Introduction to Reproducible Research in R and R Studio.

Susan Johnston

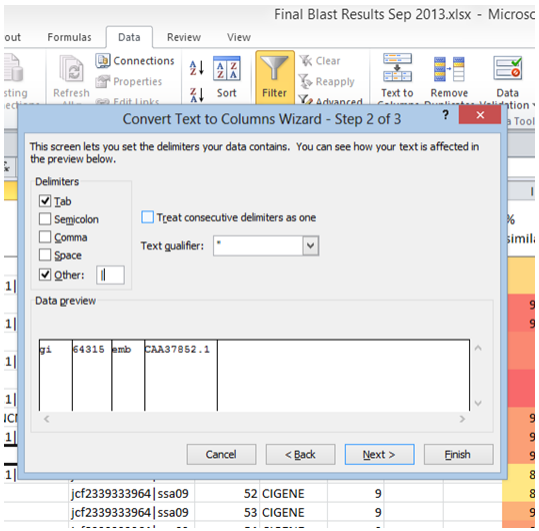
April 23, 2015

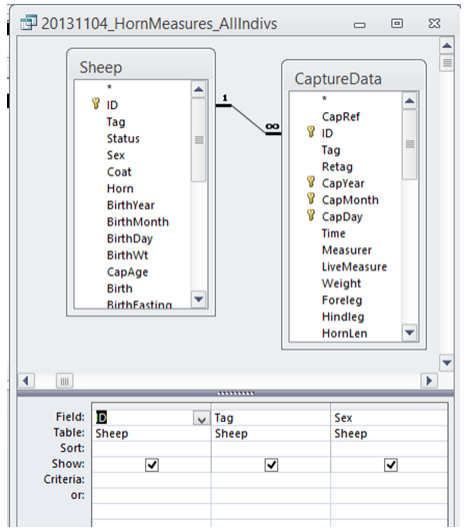
What is Reproducible Research?

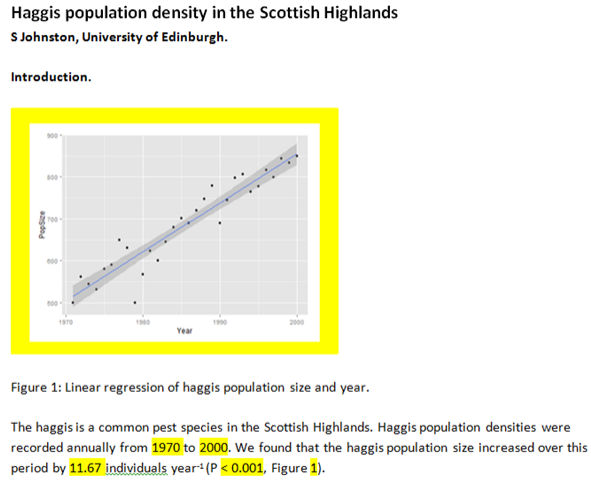
Reproducibility *is the ability of an entire experiment or study to be reproduced, either by the researcher or by someone else working independently, [and] is one of the main principles of the scientific method.*

Wikipedia

Many of us are used to clicking, copying and pasting...







Haggis population density in the Scottish Highlands

S Johnston, University of Edinburgh.

Introduction.

Figure 1: Linear regression of haggis population size and year.

The haggis is a common pest species in the Scottish Highlands. Haggis population densities were recorded annually from 1970 to 2000. We found that the haggis population size increased over this period by 11.67 individuals year^{-1} ($P < 0.001$, Figure 1).

- Can you repeat all of this again...
  - When new data is added to the dataset?
  - When a journal editor wants you to change a model parameter?
  - When you find an error, but not sure where you went wrong?
- ...and would you get the same results every time?

Worst Case Scenario

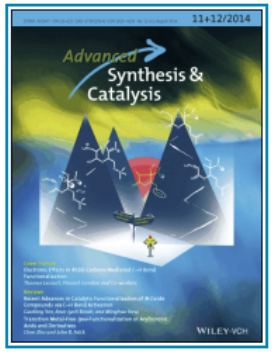
Retraction Watch

Tracking retractions as a window into the scientific process

Archive for the 'not reproducible' Category

Molecular mixup burns chemistry paper

without comments



Chemists at Lanzhou University in China did the right thing last month, retracting a paper in *Advanced Synthesis & Catalysis* because of issues with a reactant that could only be corrected by changing "all the text and quantities."

When the scientists were adding what was labeled Reactant 1 to the mix, they believed it was α-ethoxycarbonyl-α-azido-*N*-phenylacetamides. Unfortunately, what they were actually using was a decomposed version of the molecule, which threw everything off.

Here's the notice for "*tert*-Butyl Hydroperoxide and Tetrabutylammonium Iodide- Promoted Free Radical Cyclization of α-Azido-*N*-arylamides": Read the rest of this entry »

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Written by Cat Ferguson
April 14th, 2015 at 11:30 am

Posted in Advanced Synthesis and Catalysis,chemistry retractions,china retractions,doing the right thing,freely available,not reproducible,wiley

Two more retractions bring lab break-in biochemist up to eleven

without comments

Karel Bezouška, the Czech biochemist who was caught on hidden camera breaking into a lab fridge to fake results, has turned it up to eleven with two new retractions.

Both retractions appeared in *Biochemical and Biophysical Research Communications,* one in October 2014 and one in January 2015. His story began two decades ago in 1994, when he published a paper in *Nature* that couldn't be reproduced, and was eventually retracted in 2013.

The best part of the story, of course, is that when his university was attempting to recreate his experiments, Bezouška broke into a lab fridge to tamper with the experiments. Unbeknownst to him, he was caught on hidden camera. Read the rest of this entry »

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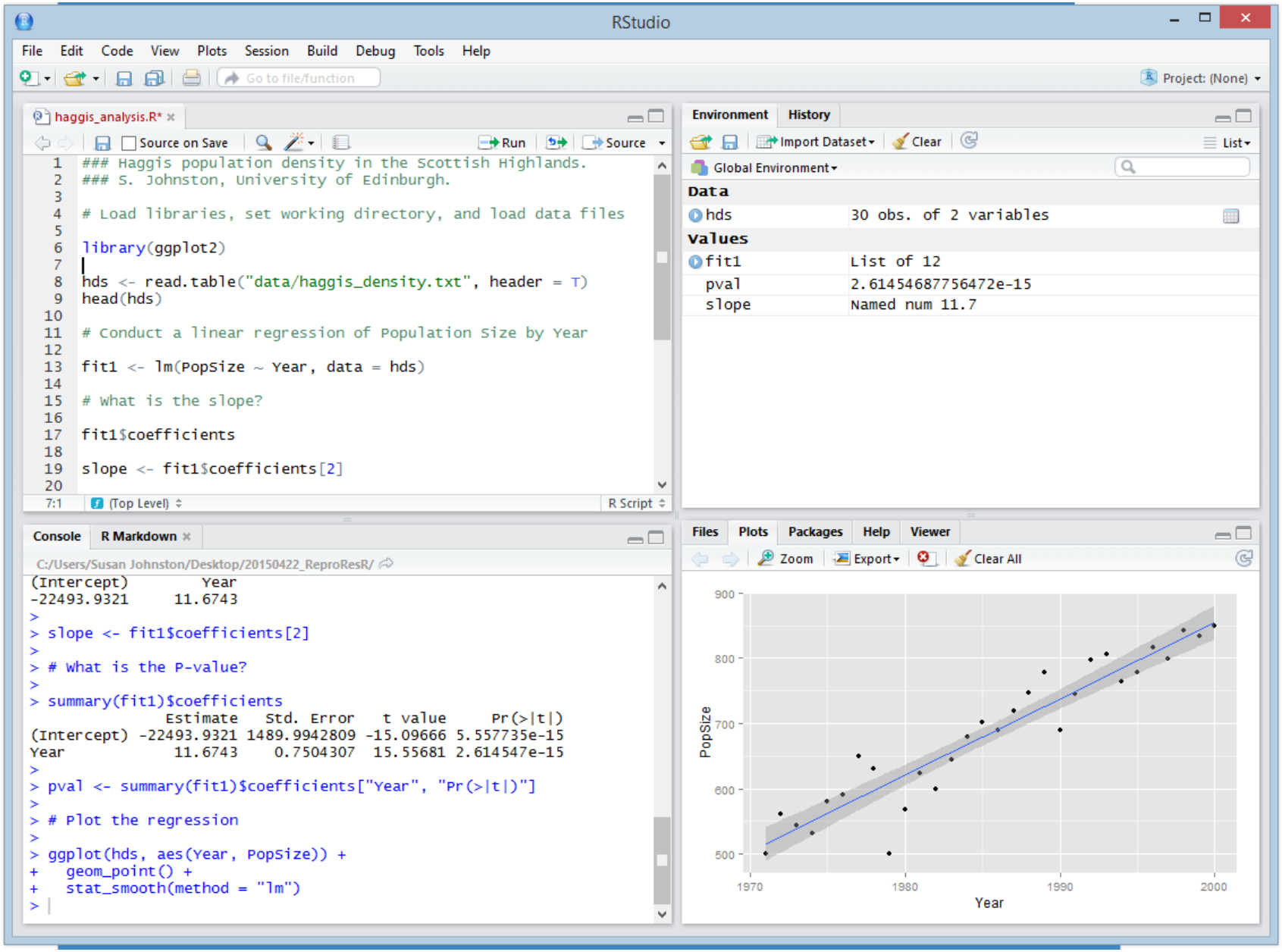
Three rules for reproducibility

1. Avoid manual data manipulation steps.
   - Automate analyses using scripts
   - "This is R. There is no 'if'. Only 'how'."

2. Connect textual statements to underlying results.
   - Create documents where results and figures update automatically.

3. Version control all custom scripts and documents.
   - It should be possible to revert to a previous version of an analysis.

The RStudio Environment: http://www.rstudio.com



Reproducible Research in RStudio

1. Creating a Portable Project (.Rproj)
2. Dynamic report writing with R Markdown and `knitr`
3. Version control using `git`

Reproducible Research in RStudio.

1. Creating a Portable Project (.Rproj)
2. Dynamic report writing with R Markdown and `knitr`
3. Version control using `git`

Bad habits can hinder portability.

https://support.rstudio.com/hc/en-us/articles/200526207-Using-Projects

Hadley Wickham @hadleywickham · Jan 27

Never plan on sharing your code? Using **setwd**() means that old code will break if you ever reorganise your directories

7 6

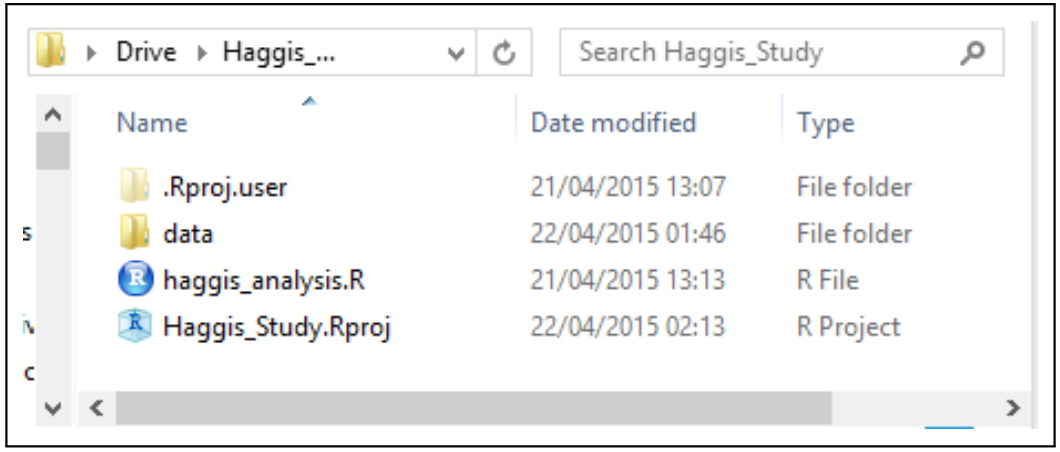
```
setwd("C:/Users/susjoh/Desktop/SalmoAnalysis")
setwd("C:/Users/Susan Johnston/Desktop/SalmoAnalysis")
setwd("C:/Users/Susan Johnston/Drive/SalmoAnalysis")

source("../../OvisAnalysis/GWASplotfunctions.R")
```

An analysis should be contained within a directory, and it should be easy to move it or pass on to someone new.

