SATVI Computational Course

Session Guide

SATVI Computational Group

2024-03-05

Table of contents

Preface

This is a session guide book for the SATVI Computational Course.

This is a version-controlled living document that will be updated as needed as the course progresses. All changes are tracked using git.

1 Introduction

Welcome to the SATVI Computational Course! This course is designed to strengthen fundamental coding skills for SATVI trainees and staff. The curriculum will take you through the basics of R, using the terminal, creating and using git controlled projects, as well as more advanced data analysis methods commonly used at SATVI.

All lessons will be stored on the SATVI GitHub under the repository SATVI_ComputationalCourse.
To access all relevant course content, navigate to https://github.com/SATVILab/SATVI_ComputationalCourse.

A static webpage version of the course is also available at https://satvilab.github.io/SATVI_ComputationalCours

Your instructors are SATVI members with experience in each topic. For session-specific questions, please contact the relevant instructor:

1.1 Instructor contacts


```
Carly Young-Baile: carly.young-bailie@uct.ac.za

Monika Looney: monika.looney@uct.ac.za

Miguel Rodo: miguel.rodo@uct.ac.za

Simon Mendelsohn: simon.mendelsohn@uct.ac.za

Munyaradzi Musvosvi: munyaradzi.musvosvi@uct.ac.za

Denis Awany: denis.awany@uct.ac.za
```


The full curriculum can be found on the "Syllabus" page.

Happy coding!

This is a book created from markdown and executable code.

See Knuth (1984) for additional discussion of literate programming.

2 Syllabus

2.1 Description

This page serves as a syllabus for the SATVI Computational Course. Details for each session can be found on their dedicated page.

2.2 Module 1: Intro to R and MaRcus Training Course

2.2.1 Session 1: Intro to R and swirl

Topic: Introduction to R language and environments, RStudio, and swirl self-teaching tools.

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 05 MAR 2024

Time: 10h30 - 11h30

Location: Lekgotla 4A and 4B

Homework: Complete swirl "R Programming" interactive learning sessions at own pace.

2.2.2 Session 2: MaRcus Training Course lesson 1

Topic: Importing data into R environment and basic visualizations with ggplot2

Instructor: Carly Young-Baile: carly.young-bailie@uct.ac.za

Date: 19 MAR 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: See assignment from https://haswal.github.io/MaRcus/01_session.html

2.2.3 Session 3: MaRcus Training Course lesson 2

Topic: Creating histograms and statistical summaries; combining and exporting plots

Instructor: Carly Young-Baile: carly.young-bailie@uct.ac.za

Date: 26 MAR 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: See assignment from https://haswal.github.io/MaRcus/02_session.html

2.2.4 Session 4: MaRcus Training Course lesson 3

Topic: Basic data transformation using dplyr

Instructor: Carly Young-Baile: carly.young-bailie@uct.ac.za

Date: 02 APR 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: See assignment from https://haswal.github.io/MaRcus/03_session.html

Note - MaRcus Training Course lesson 4 was skipped as it covers R Markdown which will be replaced by a session on Quarto later.

2.2.5 Session 5: MaRcus Training Course lesson 5

Topic: Continuation of data transformation using dplyr and data wrangling

Instructor: Carly Young-Baile: carly.young-bailie@uct.ac.za

Date: 09 APR 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: See assignment from https://haswal.github.io/MaRcus/05_session.html

2.2.6 Session 6: MaRcus Training Course lesson 6

Topic: Clean up data using tidyr

Instructor: Carly Young-Baile: carly.young-bailie@uct.ac.za

Date: 30 APR 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: See assignment from https://haswal.github.io/MaRcus/06_session.html

2.2.7 Session 7: MaRcus Training Course lesson 7

Topic: Manipulating strings with stringr and intro to regular expressions

Instructor: Carly Young-Baile: carly.young-bailie@uct.ac.za

Date: 07 MAY 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: See assignment from https://haswal.github.io/MaRcus/07_session.html

2.2.8 Session 8: Exporting data from R

Topic: Exporting data and plots from R in different formats including csv, pdf, and jpeg

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 21 MAY 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: Export data frame to csv and save plots as pdf and jpeg;

2.3 Module 2: Quarto, GitHub, and GUIs

2.3.1 Intro to Quarto

Topic: Intro to technical publishing using Quarto

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 04 JUN 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: Initialize a Quarto project for your own study; Make GitHub account, access SATVILab GitHub, and download GitHub Desktop

2.3.2 Intro to GitHub

Topic: Intro to version control using Git and GitHub

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 18 JUN 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: Set up a version controlled project; Download VS Code

2.3.3 Intro to VS Code

Topic: Intro to VS Code as an alternative GUI to RStudio and git-aware terminals

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 02 JUL 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework: Write a script in the VS Code GUI

2.4 Module 3: Statistics

2.4.1 Basic statistical tests

Topic: Computing commonly needed statistics and confidence intervals in R

Instructor: Miguel Rodo: miguel.rodo@uct.ac.za

Date: 16 JUL 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.4.2 Correlations

Topic: Computing correlation metrics in R

Instructor: Miguel Rodo: miguel.rodo@uct.ac.za

Date: 30 JUL 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.5 Module 4: Commonly needed analyses for Immunology

2.5.1 Heatmaps

Topic: Plotting and manipulating heatmaps

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 27 AUG 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.5.2 Dimensionality reduction

Topic: Understanding and conducting dimensionality reduction using PCA and UMAP

Instructor: Monika Looney: monika.looney@uct.ac.za

Date: 03 SEP 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.5.3 Receiver operating characteristic (ROC) curves

Topic: Understanding and computing ROC curves

Instructor: Simon Mendelsohn: simon.mendelsohn@uct.ac.za

Date: 17 SEP 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.5.4 Background subtraction

Topic: Learning how to apply a function for background subtraction

Instructor: Miguel Rodo: miguel.rodo@uct.ac.za

Date: 01 OCT 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.5.5 Basic flow cytometry analysis

Topic: Plotting background subtracted frequencies and MFIs from flow cytometry data

Instructor: Munyaradzi Musvosvi: munyaradzi.musvosvi@uct.ac.za

Date: 15 OCT 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.5.6 Automatic gating

Topic: Generating inputs for and carrying out automated gating for flow cytometry data

Instructor: Munyaradzi Musvosvi: munyaradzi.musvosvi@uct.ac.za

Date: 29 OCT 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

2.6 Module 5: Other coding languages

2.6.1 Intro to Python

Topic: Basics of using python and applications for computational immunology

Instructor: Denis Awany: denis.awany@uct.ac.za

Date: 12 NOV 2024

Time: 11h00 - 12h00

Location: Lekgotla 4A and 4B

Homework:

3 Installations

3.1 Description

This document provides installation guides for basic programming tools.

