Markdown and the knitr Package in R



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Baggerly and Coombes' Replication Work A Strategy for Reproducible Research

The Markdown Language

Choosing an Output and Compiling
The Header
Publishing the HTML Output

Syntax

Bold, Italics, etc.

Sectioning

Tabbing

Equations

Lists

Tables (by hand)

Graphics (from external files)

Embedding Code

In-line Code for Display Only

In-line Code that gets Evaluated

Code Chunks

Code Chunk Options

Caching

Tables and Figures (from code)

There's a really infamous talk from 2010, called

The Importance of Reproducible Research in High-Throughput Biology: Case Studies in Forensic Bioinformatics: https://www.youtube.com/watch?v=7gYls7uYbMo

by Keith Baggerly and Kevin R. Coombes.





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Their talk illustrates what can go seriously wrong when people working with data are not transparent about how they get their results.

Baggerly and Coombes are bioinformaticians who study cancer. They attempted to replicate this study:

Genomic signatures to guide the use of chemotherapeutics

Anil Potti^{1,2}, Holly K Dressman^{1,3}, Andrea Bild^{1,3}, Richard F Riedel^{1,2}, Gina Chan⁴, Robyn Sayer⁴,
Janiel Cragun⁴, Hope Cottrill⁴, Michael J Kelley², Rebecca Petersen⁵, David Harpole⁵, Jeffrey Marks⁵,
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This was an important finding and was published in a prominent journal.

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The study's original, raw clinical data

The results published in the paper

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As a result, Baggerly and Coombes had to reproduce the results in a "forensic" way: figuring out after-the-fact what the authors must have done to get these results.

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- 2. The treatment was coded as 1 or 2, but someone along the way confused what 1 and 2 meant. So the treated patients were reported as control, and vice versa.

That means that the reported positive effect for the treatment group is actually a positive effect for the control group. In other words, the treatment harms people.

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The study continued for many months. It was only stopped when it was revealed that the principal investigator on the original study had lied on his CV about being a Rhodes Scholar.

So, what exactly went so wrong here?

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- 3. Self-interest and ego: covering up mistakes instead of risking the penalties of correcting them, thereby making the mistakes worse.
- 4. Magical thinking: because the work involves data, there's a tendency by most people to simply believe that the work is correct without digging in to it (not Baggerly and Coombes though!)

If we are going to be working with data, **how can we avoid the mistakes** that Baggerly and Coombes discovered?

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- 3. We can feed our egos in a different way: clear and professional documentation looks impressive to others.
- 4. Working with code and explaining what each part of the code does goes a long way towards dispelling the anxiety people have about data, and overcomes magical thinking.

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This afternoon we will walk through an entire research pipeline using R markdown, documenting everything we need to do to raw data to prepare it for analysis, and including the final results in the document.

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Practice on your own computer as we discuss the steps for creating a markdown document.



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Pros: Creates a beautiful, readable document by placing text, code, and the output of the code all in the same document (this is also called weaving: hence the name knitr). Able to create HTML, PDF, or Word files.

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- ► <u>Cons</u>: More syntax to learn in addition to R code. Might take a while to compile documents.

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This will call up an example page with some text and code already in it. (You will end up deleting this example text and code and writing your own.)

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- For PDF output, output: pdf_document
- ► For Word output, output: word_document

To create a table of contents that lists up to 5 levels of sectioning:

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By default the table of contents appears at the top of the document, just under the title. But, you can also use a floating and collapsable table of contents window like this:

```
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    toc: true
    toc_depth: 5
    toc_float: true
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Other options for the header are listed here:

http://rmarkdown.rstudio.com/html_document_format.html

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If you need space on the web to host this page, click on "**Publish**", then click "**RPubs**". RPubs is a free service, run by R Studio, that provides server space for your markdown documents. If you post online using RPubs, you can use a URL to share your work with your audience.

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*this will be italicized*

**this will be bold**

~~this will be struck out~~
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For block quotes, push Enter/Return TWICE then start every line of the quote with > and a space.

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Here's a profound quote:
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- > I'd rather have this bottle in front of me
- > than a frontal lobotomy

Sectioning

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If the toc: true option is specified, the section titles will appear in the **table of contents** automatically.



Tabbing

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{.tabset .tabset-fade} does the same thing, but include a nice fade-in animation when switching between tabs.

{.tabset .tabset-fade .tabset-pills} places the tabs into squares with rounded-edges.

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Some special math characters:

• capponentiation • $\sqrt{5}$ value $\sqrt{5}$ subscripts • $\sqrt{5}$ frac $\{1\}\{2\}$ $\frac{1}{2}$

A list of the code for many other math symbols is here: http://reu.dimacs.rutgers.edu/Symbols.pdf



For example, to include the quadratic formula in your document,

$$x = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

type

$$\ x = \frac{-b \pm 6^2 - 4ac}{2a}$$

(Here the \setminus pm refers to the "plus or minus" symbol)

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- - * Item 2a
 - * Item 2b

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```
* Item 1
* Item 2
```

* Item 2a

* Item 2b

To create an ordered list (numbered), type:

```
1. Item 1
```

- 2. Item 2
- 3. Item 3

a. Item 3a

b. Item 3b

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- 2. To create a sublist, you need to **tab twice**. Once won't register differently from the other items
- 3. For numbered lists, the top level must be regular (Arabic) numbers (1,2,3,...). The next levels can be lowercase letters or lowercase Roman numerals
- 4. You can change the first number to anything you want. But the following numbers will always count up by 1 from the first number, no matter what you type there

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The table will appear in a neatly formatted way when you compile.

Graphics (from external files)

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Or pull them directly off the web by entering the image's URL:

Embedding Code

Remember that the purpose of an R markdown file is to weave text, code, and the results of code together in one, readable document. There are three ways to include code in a document:

- 1. in-line for display only,
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To write in-line code, use single, forward-sloping quotes ' (on the same key as the tilde). Then if you write about the lm() function, or the ggplot2 package, it will appear in this different font and have a grey background.

If you use the single, forward-sloping quotes, the code is displayed but not run. Alternatively, if you type r prior to any code within the quotes, markdown will evaluate the code and display the output in the text.

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This feature is great for filling in details about the data into your text automatically.

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End a code chunk by typing three more forward single-quotes on a new line:

```
...
```

Code Chunks

You can type as many lines of R code as you want inside one code chunk. But, best practice is to only write a few lines at a time in one code chunk.

The reason is that you are trying to bring a reader along and explain your code. It's easier to explain a few lines at a time.

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Take a moment to try out some code chunks in your markdown document.

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Other options are listed here: https://yihui.name/knitr/options/



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You can set other global options here if you want them applied to all code chunks. Just write knitr::opts_chunk\$set(option) in this chunk.

Caching

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To cache the output of a code chunk, use the option cache=TRUE.

This option saves A LOT OF TIME when using commands that take a while to run, such as loading a big dataset or running a complicated model. But don't use this option for every chunk, as it can cause problems with the keeping results accurate as code changes.

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For example:

```
```{r plot, fig.width=6, fig.height=8}
ggplot(mtcars, aes(x=wgt, y=mpg)) + geom_point()
```
```