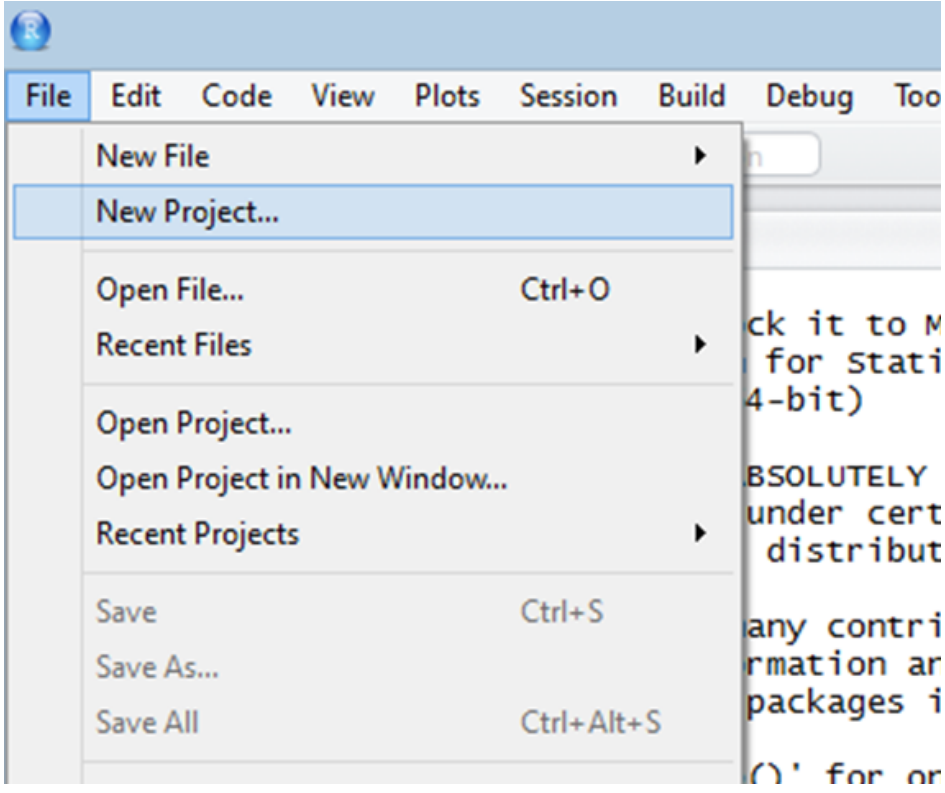
Solution: using RStudio Projects.

https://support.rstudio.com/hc/en-us/articles/200526207-Using-Projects



- Establishes a directory with associated `.Rproj` file.
- Automatically sets the working directory.
- Can save and source `.Rprofile`, `.Rhistory`, `.Rdata` files.
- Allows version control within R Studio.

Creating a Portable Project (.Rproj)



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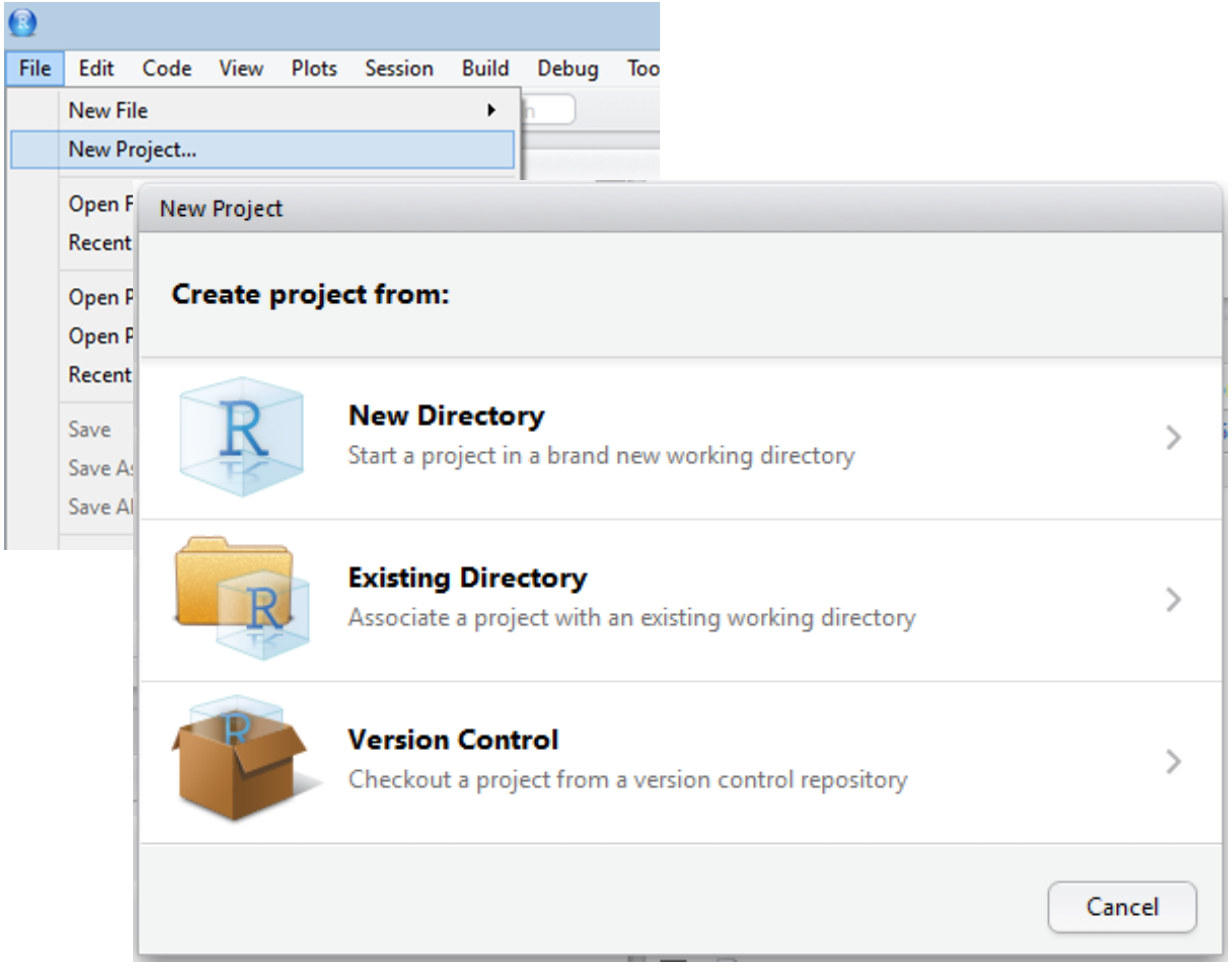

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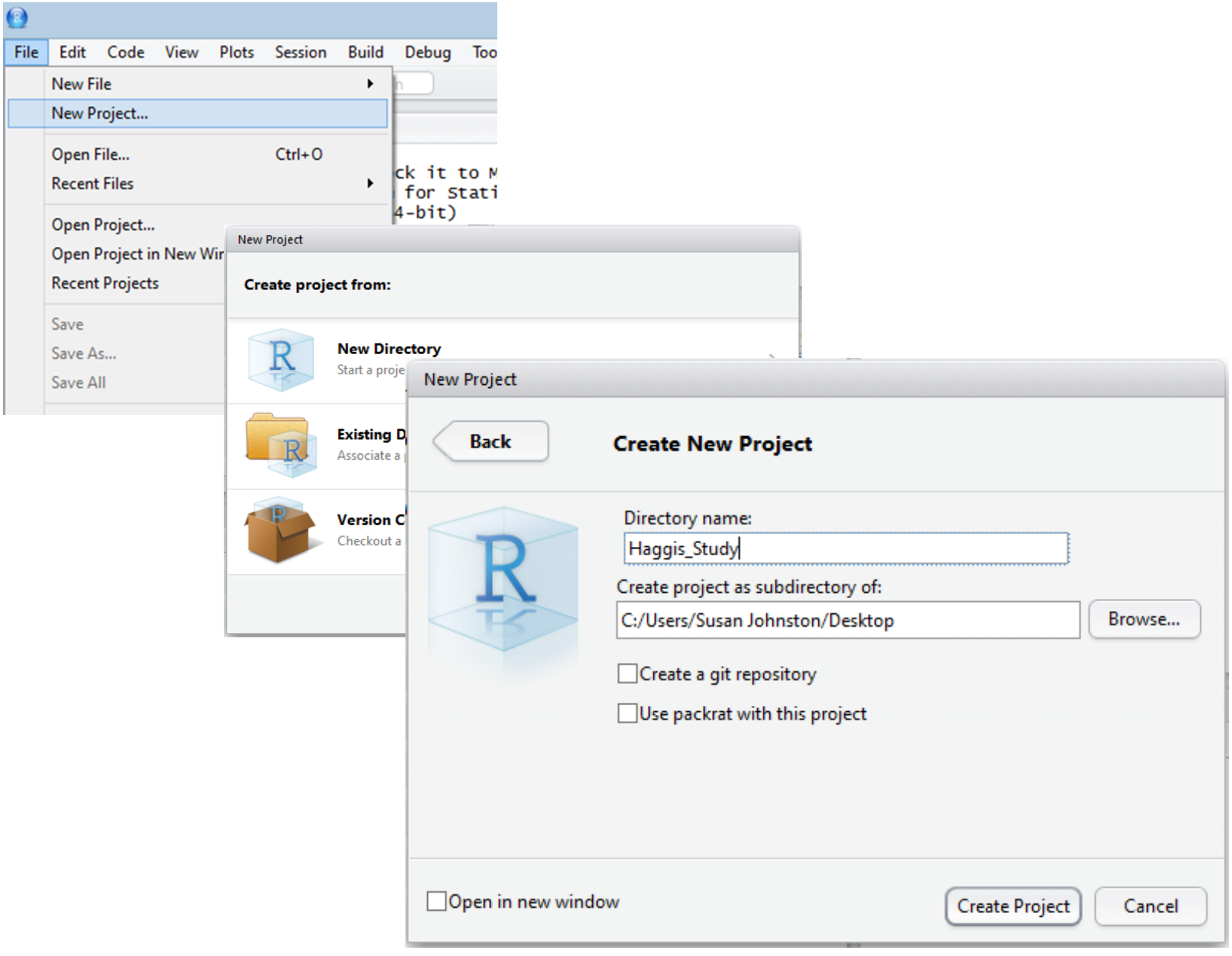

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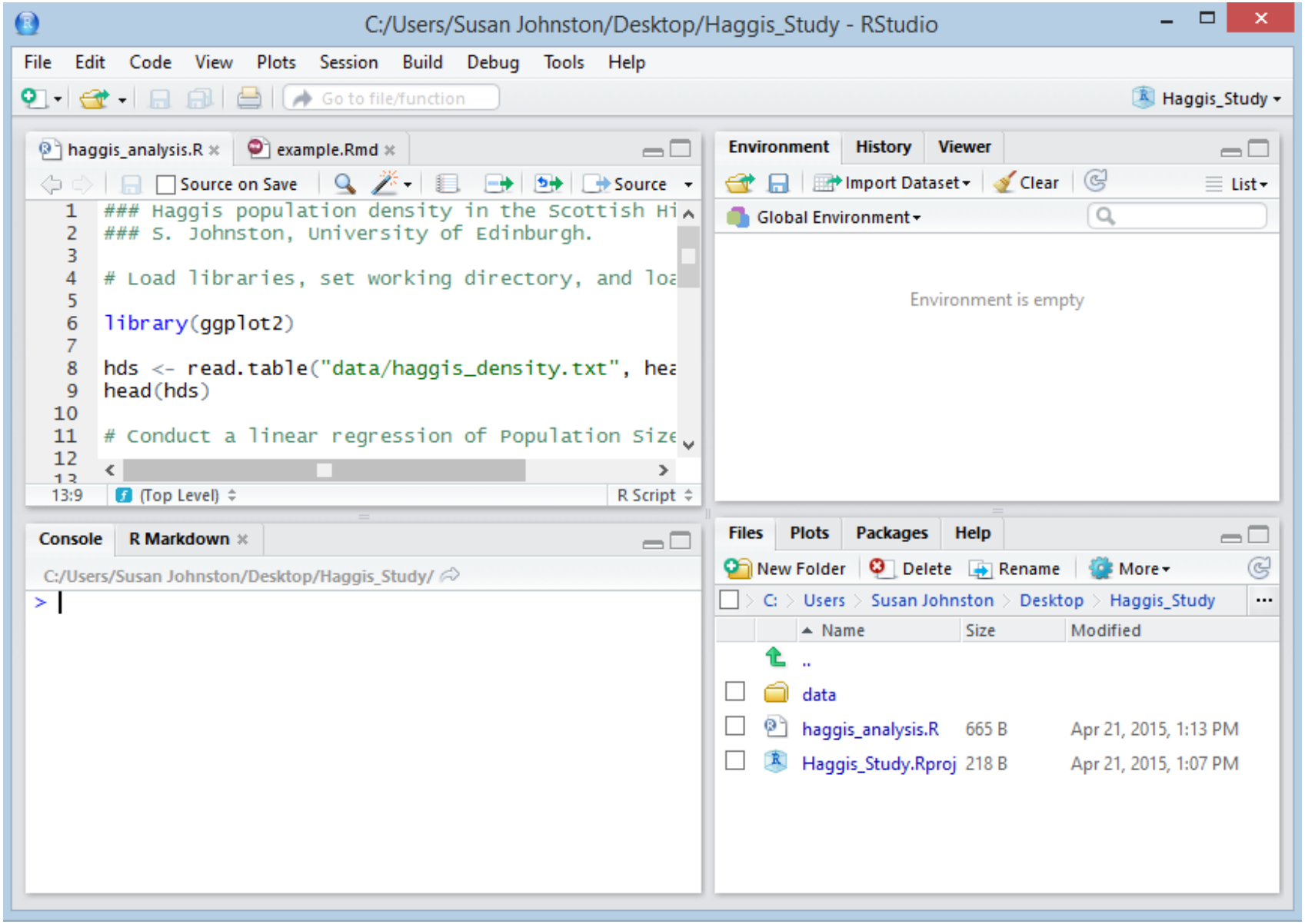
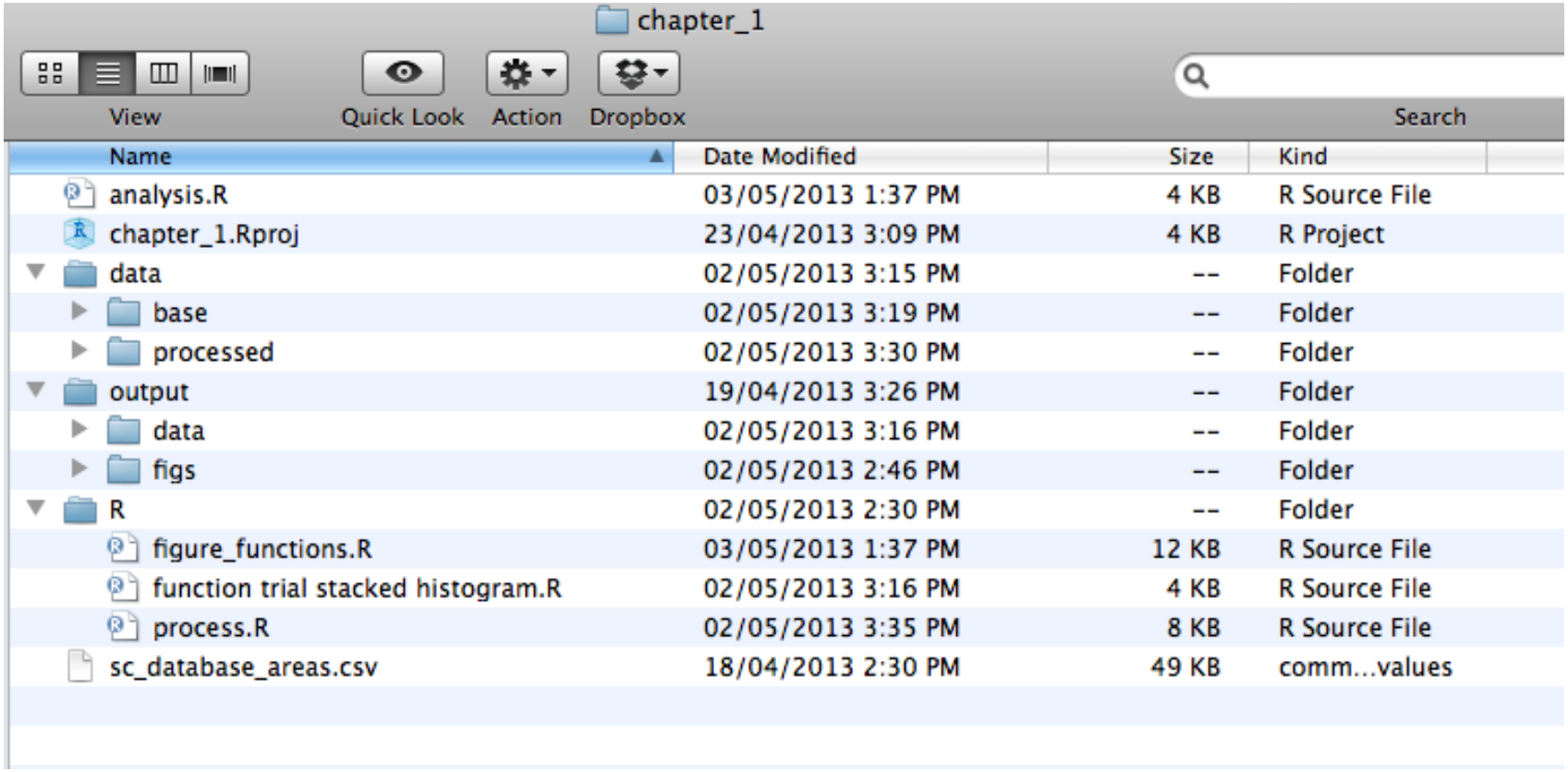