3.2 R

R is a commonly used coding language for computational biologists and immunologists. Many software packages and analysis pipelines depend on R. R is also a computational environment used for computing and generating graphics.

To install R for Windows or Mac, follow the instructions provided by The Comprehensive R Archive Network (CRAN) found here: https://cran.r-project.org/

It is recommended to download the precompiled binary distribution appropriate for your machine.

To learn more about R, read the following introduction provided by CRAN: https://www.r-project.org/about.html

3.3 R Studio

RStudio is an integrated development environment (IDE) based on R. It provides a user-friendly option for building code and can incorporate multiple languages including python, which is also commonly used by computational immunologists.

To donwload and install RStudio Desktop, follow this link and the provided instructions: https://posit.co/download/rstudio-desktop/#download

3.4 GitHub Desktop

GitHub Desktop is a desktop application that interfaces with version-controlled code, GitHub, and other Git services. It provides a user friendly GUI where you can review changes made to code and perform Git commands. It is open source and free to use.

First sign up for a GitHub account at https://github.com

Now download and install GitHub Desktop, follow this link and the provided instructions: https://desktop.github.com. Sign in with your GitHub account login.

3.5 Visual Studio Code (VS Code)

VS Code is a text and code editor commonly used by developers. It can be used as an alternative for RStudio and supports multiple coding languages and various extensions for debugging and version control.

To download and install VS Code, follow this link and the provided instructions: https://code.visualstudio.com/download

4 swirl

4.1 Description

swirl (https://swirlstats.com/) is an interactive R package that helps you self-teach the basics of R. It is run from directly from the R console.

This session guide follows the instructions provided by swirl. Visit the following link to access the full tutorial: https://swirlstats.com/students.html

You can also find the full swirl course tutorial on GitHub at https://github.com/swirldev/swirl_courses

4.2 Install swirl

swirl requires R 3.1.0 or later installed on your computer. It is also recommended that you have RStudio installed which will provide a user-friendly environment to work with.

For instructions on how to install R and RStudio, visit the Installations session guide page.

Once you have downloaded R and RStudio, perform the following steps:

```
1. Open RStudio.
2. In the RStudio console, type the following where you see the command prompt > :

    install.packages("swirl")
```

4.3 Initialize swirl

Whenever you want to run swirl, you must load and initialize the package.

```
1. In the console, type the following:

    library("swirl")
    swirl()

2. Follow any prompts that come up in the console. i.e. if swirl asks "What shall I call you
```

4.4 Install an interactive course

The first time you initialize swirl, you will need to install a course.

For the SATVI Computational Course, we recommend that those who are new to coding start with "R Programming". This course will cover the basics of programming in R.

There are many courses to choose from, so those who are more advanced may opt for an intermediate or advanced course to work through in their own time. A repository with all available swirl courses can be found here: https://github.com/swirldev/swirl_courses#swirl-courses.

There is also an expansive swirl Network that expands further on open sourse interactive R lessons. You can access the Network and associated courses or become a swirl course author here: https://swirlstats.com/scn/

To install a course that is not part of the swirl course repository, type the following into the console:

```
?InstallCourses
```

4.5 Run swirl

For now, we will assume that we are starting with the basics and have chosen to install the "R Programming" course.

To run the interactive lessons:

Select a new lesson. The R Programming course offers 14 different short interactive lessons. Go through each one in order as the information from earlier lessons is required in later lessons.

4.6 Exit swirl

If at any time you need to exit a swirl lesson before it is complete, simply press the Esc key.

If you need to exit from a prompt, exit and save your work by typing: bye()

4.7 Interactive commands

While you are working in swirl, you may find that you want to skip a section that you are already comfortable with, or to work more on the current topic outside of an interactive session.

Below are some helpful commands for getting the most out of your swirl sessions:

From the R prompt (>):

```
To skip the current question: skip()

To experiment with R on your own without swirl interaction: play()

To re-initiate swirl interaction after playing: nxt()

To exit and save: bye()

To return to swirl's main menu: main()

To display these command options: info()
```

If you see a swirl output followed by ... press Enter to continue.

4.8 Homework

As beginners, regular practice is critical! It is recommended that you go through one or two lessons daily to improve and retain these fundamentals.

Over the next week, in your own time, complete the 14 short interactive lessons from the "R Programming" swirl course.

4.9 FAQ

Q1: Can funcitons learned in swirl be applied when writing my own R scripts?

```
A: Absolutely! The functions that you use in swirl are all base R functions that can be used
```

Q2: If I need to use an R package, do I need to install the package each time I start a new session?

A: Nope! Once a package is installed, you do not have to re-install when you open a new R ses

5 MaRcus R Training

5.1 Description

The Marcus R Training program was developed by Hasse Walum of Emory University. The program will cover the following:

1. Importing data
2. Basic data visualization
3. Exporting and saving plots
4. Data transformation
5. R Markdown basics
6. Summarizing data
7. String manipulation and data joining

Rather than reinventing what is covered in the Marcus R Training program, we have been granted permission to use the materials for our SATVI Computational Course.

Over the next 6 weeks, we will refer to the Marcus R Training materials for our sessions.

5.2 Content access

The course and all associated resources are available at:

https://haswal.github.io/MaRcus/index.html

5.3 Homework

Please refer to the MaRcus R Training program session guides to access your homework assignments.

5.4 FAQ

5.4.0.1 Session 1

Q1: What are the best ways to set your working directory?

