to install the package. The package should be in your “Packages” pane.

Doing `?get_work_references` will bring up the help page with working links. We can successfully run the example. But if input is not a character, the function doesn’t work.

8.6.7 Input checking

You cannot account for every possible scenario where the function doesn’t work. Or there are certain variables you know have to be in a specific form.

You can add checks for inputs within the function.

For example, the DOI should be a character string. We can add a test for the input and stop the function with an error if the input isn’t a character string.

```
get_work_references<-function(DOI){
  if (!is.character(DOI)) stop(" 'DOI' must be a character string")
  url<-paste0("https://api.crossref.org/works/",DOI)
  result<-jsonlite::fromJSON(url)
  return(as.data.frame(result$message$reference))
}
```

Re-install and you have a working package!

8.6.8 Make it public

Before going public:

1. Create a public GitHub repository and push your project
2. Flesh out documentation and meta-data
3. Error checking with `devtools` library * `spell_check()` * `check_rhub()` – use rhub to check for errors. More about RHub. * `check_win_release()` – check for errors on Windows with latest release version of R * `check_win_devel()` – check for errors on Windows with latest pre-release of R * `release()` – release to the world!
4. Tag the latest release on GitHub

For details on this and more: http://r-pkgs.had.co.nz/release.html

8.6.9 References:

Hadley Wickham, 'R packages' http://r-pkgs.had.co.nz/

Hilary Parker, 'Writing an R package from scratch', https://hilaryparker.com/2014/04/29/writing-an-r-package-from-scratch/