Maintaining a portable R Project.

http://nicercode.github.io/blog/2013-05-17-organising-my-project/



All data, scripts and output should be kept within the project directory.

Reproducible Research in RStudio.

1. Creating a Portable Project (.Rproj)
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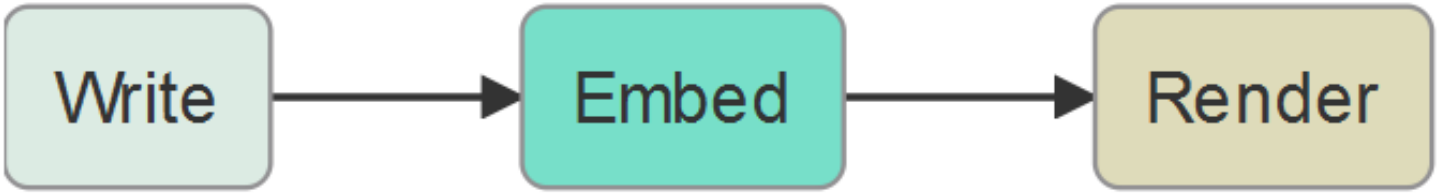
3. Version control using `git`

knitr

Elegant, flexible and fast dynamic report generation with R



The knitr package allows R code and document templates to be compiled into a single report containing text, results and figures.

knitr

Elegant, flexible and fast dynamic report generation with R

Write reports directly in R

haggis_analysis.R | example.Rmd

Knit HTML | Chunks

```
1  ### Example of using "R Markdown" and `knitr`
2
3  This is an R Markdown Document. Markdown is a
   simple formatting syntax for authoring
   documents. For example, text can be emphasise
   d with *italics* and **bold**.
4
5  Wrap code to be evaluated in R in an R
   "chunk"
6
7  ```{r}
8  nrow(cars)
9  ```
10
11 Code can be evaulated in-line using backticks
   . For example, we can write 1 + 1 = `r 1+1`.
12
13 Plots will also be printed.
14
15 ```{r fig.width = 3, fig.height = 3}
16 library(ggplot2)
17 ggplot(cars, aes(speed, dist)) +
18   geom_point()
19 ```
20
```

8:11 | Chunk 1 | R Markdown

knitr

Elegant, flexible and fast dynamic report generation with R

Write reports directly in R

C:/Users/Susan Johnston/Desktop/Drive/Haggis_Study/example.html

example.html | Open in Browser | Publish | Find

Example of using "R Markdown" and `knitr`

This is an R Markdown Document. Markdown is a simple formatting syntax for authoring documents. For example, text can be emphasised with *italics* and **bold**.

Wrap code to be evaluated in R in an R "chunk"

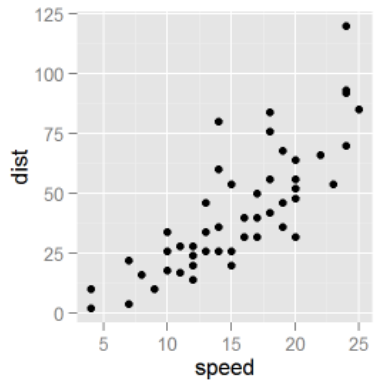
```
nrow(cars)
```

```
## [1] 50
```

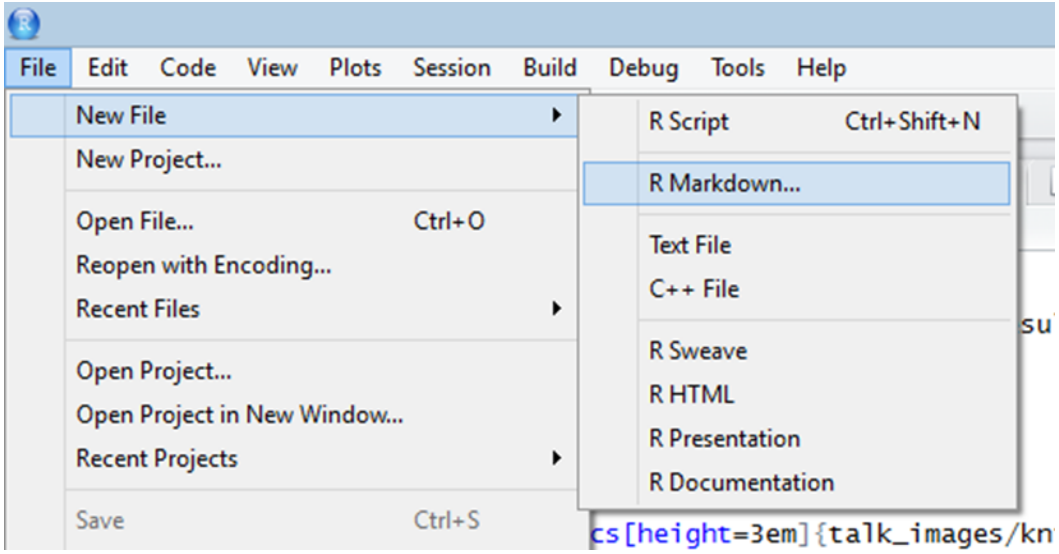
Code can be evaulated in-line using backticks. For example, we can write 1 + 1 = 2.

Plots will also be printed.

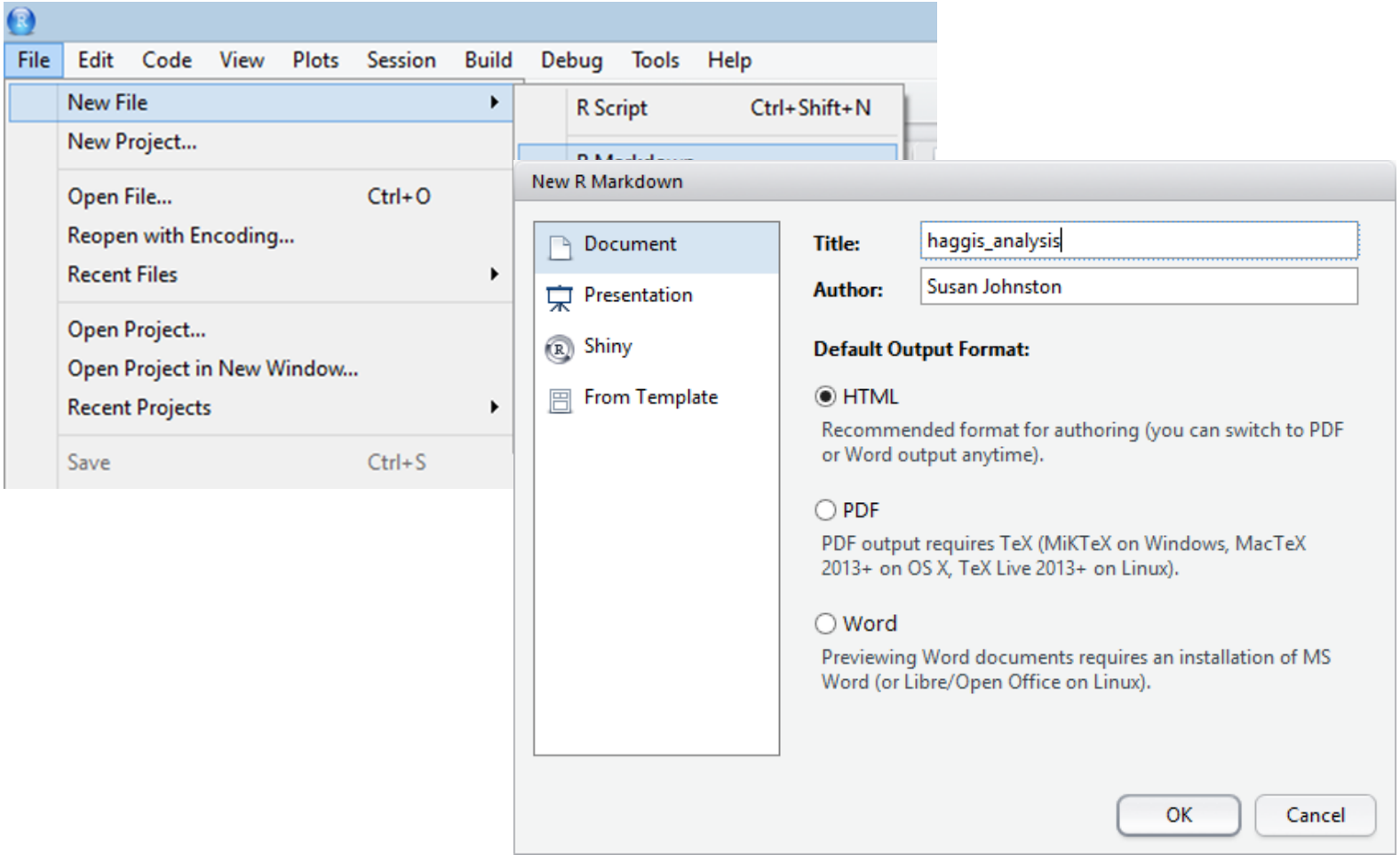
```
library(ggplot2)
ggplot(cars, aes(speed, dist)) +
  geom_point()
```



Creating an R Markdown Script (.Rmd).



Creating an R Markdown Script (.Rmd).