A: There are a few ways to do this:

1. If you are using Mac, you can navigate to the directory you would like to work in usi

2. You can also set the working directory using point and click in RStudio. To do so, na

3. A note about setting working directories in scripts. It is good practice to avoid usi

Q2: When generating a plot using ggplot2, does the name used in the script for the row or column we want to plot have to match the col or rowname of the associated dataframe exactly?

A: Yes. The names must match exactly because R searches the dataframe for col or rownames as

Q3: What is the difference between facet_wrap() and facet_grid()?

A: Both are options that can be applied to ggplot2. facet_wrap() wraps a 1d sequence of panel

Q4: When should I specify aes globally vs. locally?

A: In general, specify aes in mapping (global) so that the specifications are applied to all

Q5: What are HEX codes?

A: HEX codes are unique alphanumeric codes assigned to specific colors. They can be used to a

Q6: What are your recommendations for using Chat GPT for help with coding?

A: Chat GPT is a quickly growing tool used by coders. It can be very helpful for designing /

5.4.0.2 Session 2

Q1: What is the difference between top and bottom windows in R Studio?

```
A: It can help to think of this an analogy: In R Studio, the top left (script) is your recip
```

Q2: Can you plot confidence intervals automatically using geom_errorbar or do you have to calculate them separately first?

```
A: Confidence intervals should be calculated separately.
```

5.4.0.3 Session 3

Q1: How can you save the contents of the R console when I finish a session?

```
A1: You can save the contents of the base R console using the 'sink()' function. Here you wi
```

```
For example:
```

```
sink("output/console_content.txt")
```

```
Run code of your choice
```

```
sink()
```

```
A2: If using RStudio, you can do this via point and click. Navigate to "History" in the top
```

Q2: How does 'filter()' work?

```
A: The 'filter()' function from the 'dplyr' package is used to subset data frames based on s
```

```
filter(.data, condition)
```

```
Here .data is any data frame in your environment that you want to filter. Condition needs to
```

```
filtered.data <- filter(original.data, original.data$frequency > 0.05)
```

```
filtered.data have rows with frequency > 0.05 removed.
```

Q3: What is the difference between a function and an operator?

A: A function is a chunk of code that is designed to perform a specific task. They typically

Alternatively, an operator is a simple symbol that is used to perform arithmetic, logical, o

Q4: Why does the 'is.na()' function work if the NA in my data frame is uppercase? Isn't it case-specific?

A: Though most things in R are case specific, is.na() isn't actually looking for the specifi

6 Exporting and Importing Data Formats in R

6.1 Description

This script will demonstrate methods for exporting and importing various data and plot formats from an R script. We will be using the built-in "iris" and "mtcars" datasets available in R. We encourage you to go through these steps with a dataset of your own and export formats that are relevant to your study. This session will cover commonly needed formats, including .xlsx, .csv, .pdf, .png, and .jpeg. However, there are many additional data formats that can be used and we recommend exploring these independently. Keep in mind that there are many different ways to do similar things in R, i.e. multiple packages to export to .xlsx. This script is intended to provide some helpful examples, but is not comprehensive.

6.1.1 Clear environment

```
ls()
rm(list=ls())
```

6.1.2 Set output directory

```
dir.create("output")
dir_save <- "output/"
```

6.1.3 Load libraries

```
library(tidyverse) # Needed for 'glimpse()'
library(openxlsx) # Needed to export data.frame to .xlsx
library(dplyr) # Needed to convert rownames to column and simultaneously delete rownames
library(rio) # Needed for 'import' function
library(readxl) # Needed for alternative method for importing .xlsx
```

6.1.4 Load datasets

We will load the built-in "iris" and "mtcars" datasets for demonstration purposes.

```
data("iris")
data("mtcars")
```

6.1.5 Examine data structure

```
head(iris)
```

```
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1          5.1         3.5          1.4         0.2  setosa
2          4.9         3.0          1.4         0.2  setosa
3          4.7         3.2          1.3         0.2  setosa
4          4.6         3.1          1.5         0.2  setosa
5          5.0         3.6          1.4         0.2  setosa
6          5.4         3.9          1.7         0.4  setosa
```

```
head(mtcars)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

```
glimpse(iris)
```

```
Rows: 150
Columns: 5
$ Sepal.Length <dbl> 5.1, 4.9, 4.7, 4.6, 5.0, 5.4, 4.6, 5.0, 4.4, 4.9, 5.4, 4.~
$ Sepal.Width  <dbl> 3.5, 3.0, 3.2, 3.1, 3.6, 3.9, 3.4, 3.4, 2.9, 3.1, 3.7, 3.~
$ Petal.Length <dbl> 1.4, 1.4, 1.3, 1.5, 1.4, 1.7, 1.4, 1.5, 1.4, 1.5, 1.5, 1.~
$ Petal.Width  <dbl> 0.2, 0.2, 0.2, 0.2, 0.2, 0.4, 0.3, 0.2, 0.2, 0.1, 0.2, 0.~
$ Species      <fct> setosa, setosa, setosa, setosa, setosa, setosa, setosa, s~
```

```
glimpse(mtcars)
```

```
Rows: 32
Columns: 11
$ mpg  <dbl> 21.0, 21.0, 22.8, 21.4, 18.7, 18.1, 14.3, 24.4, 22.8, 19.2, 17.8,~
$ cyl  <dbl> 6, 6, 4, 6, 8, 6, 8, 4, 4, 6, 6, 8, 8, 8, 8, 8, 8, 4, 4, 4, 4, 8,~
$ disp <dbl> 160.0, 160.0, 108.0, 258.0, 360.0, 225.0, 360.0, 146.7, 140.8, 16~
$ hp   <dbl> 110, 110, 93, 110, 175, 105, 245, 62, 95, 123, 123, 180, 180, 180~
$ drat <dbl> 3.90, 3.90, 3.85, 3.08, 3.15, 2.76, 3.21, 3.69, 3.92, 3.92, 3.92,~
$ wt   <dbl> 2.620, 2.875, 2.320, 3.215, 3.440, 3.460, 3.570, 3.190, 3.150, 3.~
$ qsec <dbl> 16.46, 17.02, 18.61, 19.44, 17.02, 20.22, 15.84, 20.00, 22.90, 18~
$ vs   <dbl> 0, 0, 1, 1, 0, 1, 0, 1, 1, 1, 1, 0, 0, 0, 0, 0, 0, 1, 1, 1, 1, 0,~
$ am   <dbl> 1, 1, 1, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 1, 1, 0, 0,~
$ gear <dbl> 4, 4, 4, 3, 3, 3, 3, 4, 4, 4, 4, 3, 3, 3, 3, 3, 3, 4, 4, 4, 3, 3,~
$ carb <dbl> 4, 4, 1, 1, 2, 1, 4, 2, 2, 4, 4, 3, 3, 3, 4, 4, 4, 1, 2, 1, 1, 2,~
```