A Quick Start Guide

http://nicercode.github.io/guides/reports/

1. Type report text into .Rmd file

```
Lorem ipsum dolor sit amet, consectetuer adipiscing elit.
```

2. Enclose code to be evaluated in chunks

````
```{r}
model1 <- lm(speed ~ dist, data = cars)
```
````

3. Evaluate code inline

````
The slope of the model is `r coefficients(model1)[2]`
````

The slope of the model is 0.16557

4. Compile report as .html, .pdf or .doc

A Quick Start Guide

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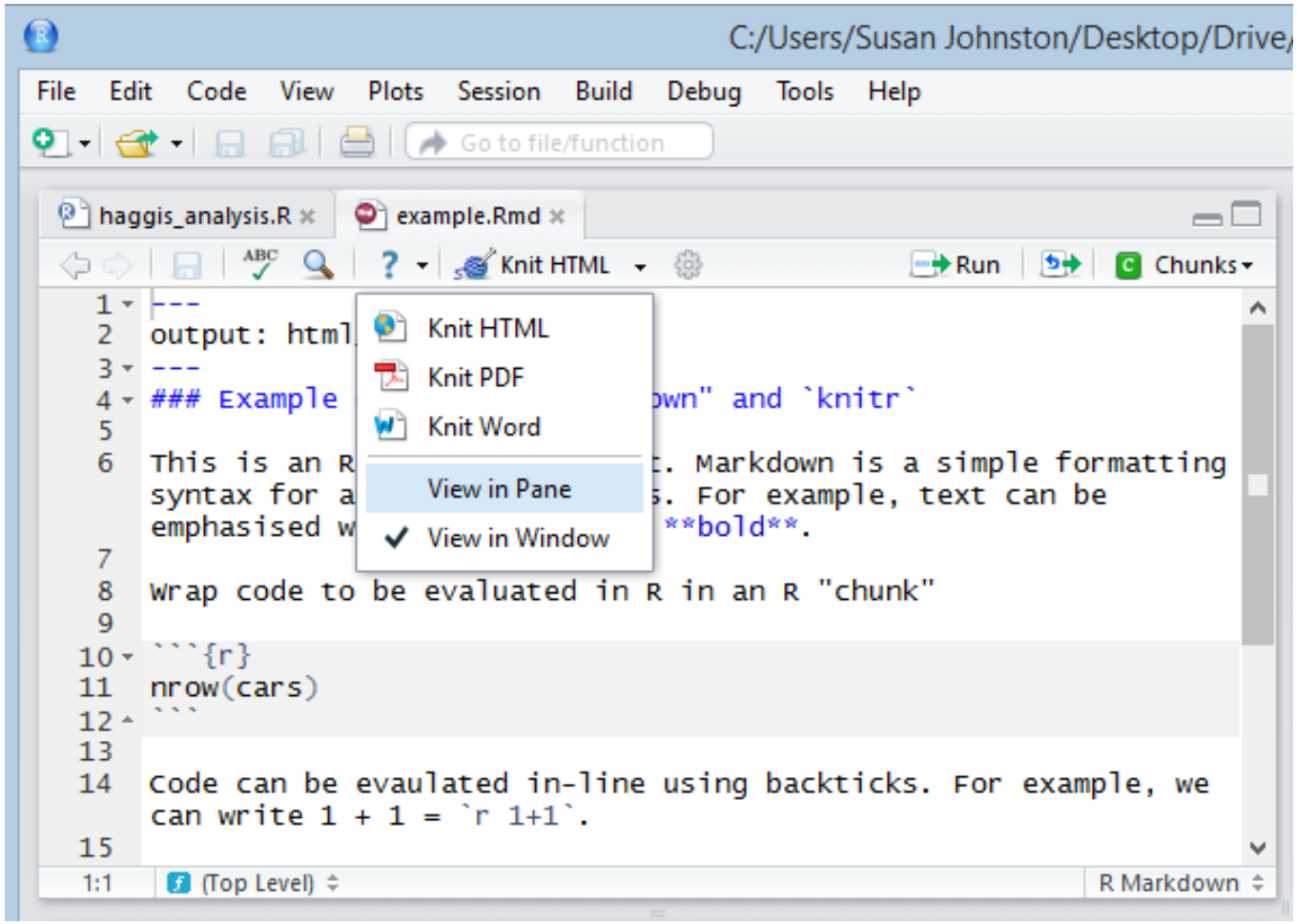

NB. PDF and Word docs require additional software.

http://rmarkdown.rstudio.com/?version=0.98.1103&mode=desktop

A Quick Start Guide

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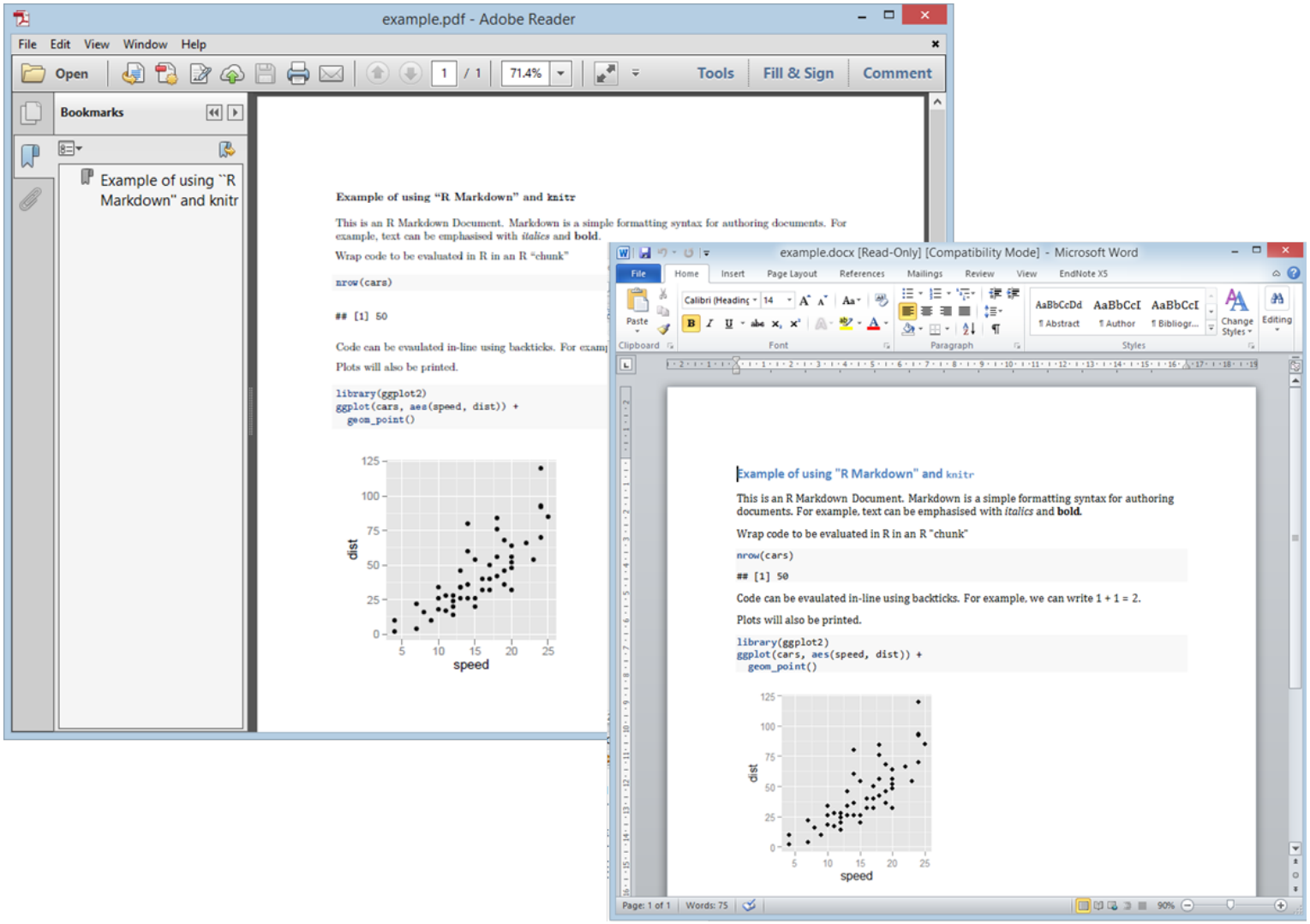

http://rmarkdown.rstudio.com/?version=0.98.1103&mode=desktop

Advanced Tips

- Control how chunks are reported and evaluated

````
```{r echo = F, warning = F, fig.width = 3}
model1 <- lm(speed ~ dist, data = cars)
plot(model1)
```
````

- `spin()`: compile .R files using #' and #+

  http://deanattali.com/2015/03/24/knitrs-best-hidden-gem-spin/

- LaTeX documents, Presentations, Shiny, etc.

Reproducible Research in RStudio.

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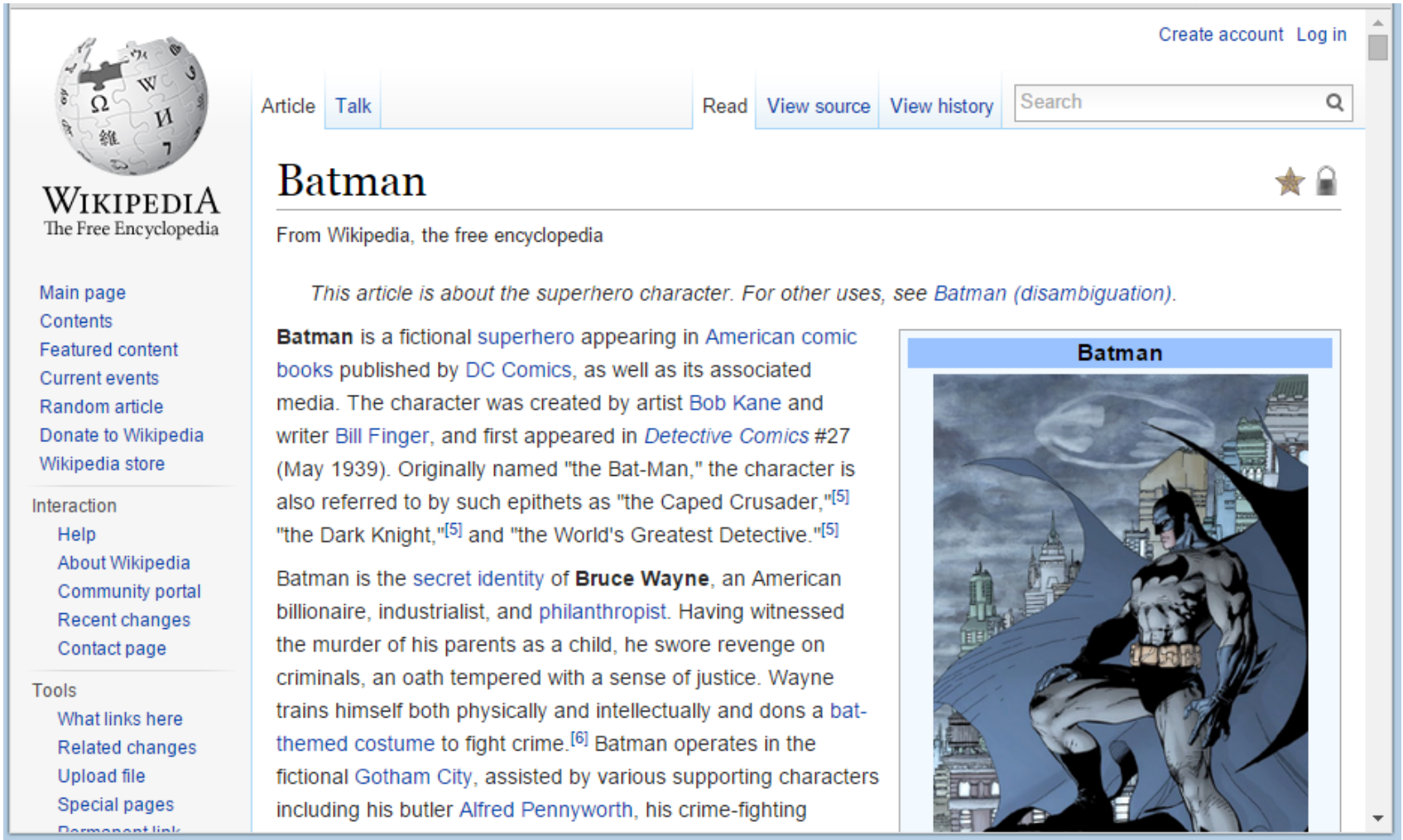

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Batman

From Wikipedia, the free encyclopedia

This article is about the superhero character. For other uses, see Batman (disambiguation).

Batman is a fictional superhero appearing in American comic books published by DC Comics, as well as its associated media. The character was created by artist Bob Kane and writer Bill Finger, and first appeared in *Detective Comics* #27 (May 1939). Originally named "the Bat-Man," the character is also referred to by such epithets as "the Caped Crusader,"[5] "the Dark Knight,"[5] and "the World's Greatest Detective."[5]

Batman is the secret identity of **Bruce Wayne**, an American billionaire, industrialist, and philanthropist. Having witnessed the murder of his parents as a child, he swore revenge on criminals, an oath tempered with a sense of justice. Wayne trains himself both physically and intellectually and dons a bat-themed costume to fight crime.[6] Batman operates in the fictional Gotham City, assisted by various supporting characters including his butler Alfred Pennyworth, his crime-fighting

Batman

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- (cur | prev) 14:23, 15 April 2015 Kinfoll1993 (talk | contribs) **m** . . (118,704 bytes) (+10) . . *(→Personality)*
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- (cur | prev) 13:25, 15 April 2015 Kinfoll1993 (talk | contribs) **m** . . (117,625 bytes) (+34) . . *(Category:fictional antiheroes per citations at list of fictional antiheroes)*
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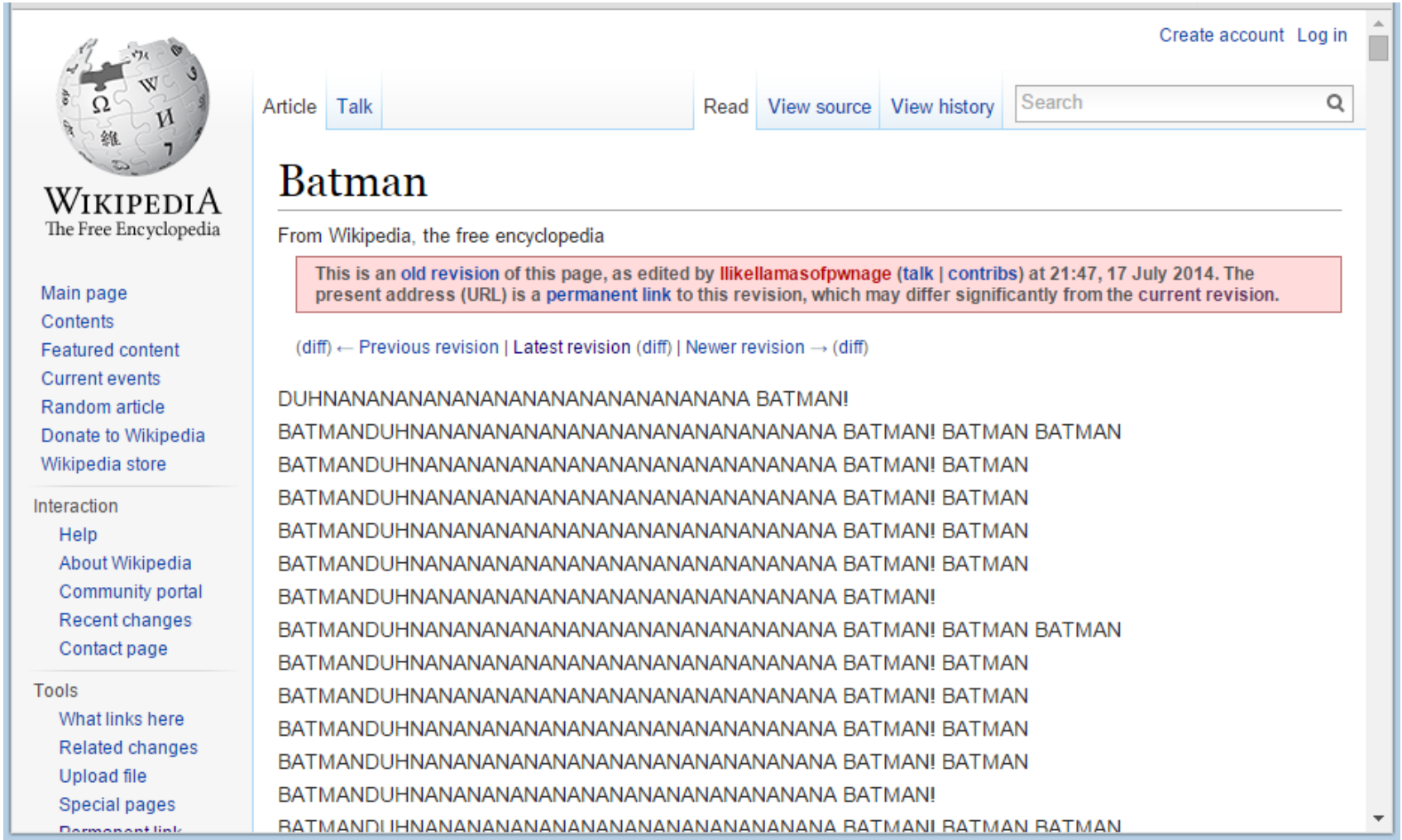

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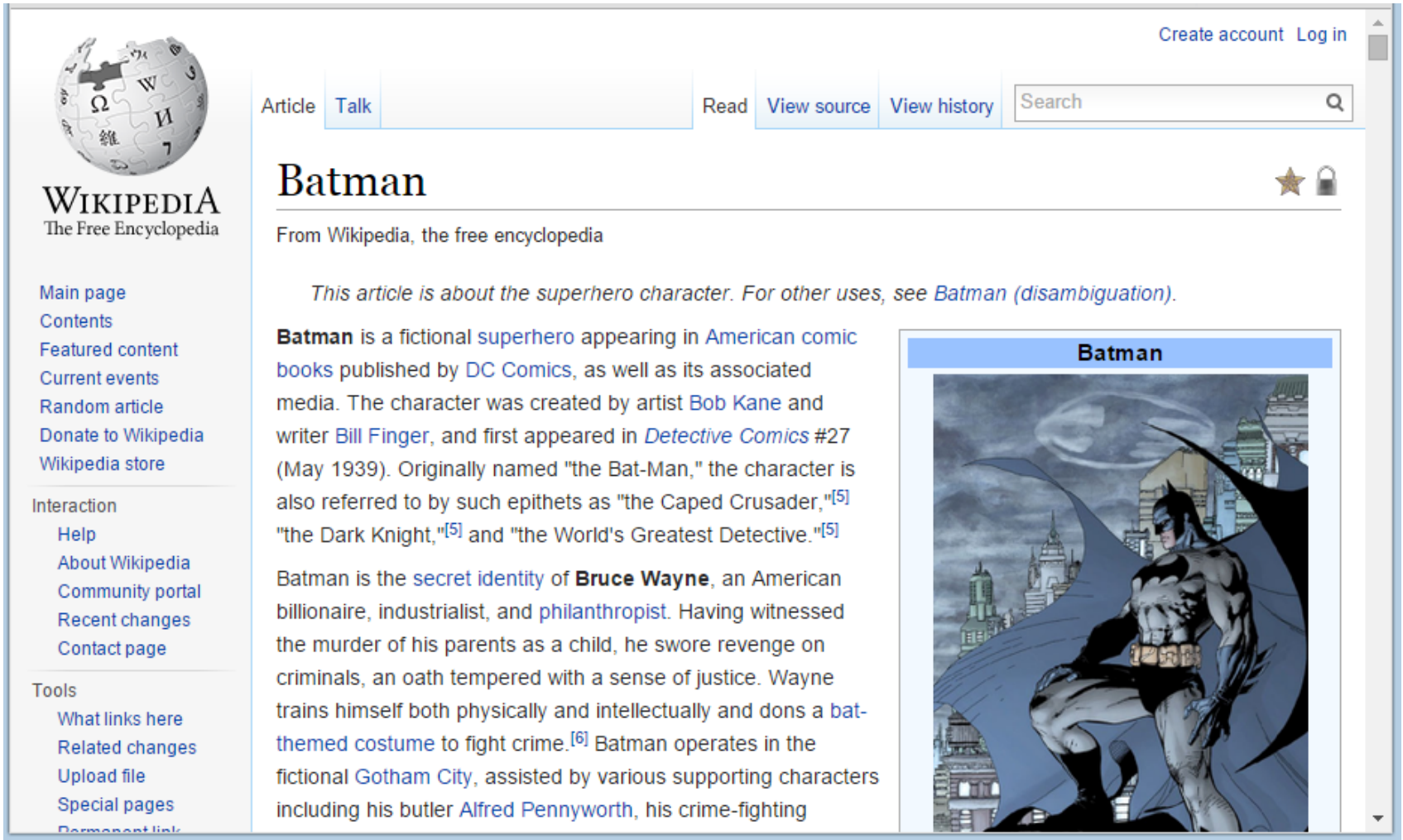

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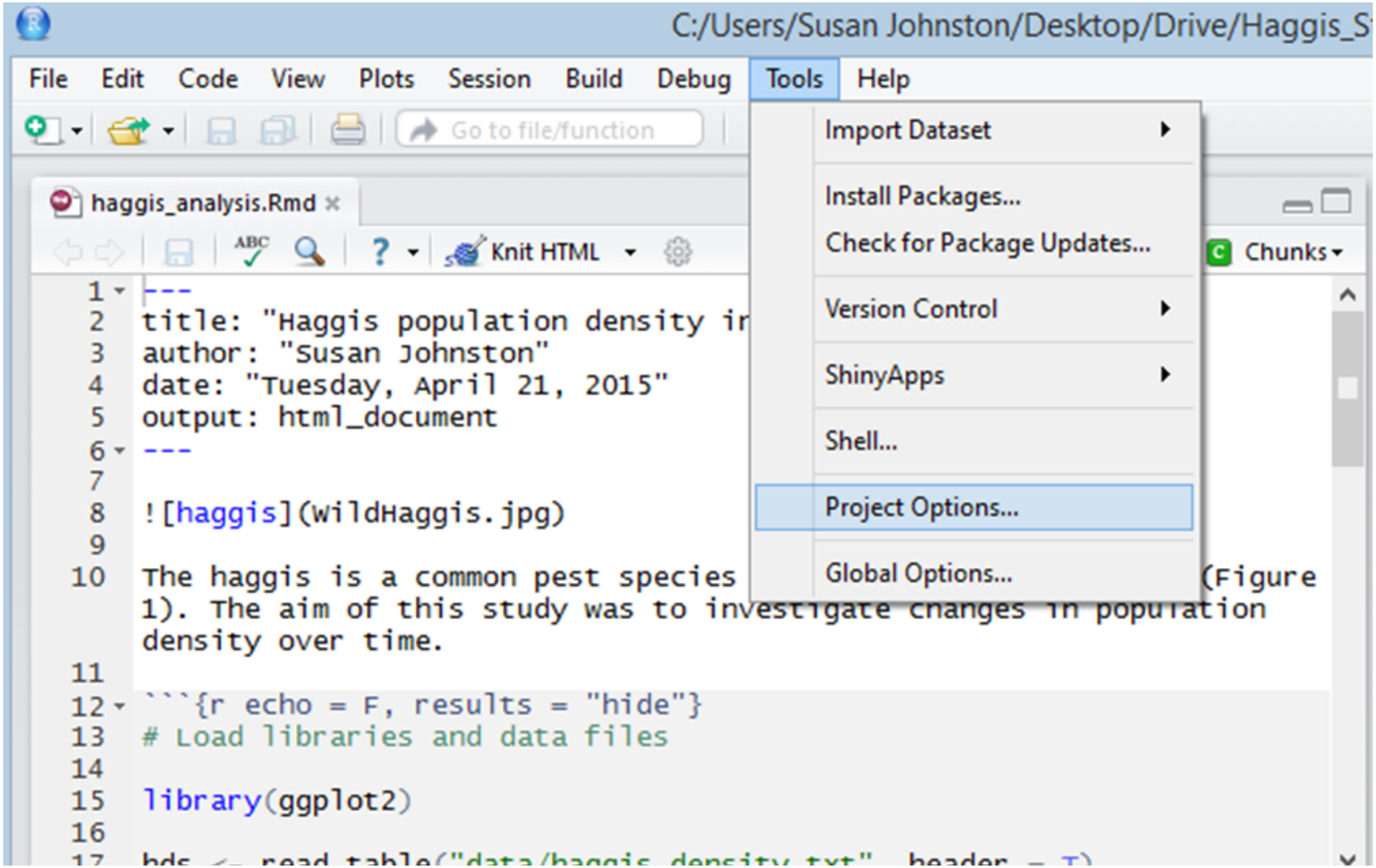
Version Control Using git.

https://support.rstudio.com/hc/en-us/articles/200532077-Version-Control-with-Git-and-SVN

Git can be installed on all platforms, and can be used to implement version control within an R Studio Project.