```
class(iris)
```

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

```
class(mtcars)
```

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

6.1.6 Export data to .xlsx

Here we will use dir_save to specify where we want to save our files. Alternatively, you can write out the full path to your output directory.

```
# To export a single data.frame to .xlsx

write.xlsx(iris, paste0(dir_save, "iris_data.xlsx"))


# To export multiple data.frames into different sheets, create a list of data.frames to be us

data.frames <- list('Sheet1' = iris, 'Sheet2' = mtcars)
write.xlsx(data.frames, file = paste0(dir_save, "iris_mtcars_data.xlsx"))
```

```r
# Write to .xlsx including colnames and rownames for all sheets

write.xlsx(data.frames, file = paste0(dir_save, "iris_mtcars_data_colrow.xlsx"), colNames = T


# Alternatively, convert rownames from specific data.frames to a named column and export with

mtcars <- tibble::rownames_to_column(mtcars, "Model")
data.frames <- list('Sheet1' = iris, 'Sheet2' = mtcars)
write.xlsx(data.frames, file = paste0(dir_save, "iris_mtcars_data_rownamestocol.xlsx"))
```

6.1.7 Export data to .csv

```r
# Let's first export iris as is and restore mtcars to its original format before exporting to

write.csv(iris, file = paste0(dir_save, "iris_data.csv"))

mtcars <- column_to_rownames(mtcars, var = "Model")
write.csv(mtcars, file = paste0(dir_save, "mtcars_data.csv"))

# You'll notice that the default for write.csv is to set col.names and row.names = TRUE

write.csv(mtcars, file = paste0(dir_save, "mtcars_data_colrowfalse.csv"), col.names = FALSE,
```

```
Warning in write.csv(mtcars, file = paste0(dir_save,
"mtcars_data_colrowfalse.csv"), : attempt to set 'col.names' ignored
```

```r
# When using write.csv, colnames will still be written. If you want to eliminate colnames, us

write.table(mtcars, file = paste0(dir_save, "mtcars_data_colfalse.csv"), col.names = FALSE, r
```

6.1.8 Import data from .xlsx

```r
# Import a data.frame from a specific sheet in a .xlsx file

df.iris.xlsx <- read.xlsx(xlsxFile = "output/iris_mtcars_data_colrow.xlsx",
                          sheet = 1,
```

```
                      rowNames = TRUE)

class(df.iris.xlsx)
```

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

```
head(df.iris.xlsx)
```

```
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1          5.1         3.5          1.4         0.2  setosa
2          4.9         3.0          1.4         0.2  setosa
3          4.7         3.2          1.3         0.2  setosa
4          4.6         3.1          1.5         0.2  setosa
5          5.0         3.6          1.4         0.2  setosa
6          5.4         3.9          1.7         0.4  setosa
```

```
# A common alternative method relies on the 'readxl' package, but functions differently

df.mtcars.xlsx <- read_xlsx("output/iris_mtcars_data_colrow.xlsx",
                      sheet = 2)
```

```
New names:
* `` -> `...1`
```

```
class(df.mtcars.xlsx)
```

```
[1] "tbl_df"     "tbl"        "data.frame"
```

```
head(df.mtcars.xlsx)
```

```
# A tibble: 6 x 12
  ...1           mpg   cyl  disp    hp  drat    wt  qsec    vs    am  gear  carb
  <chr>        <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl> <dbl>
1 Mazda RX4     21       6   160   110  3.9   2.62  16.5     0     1     4     4
2 Mazda RX4 W~  21       6   160   110  3.9   2.88  17.0     0     1     4     4
3 Datsun 710    22.8     4   108    93  3.85  2.32  18.6     1     1     4     1
4 Hornet 4 Dr~  21.4     6   258   110  3.08  3.22  19.4     1     0     3     1
5 Hornet Spor~  18.7     8   360   175  3.15  3.44  17.0     0     0     3     2
6 Valiant       18.1     6   225   105  2.76  3.46  20.2     1     0     3     1
```

```r
# Using this method, you will need to convert to a data.frame before you can set rownames

df.mtcars.xlsx <- as.data.frame(df.mtcars.xlsx)
rownames(df.mtcars.xlsx) <- df.mtcars.xlsx[[1]]
df.mtcars.xlsx <- df.mtcars.xlsx[-1]
head(df.mtcars.xlsx)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