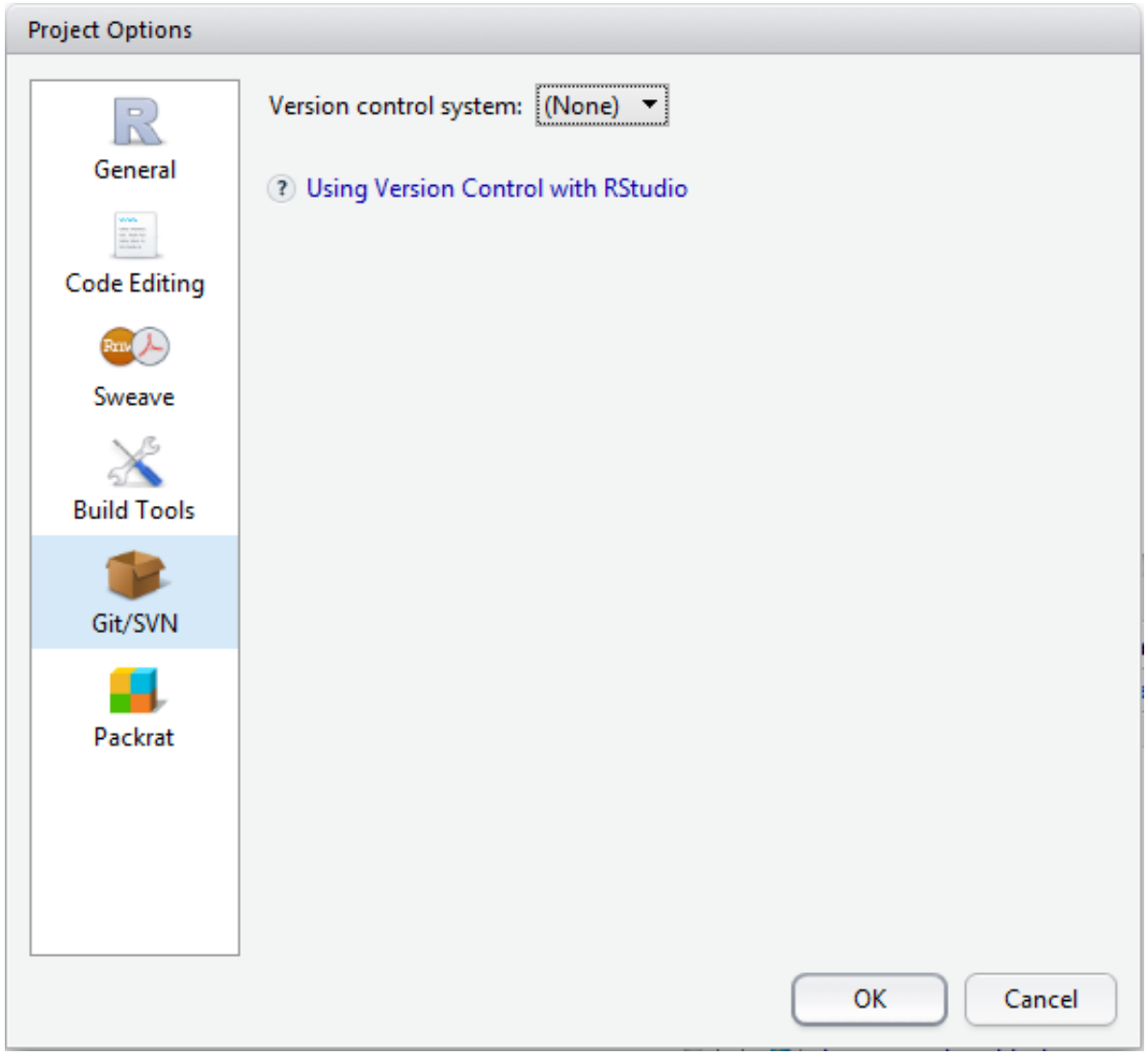
http://git-scm.com/downloads

Version Control in R Studio



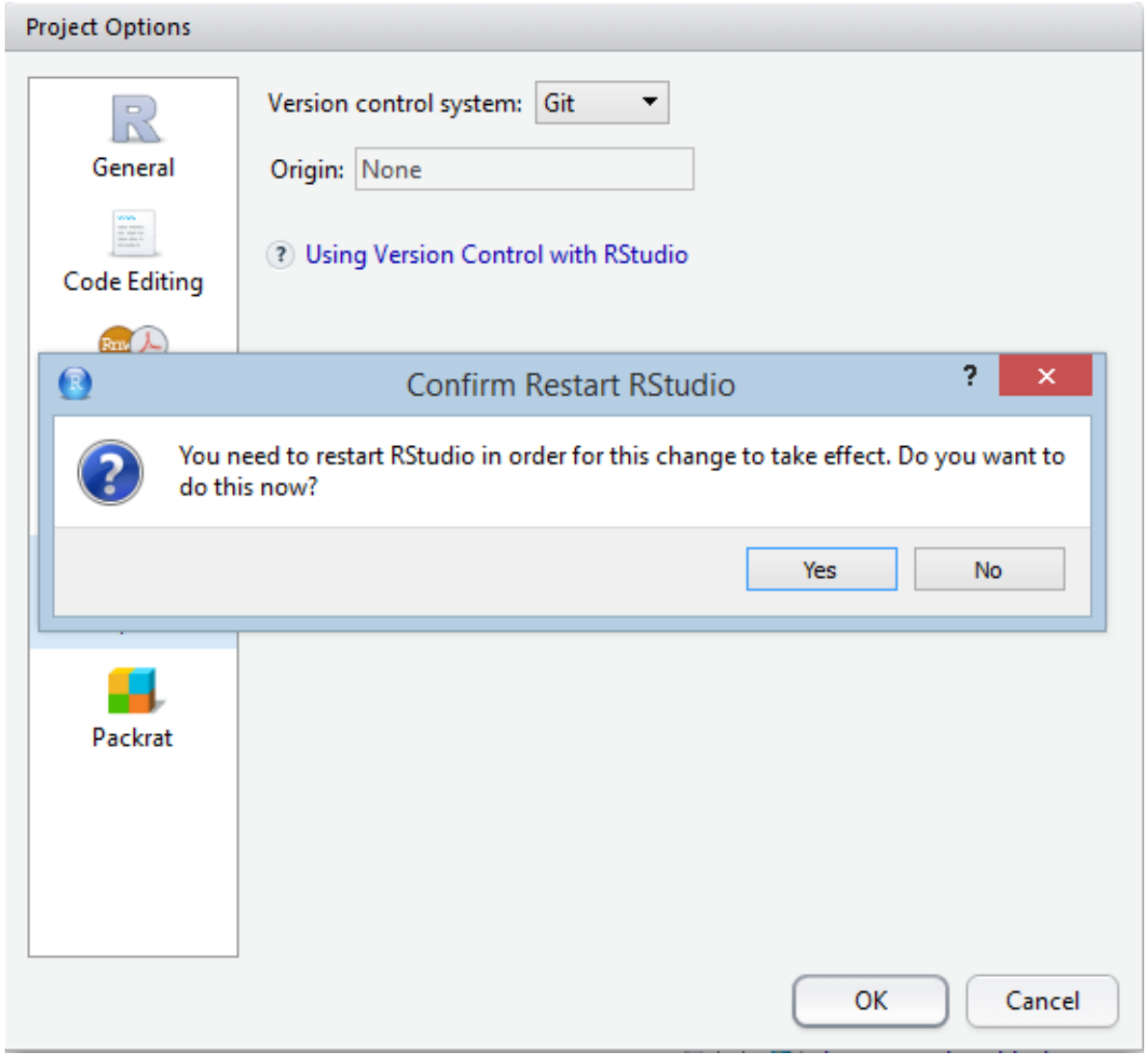
Tools >Project Options allows setup of `git` version control.

Version Control in R Studio



Select `git` as a version control system

Version Control in R Studio



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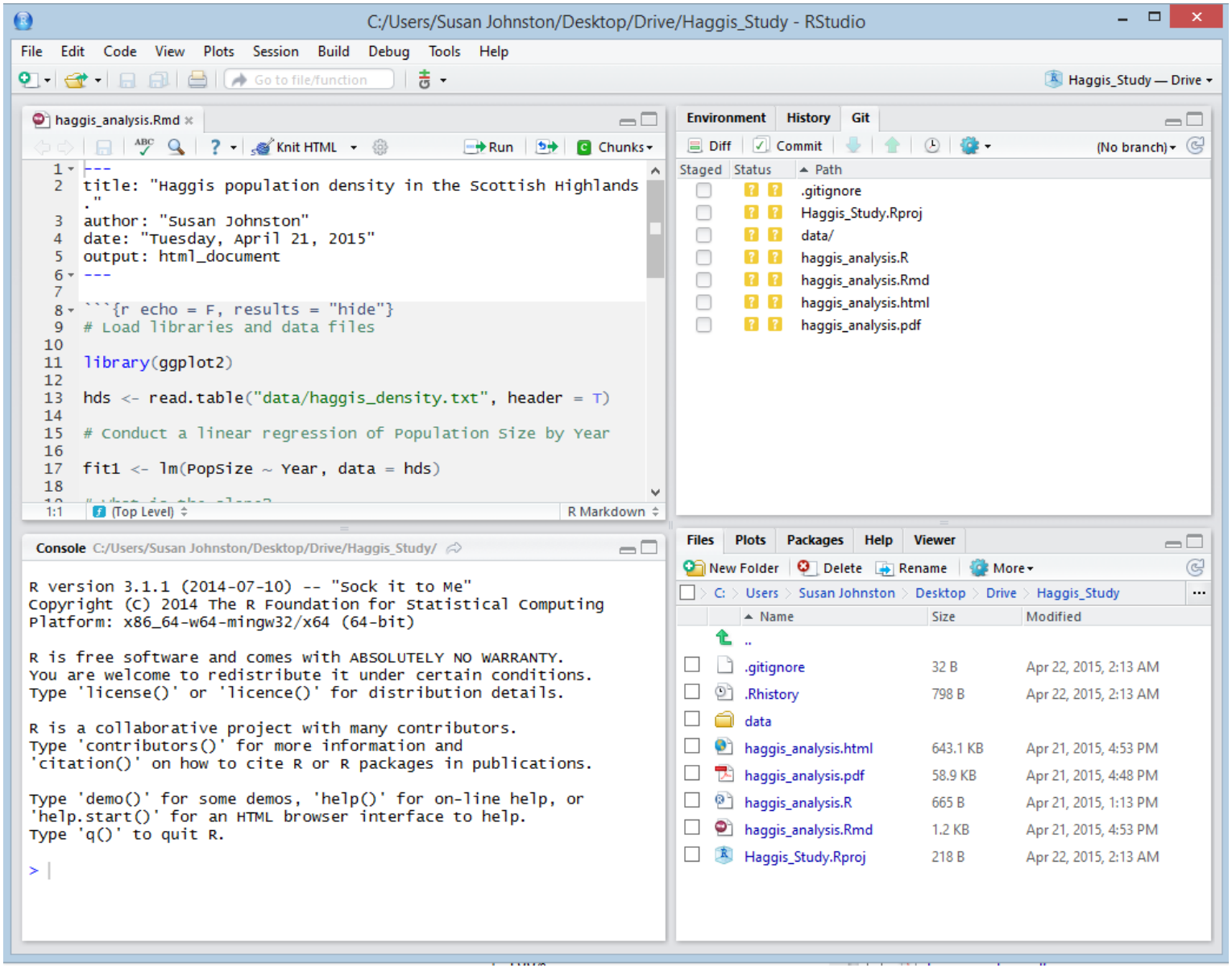
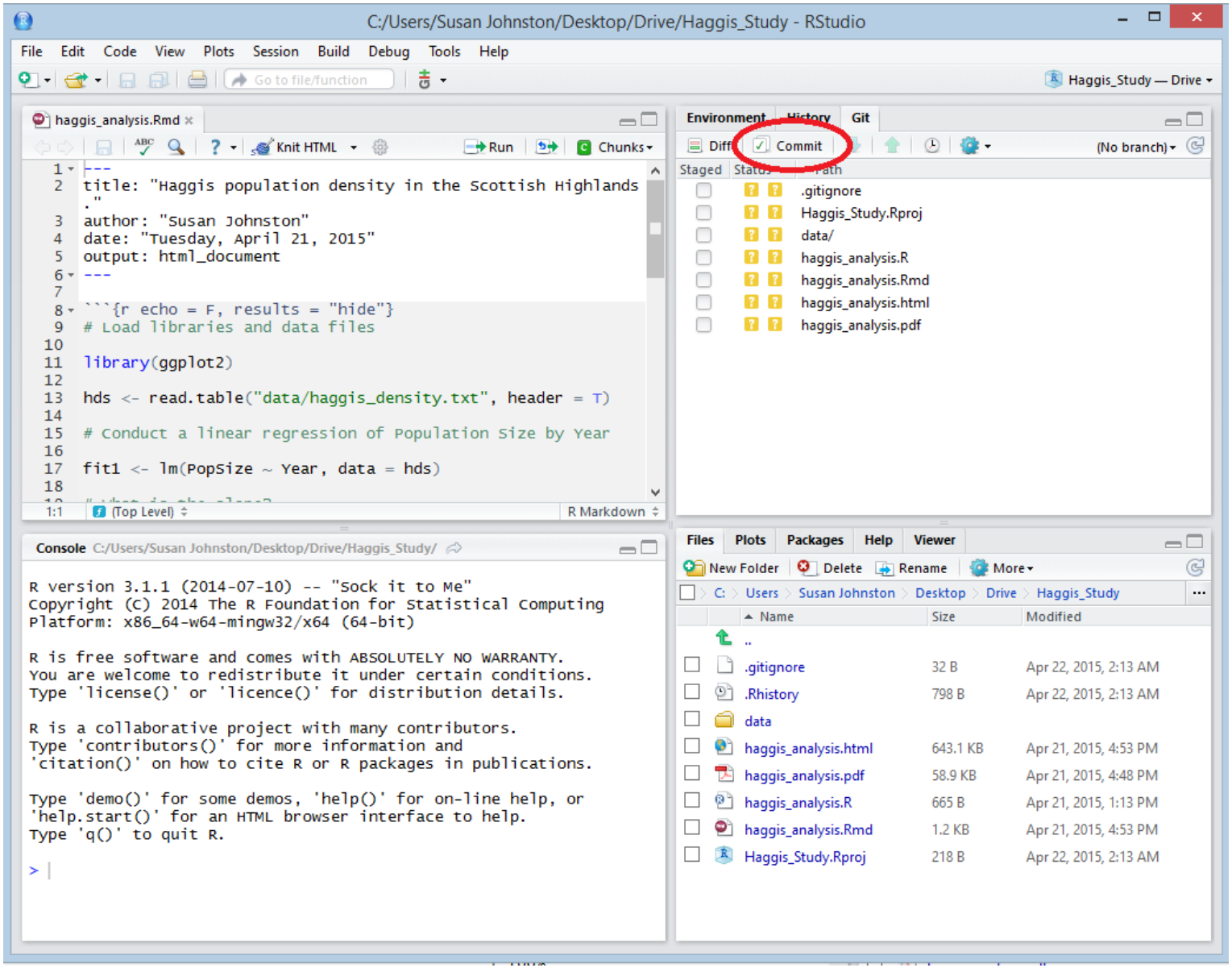


`git` information will appear in the top-right frame.