6.1.9 Import data from .csv

```r
# Import the iris data.frame as is. Below are two alternative methods.

df.iris.csv <- read.csv("output/iris_data.csv")

df.iris.csv <- import("output/iris_data.csv")

# Import and set colnames

df.iris.csv <- read.table("output/iris_data.csv", row.names = 1, header = TRUE, sep = ",")

head(df.iris.csv)
```

```
  Sepal.Length Sepal.Width Petal.Length Petal.Width Species
1          5.1         3.5          1.4         0.2  setosa
2          4.9         3.0          1.4         0.2  setosa
3          4.7         3.2          1.3         0.2  setosa
4          4.6         3.1          1.5         0.2  setosa
5          5.0         3.6          1.4         0.2  setosa
6          5.4         3.9          1.7         0.4  setosa
```

```r
df.mtcars.csv <- read.table("output/mtcars_data.csv", row.names = 1, header = TRUE, sep = ",'

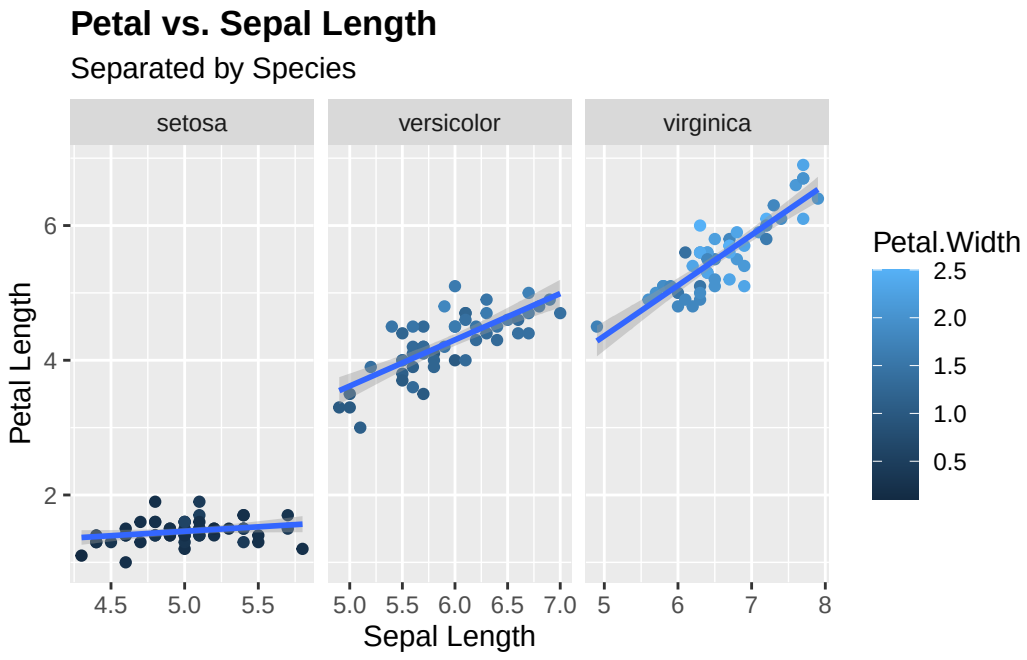
head(df.mtcars.csv)
```

```
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1
```

6.1.10 Plot data and export

```
# Create a plot and save using ggplot followed by ggsave

ggplot(data = df.iris.csv,
                mapping = aes(x = Sepal.Length, y = Petal.Length)) +
  geom_point(aes(color = Petal.Width)) +
  geom_smooth(method="lm") +
  labs(title = "Petal vs. Sepal Length", subtitle = "Separated by Species", x = "Sepal Length
  facet_wrap(~Species,
             scales = "free_x") +
  theme(plot.title = element_text(face = "bold"))
```



```
ggsave("output/iris_ggplot.pdf", width = 7, height = 7)
ggsave("output/iris_ggplot.png", width = 7, height = 7)
ggsave("output/iris_ggplot.jpeg", width = 7, height = 7)

# Alternatively, assign the plot to an object, then print and dev.off. Whereas the first meth

plot <- ggplot(data = df.iris.csv,
               mapping = aes(x = Sepal.Length, y = Petal.Length)) +
  geom_point(aes(color = Petal.Width)) +
  geom_smooth(method="lm") +
  labs(title = "Petal vs. Sepal Length", subtitle = "Separated by Species", x = "Sepal Length
  facet_wrap(~Species,
             scales = "free_x") +
  theme(plot.title = element_text(face = "bold"))

pdf("output/iris_plot.pdf", width = 7, height = 7)
print(plot)
invisible(capture.output(dev.off()))

png(filename = "output/iris_plot.png", width = 1500, height = 1500, res = 300)
print(plot)
invisible(capture.output(dev.off()))

jpeg("output/iris_plot.jpeg", width = 1500, height = 1500, res = 300)
print(plot)
invisible(capture.output(dev.off()))
```

6.1.11 Save what has been done to an .Rdata file

In some cases, it may be helpful to save a specific object or everything in your environment to an .Rdata file that can be imported all at once to be used in a different pipeline or at a later time. You can save as either an RData object or as an RDS object.

```
# To save a specific object

save(df.iris.csv, file = paste0(dir_save, "df.iris.csv.RData"))

# To save all data and values in your R environment to an RData file

save.image(paste0(dir_save, "Data_Export_Tutorial.RData"))
```

You can then load that .RData file back into R and start back up where you left off.

```
# First clear the environment so we can see how RData files are loaded

ls()
rm(list=ls())

# Now load your .RData objects

load("output/Data_Export_Tutorial.RData")
```

You can do the same thing for single objects saved as .RDS

```
saveRDS(df.iris.csv, file = paste0(dir_save, "df.iris.csv.rds"))

ls()
rm(list=ls())

# Now load your .RDS objects

reloaded_data <- readRDS("output/df.iris.csv.rds")
```

There is a workaround to save and reload an entire environment as .RDS, but it is a bit more involved and requires the use of loops, which is beyond the scope of this session. We will cover loops in a later session.

6.2 Homework

For this homework assignment, you will be using a script that you write yourself! If you have data for your own study, we suggest writing a simple script that is relevant to the analyses you will need to do. The only requirements are that you should use data that can be imported / exported in a table or dataframe format and plotted. If you do not have data of your own yet, you can use a built in dataset available from R. To find built in datasets use the following command:

data()

Now perform the following steps:

1. Clear your environment.
2. Set your working directory. This should be in a location where you perform work related to this course.

3. Set output directory. This should be a subdirectory within your working directory where you want to save any files that you generate. You can create this manually in your normal file finder or create it using R as is done in the script above.
4. Load libraries that are necessary for your script.
5. Load your dataset. Either import your own data or load one of the built in datasets.
6. Examine data structure.
7. Plot your data however you like! Refer to previous sessions for ideas and guidance.
8. Save your plots as pdf, png, and jpeg.
9. Export your data file as .xlsx and .csv. Confirm that your row and colnames are in the correct position.
10. Save a relevant object from your environment as .Rdata and .rds.
11. Load your .Rdata and .rds files back into R.
12. Consult the internet or ChatGPT and find at least one alternative method to import, export, and save your data or plots. Try these out.
13. Save your script.

7 Introduction to Quarto

7.1 Description

Quarto is an open-source new evolution of R Markdown. Quarto supports development in various coding languages and includes publishing and authoring features for individual documents, books, presentations, and websites.

Using Quarto can provide a helpful structure to organize, annotate, and share your scripts. Well-annotated Quarto documents can also promote code literacy as they are easy to read, write, and modify.

Quarto is very well documented. This tutorial will provide an introduction to some basic features, but we recommend that you explore independently. These links below may be a good place to start:

https://quarto.org/docs/get-started/hello/rstudio.html

https://quarto.org/docs/authoring/markdown-basics.html

7.1.1 Install R Markdown

To use Quarto with R you will need to install R Markdown with the rmarkdown R package. This will also install knitr which is used for rendering.

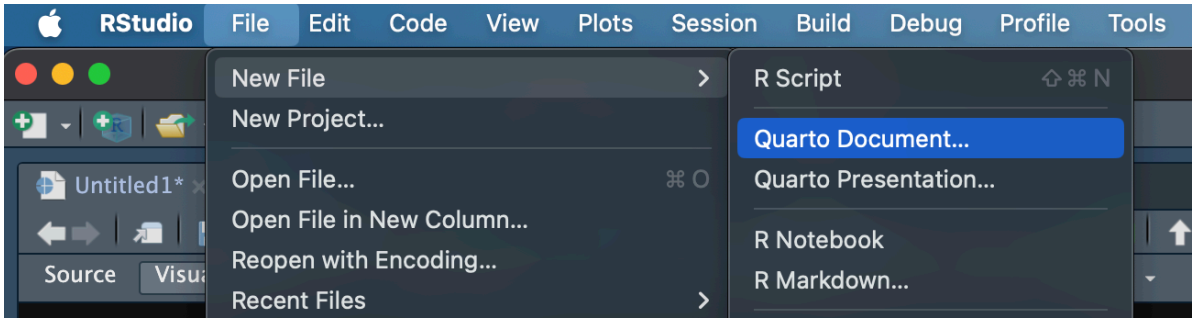
```
install.packages("rmarkdown")
```

7.1.2 Create a Quarto document

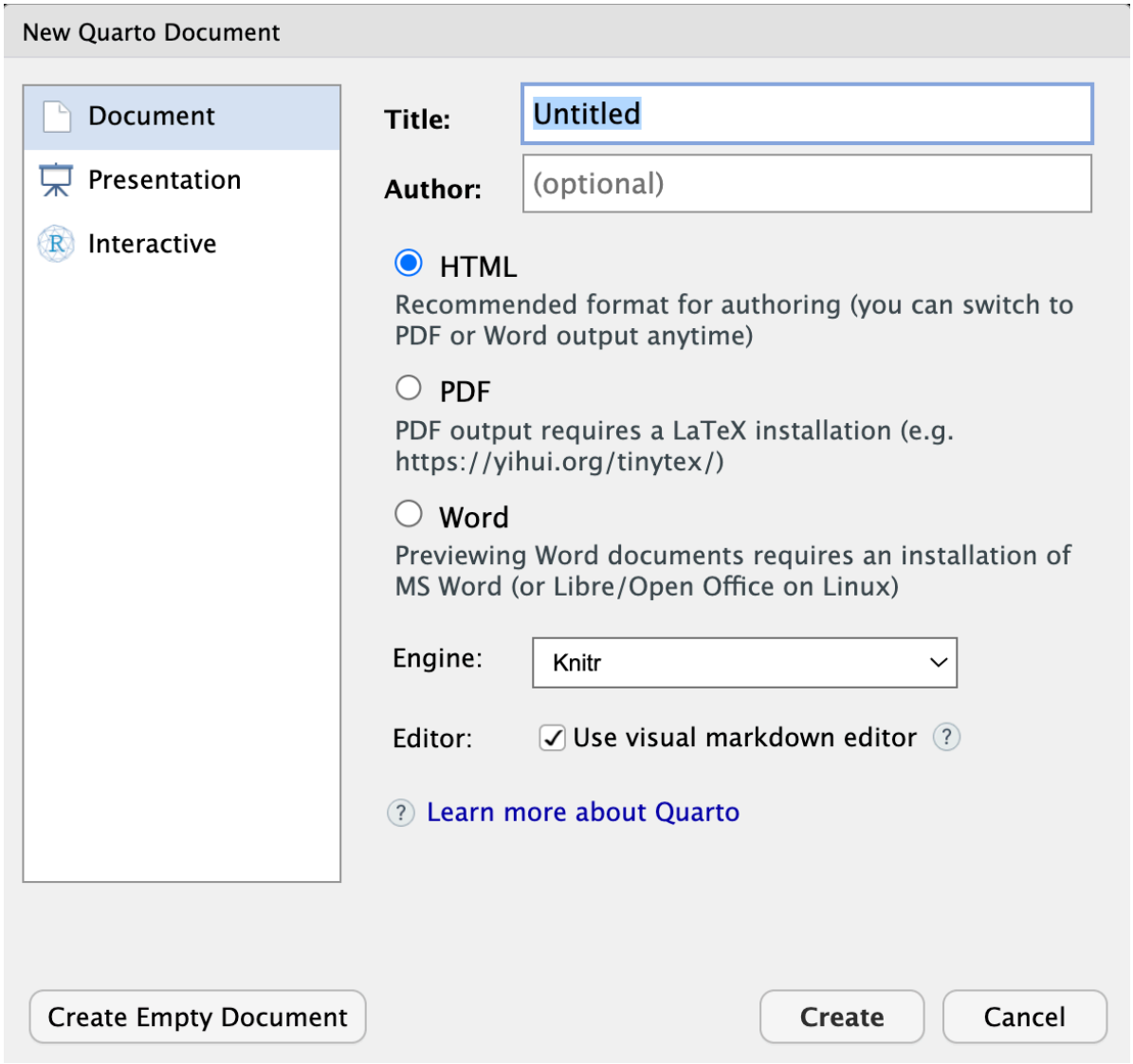
For the purposes of this session, we will introduce using Quarto documents using R. You can also create a Quarto project, which knits together multiple Quarto documents, Quarto presentations, Quarto interactive documents, or Quarto websites. Quarto is also supported by different visual editors including Visual Studio Code (VS Code) which we will cover in a later session.