Version Control in R Studio



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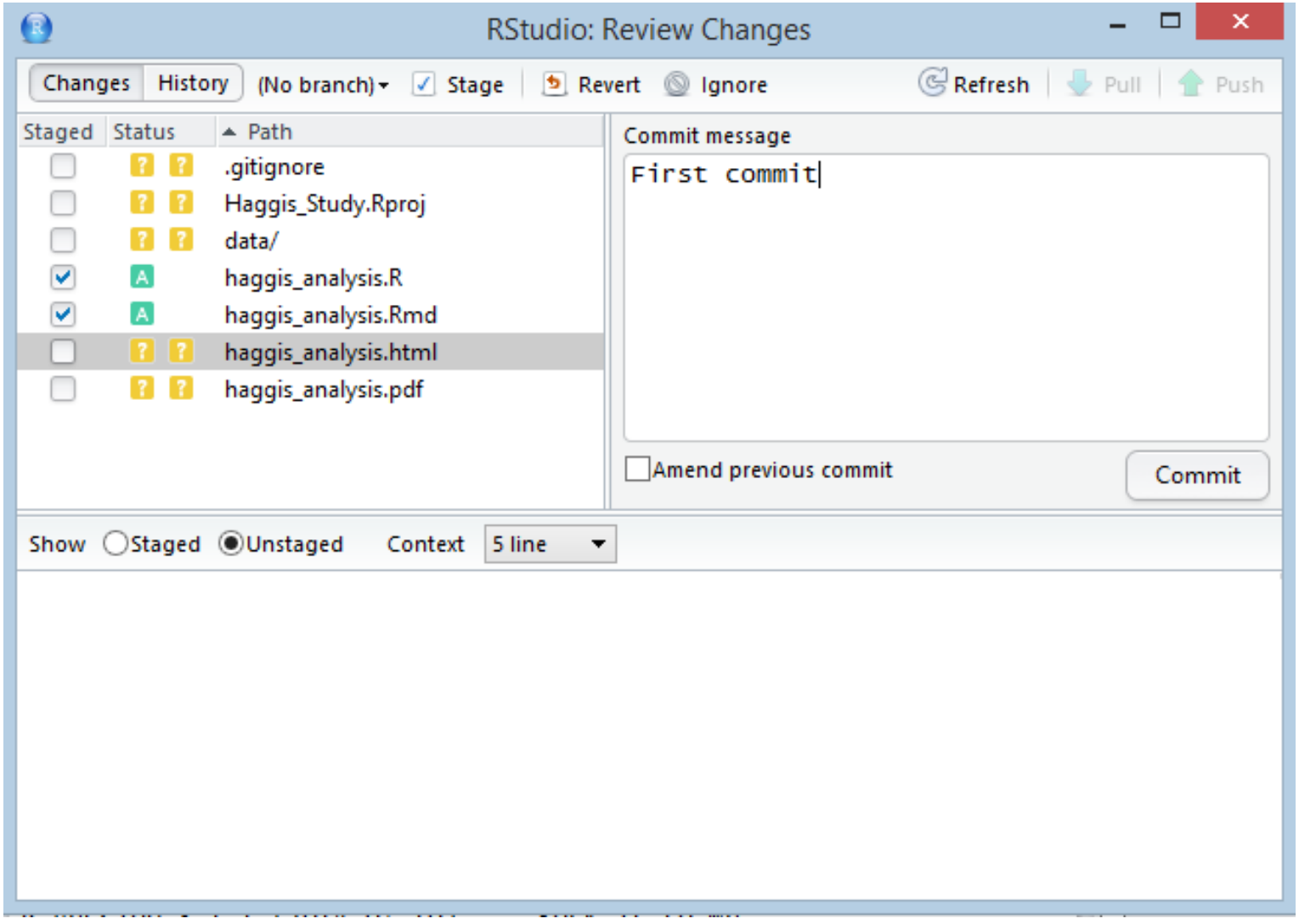
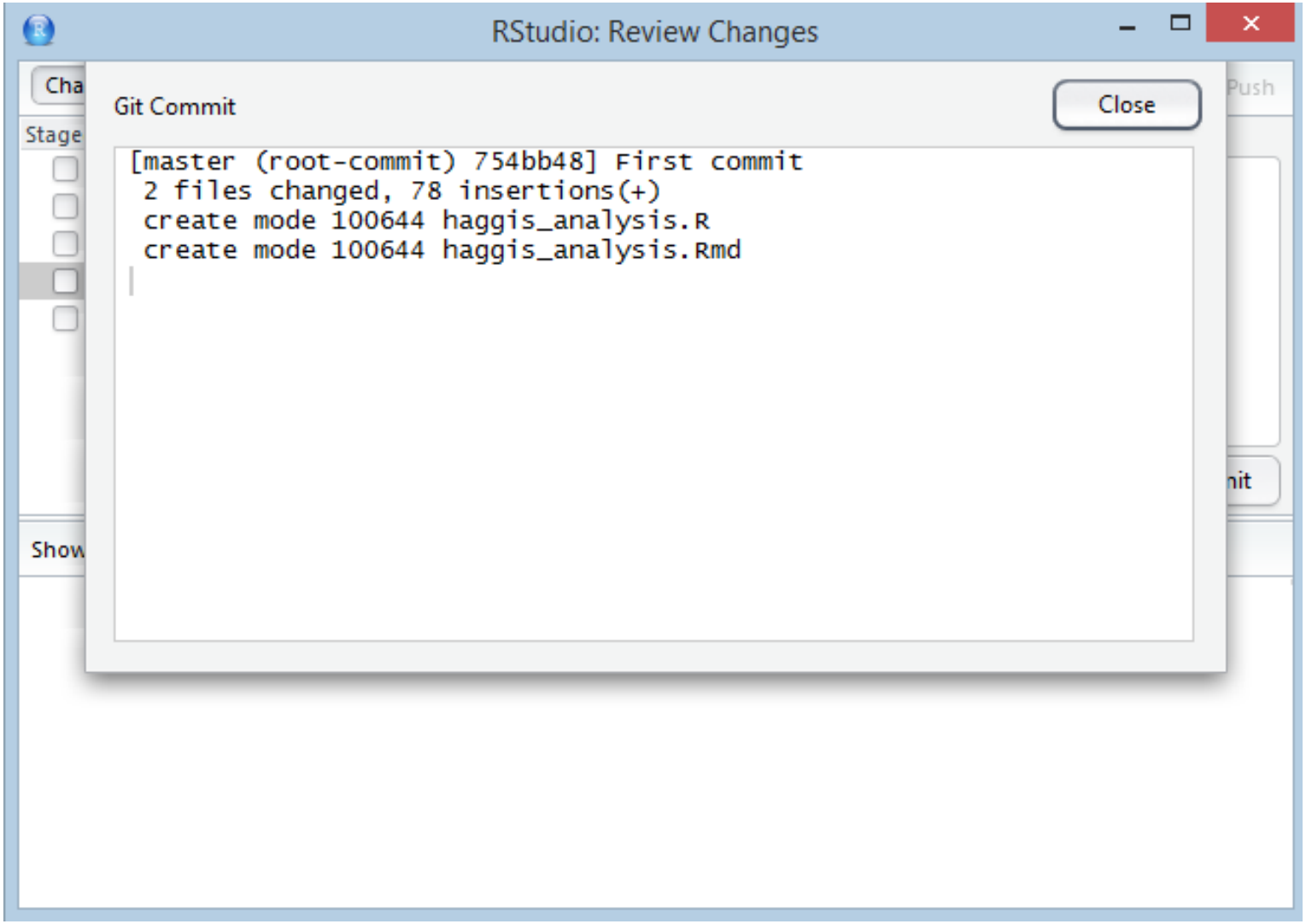


Select files to version control, write a meaningful commit message >Commit

Version Control in R Studio



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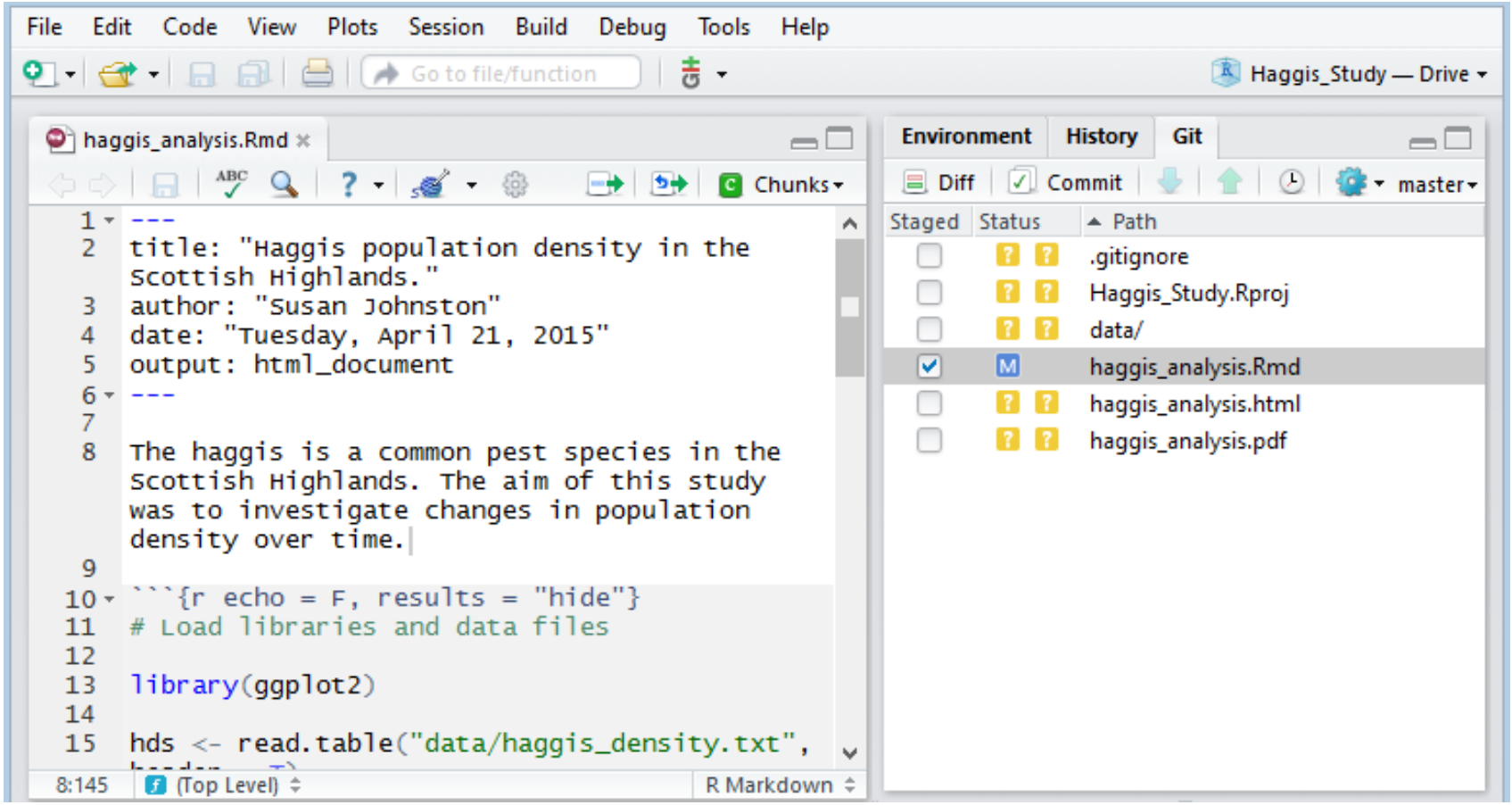
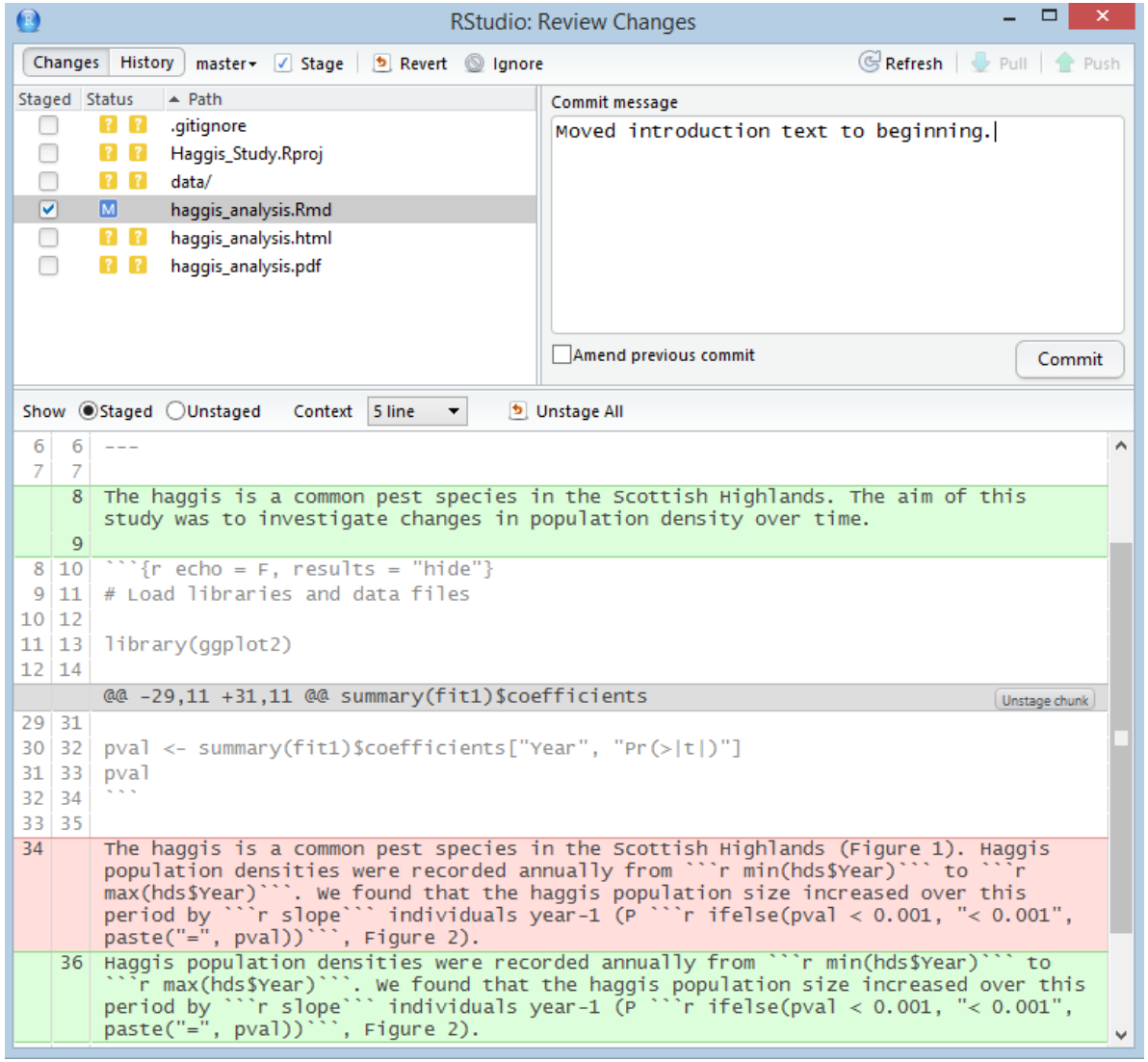


After modifying the file, repeat the process.