To begin:

1. Open RStudio
2. Create a new Quarto document. Go to File -> New File -> Quarto Document



3. Enter a name and select your preferred output format and engine. Typically we leave Knitr as the default, but you can change this if necessary.



4. Save the quarto document to your working directory.

Now we can begin with editing the document itself. The most obvious difference in features from a traditional R script is that a Quarto document incorporates code chunks which separate major segments of code into different chunks. Each chunk can be formatted and run separately as well as part of the full script. We recommend that each chunk performs a specific function that can be annotated.

Sections of code containing one or more code chunks that perform a specific task can also be denoted in an outline with headings.

7.1.3 Set the YAML header

At the top of the Quarto document, you will see a header demarcated by — at the top and bottom.

```
---
title: "Untitled"
format: html
editor: visual
---
```

Edit the YAML header to include relevant information.

```
---
title: "Introduction to Quarto"
format: html
author: SATVI Computational Group
date: today
---
```

7.1.4 Create a code chunk

You can do this manually by clicking the green chunk icon (C with a +) on the top right of the toolbar or you can use the keyboard shortcut option + cmd + I. This will produce an empty code chunk with R as the default language.

````
```{r}
#| label: R chunk

print("Hello, Quarto!")
```
````

```
[1] "Hello, Quarto!"
```

If you want to change the language, simply specify the language you would like to use in the yellow opening delimiter.

````
```{python}
# This is a Python code chunk
import math
```
````

```
# Calculate the square root of 16
sqrt_16 = math.sqrt(16)

# Print the result
print(f"The square root of 16 is {sqrt_16}")
```

```
The square root of 16 is 4.0
```

7.1.5 Tailor the code chunk output

Add options to each code chunk delimiter to show or hide specific information.

1. warning = FALSE means do not show any warnings generated by the code in the output
2. message = FALSE means do not show any messages generated by the code in the output
3. echo = FALSE means do not show the code in the output

```
```{r}
# Generate a warning
x <- -1
if (x < 0) {
  warning("x is negative!")
}
```
```

```
Warning: x is negative!
```

```
```{r}
# Generate a message
y <- 10
if (y > 5) {
  message("y is greater than 5")
}
```
```

```
y is greater than 5
```

Hide the warning from the output

````
```{r, warning = FALSE}
# Generate a warning
x <- -1
if (x < 0) {
  warning("x is negative!")
}

# Generate a message
y <- 10
if (y > 5) {
  message("y is greater than 5")
}
```
````

```
y is greater than 5
```

Hide the message from the output

````
```{r, message = FALSE}
# Generate a warning
x <- -1
if (x < 0) {
  warning("x is negative!")
}
```
````

```
Warning: x is negative!
```

````
```{r, message = FALSE}
# Generate a message
y <- 10
if (y > 5) {
  message("y is greater than 5")
}
```
````

Hide the warning and the message from the output You can achieve the same effect using Markdown syntax instead of editing the opening delimiter.

````
```{r}
#| warning: false
#| message: false

# Generate a warning
x <- -1
if (x < 0) {
  warning("x is negative!")
}

# Generate a message
y <- 10
if (y > 5) {
  message("y is greater than 5")
}
```
````

Hide the code from the output

```
Warning: x is negative!
```

```
y is greater than 5
```

More OPML options can be found here: https://quarto.org/docs/reference/formats/opml.html

7.2 Now let's test a simple script in Quarto

7.2.1 Clear environment

```r
ls()
rm(list=ls())
```

7.2.2 Set output directory

```r
dir.create("output")
dir_save <- "output/"
```

7.2.3 Load libraries

```
library(knitr) # Needed to embed an external image within a code chunk
library(quarto) # Needed to render Quarto document from R console
library(ggplot2) # Needed to plot data
```

7.2.4 Load dataset

```
data("esoph")
```

7.2.5 Examine data structure

```
head(esoph)
```

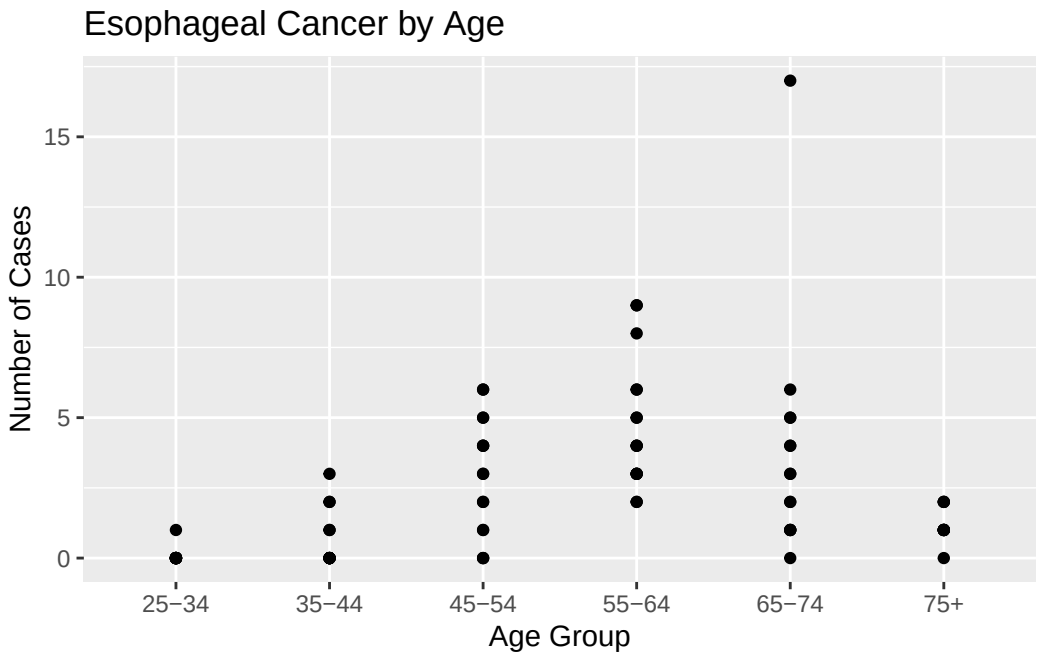
```
  agegp     alcgp    tobgp ncases ncontrols
1 25-34 0-39g/day 0-9g/day      0        40
2 25-34 0-39g/day    10-19      0        10
3 25-34 0-39g/day    20-29      0         6
4 25-34 0-39g/day      30+      0         5
5 25-34     40-79 0-9g/day      0        27
6 25-34     40-79    10-19      0         7
```

```
summary(esoph)
```

```
   agegp          alcgp          tobgp        ncases          ncontrols
 25-34:15   0-39g/day:23   0-9g/day:24   Min.   : 0.000   Min.   : 0.000
 35-44:15   40-79    :23   10-19   :24   1st Qu.: 0.000   1st Qu.: 1.000
 45-54:16   80-119   :21   20-29   :20   Median : 1.000   Median : 4.000
 55-64:16   120+     :21   30+     :20   Mean   : 2.273   Mean   : 8.807
 65-74:15                                3rd Qu.: 4.000   3rd Qu.:10.000
 75+  :11                                Max.   :17.000   Max.   :60.000
```

7.2.6 Plot data

```
ggplot(data = esoph, aes(x = agegp, y = ncases)) +
  geom_point() +  # Add points
  labs(title = "Esophageal Cancer by Age", x = "Age Group", y = "Number of Cases")
```



Quarto docs also support the import of image files stored externally. These can be arranged inline with your code or text.

7.3 Import an image

The easiest way to do this is by using R Markdown syntax outside of a code chunk.

```
![SATVI logo](images/satvi_logo.png)
```

Figure 7.1: SATVI logo

If you prefer to import from within a Quarto code chunk, you can do so using knitr

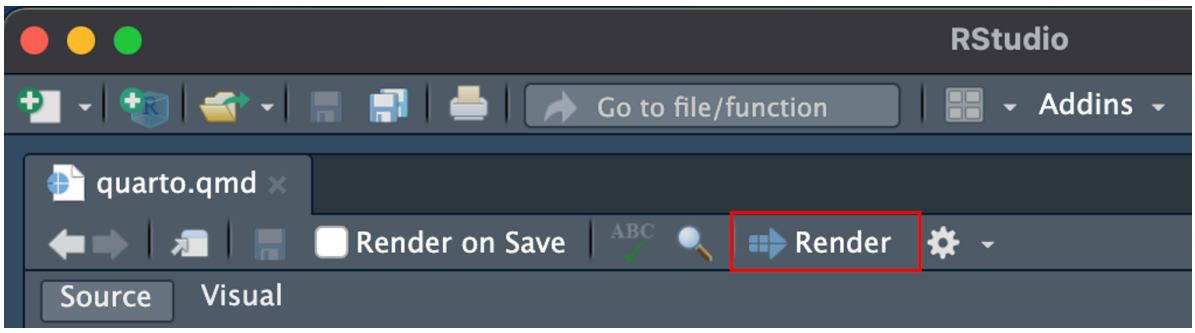
```
knitr::include_graphics("images/satvi_logo.png")
```

Documentation on embedding images can be found here: https://quarto.org/docs/authoring/figures.html

7.4 Render the document

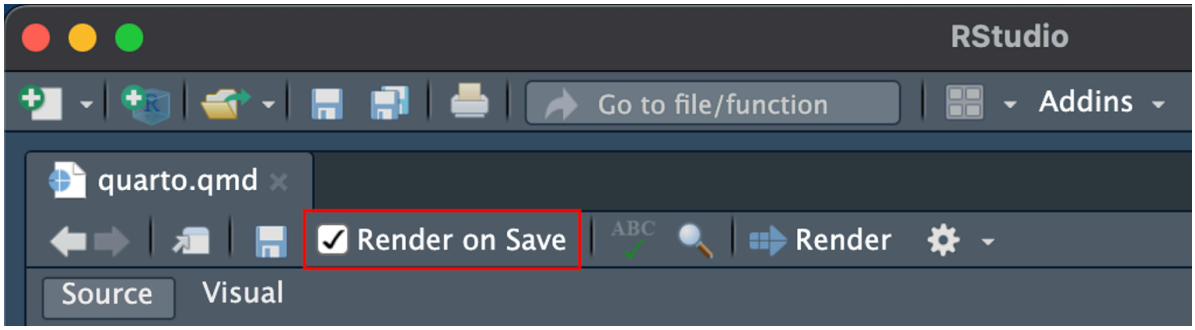
When you render your document, all code chunks and inline code will be executed automatically. You can render the document with point-and-click, directly from the RStudio console, or from the command line in the Terminal. To render your Quarto document using point-and-click:

1. Render using point-and-click



This will open a preview of your rendered document automatically. This previw will automatically update as you edit your document, so it can be helpful to render early on in the process and keep the preview open alongside your editor.

You can also choose to render on every save by checking the box in the toolbar:



2. Render from the RStudio console

You will need to download and install the Quarto command line interface (Quarto CLI, https://quarto.org/docs/get-started/). Now type the following directly into the RStudio console.

```
quarto_render("quartodocs.qmd") # This will render all formats

# You can also render to specific formats
quarto_render("quartodocs.qmd", output_format = "html")
quarto_render("quartodocs.qmd", output_format = "pdf")
quarto_render("quartodocs.qmd", output_format = "docx")
```

3. Render from the command line

Open the Terminal.

```
quarto render quartodocs.qmd # This will render all formats

# You can also render to specific formats

quarto render quartodocs.qmd --to html
quarto render quartodocs.qmd --to pdf
quarto render quartodocs.qmd --to docx
```

Further information on rendering can be found here https://quarto.org/docs/computations/r.html#rendering.

8 Summary

In summary, this book has no content whatsoever.

References

Knuth, Donald E. 1984. "Literate Programming." *Comput. J.* 27 (2): 97–111. https://doi.org/10.1093/comjnl/27.2.97.