Version Control in R Studio



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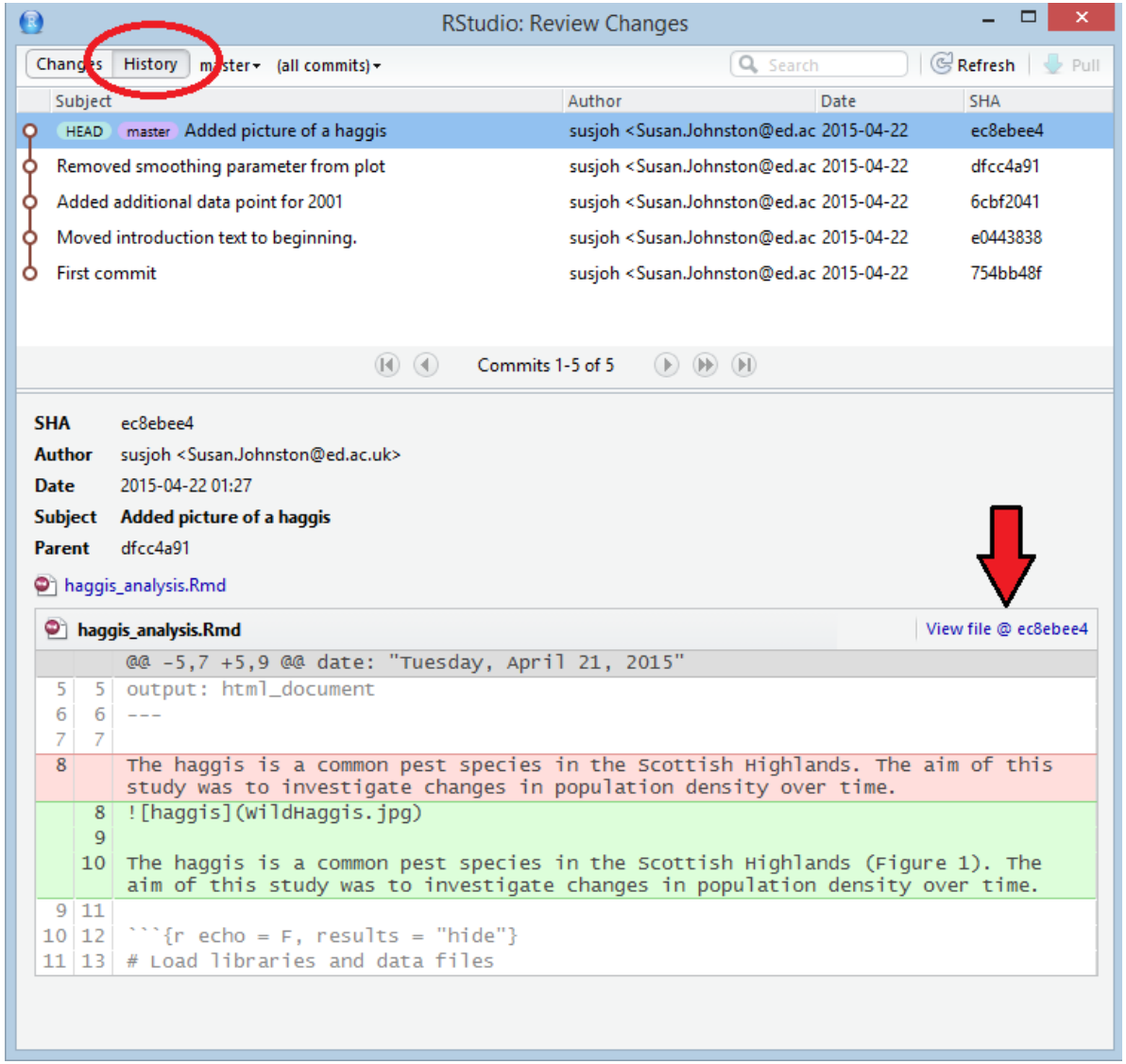
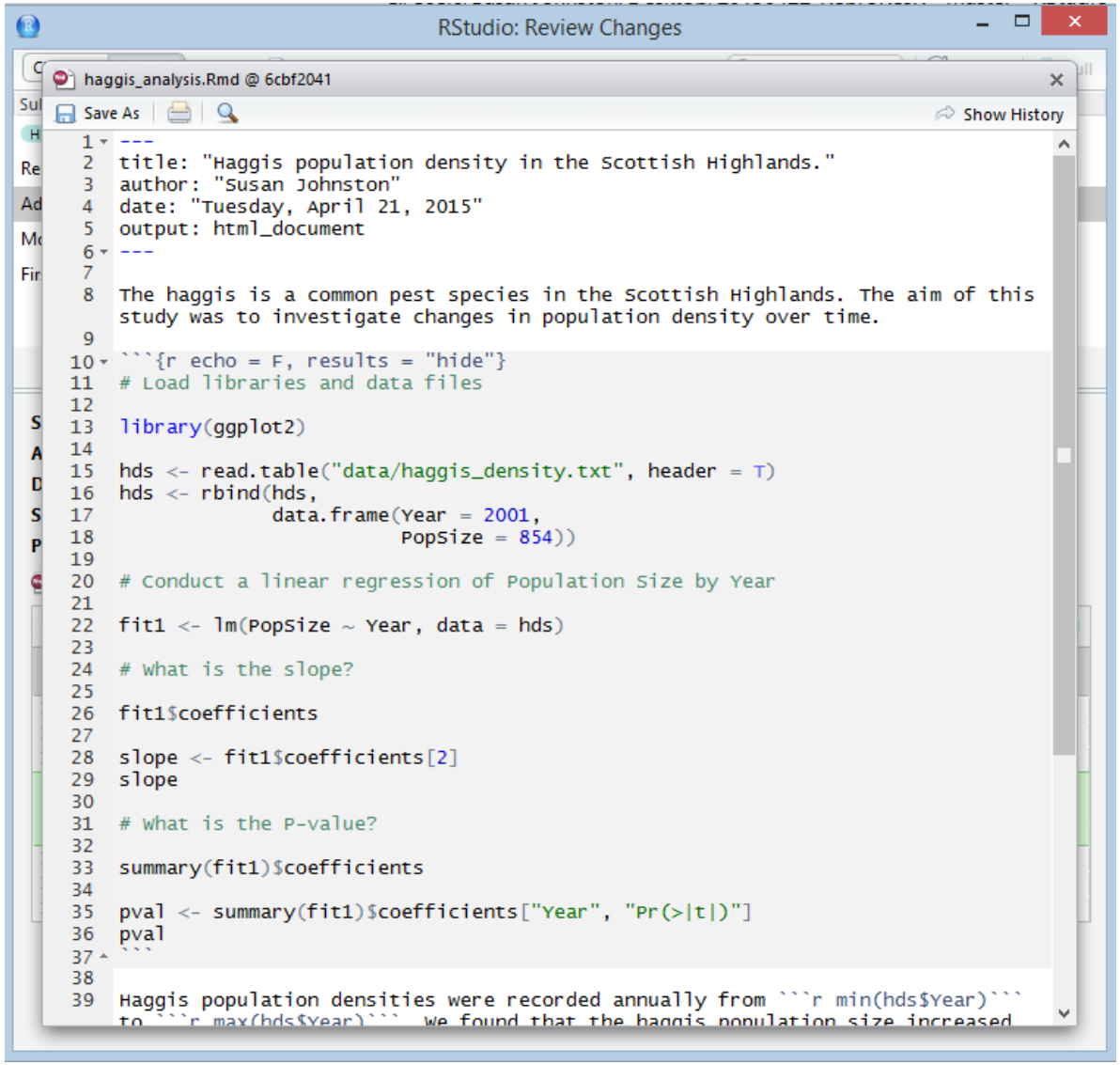


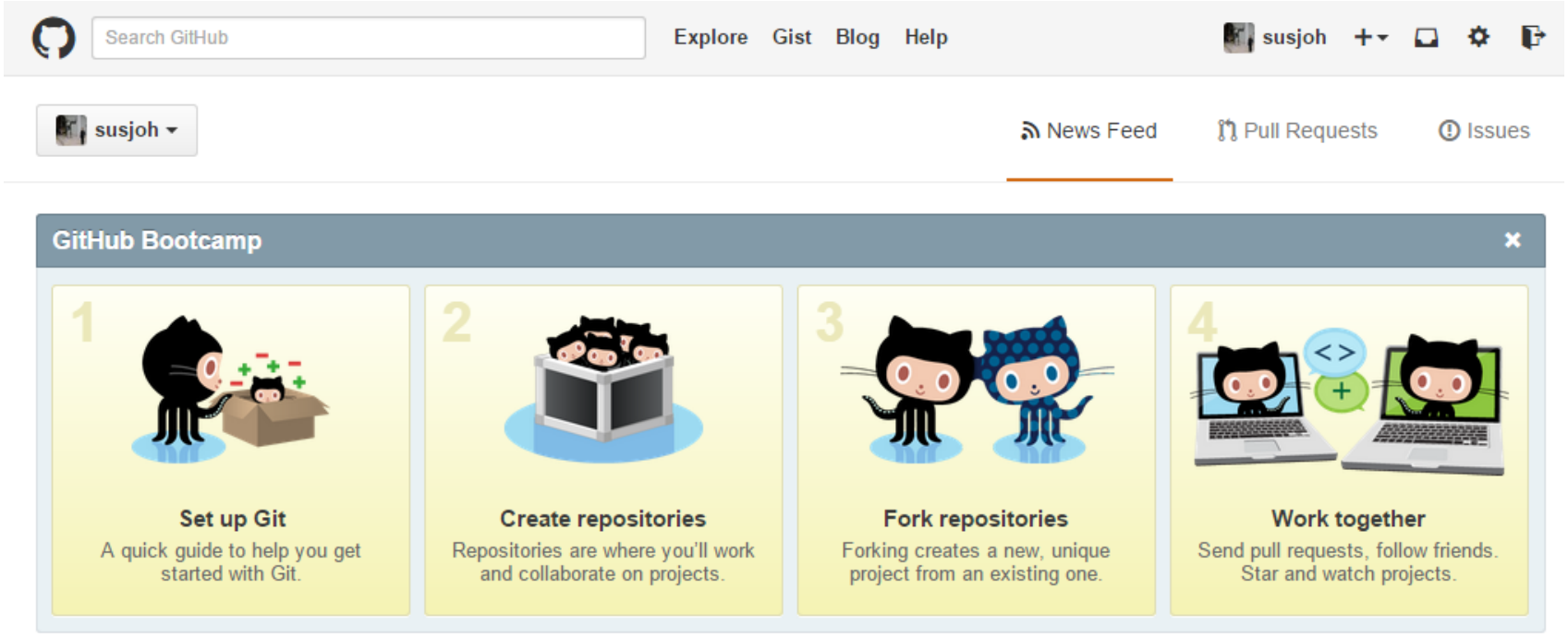
Previous versions can be viewed and restored from the History tab.

Version Control in R Studio



Previous versions can be viewed and restored from the History tab.

Advanced Steps: Github



- Forking projects
- All scripts are backed up online
- Facilitates collaboration and working on different computers

Online Resources

- RStudio: Idiot-proof guides and cheat sheets
  http://www.rstudio.com/
- Nice R Code: How-tos and advice on good coding practice
  http://nicercode.github.io/guide.html
- Ten Simple Rules for Reproducible Computational Research
  http://journals.plos.org/ploscompbiol/article?id=10.1371/journal.pcbi.1003285
- Yihui Xie's blog (knitr) http://yihui.name/en/categories/
- R Bloggers: http://www.r-bloggers.com/
- StackOverflow questions on R and knitr
  http://stackoverflow.com/questions/tagged/r+knitr