Reproducible research and `R` authoring with markdown and `knitr`

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Contents

1 Introduction

Objectives

- Understand the concept of dynamic documents are reproducible research
- Learn `R` markdown basics
- Produce a simple vignette

This content is adapted from the RStudio `R` Markdown - Dynamic Documents of R, Markdown basics and R code chunks tutorials.

This session introduces tools to author documents that include dynamically generated analysis results (tables, figures, ...) produced with `R`. Bringing data, results and their interpretation together in a single, coherent document is invaluable to keep track of long and complex analyses, assure reproducibility of the pipeline and the final report (any updates at the data or analysis level are propagated at the report level) and to comprehensively communicate these results to collaborators. A popular solution for this is *literate programming*, a technique and set of tools that permit to

1. Write text and code within a single document. Here we will use the simple *markdown* syntax and include `R` code chunks; such documents are denoted *R markdown* documents and have the `Rmd` extension. More on this in the next section.
2. Extract and execute the code: this is called *tangling*.
3. Replace the code chunks with their output into the original document: this is called *weaving*.
4. Render the document into a final, easily read format such as pdf or html.

Steps 2 to 4 are can be executed individually or automated into a single command such as `knitr::knit2html` (i.e. function `knit2html` from the package `knitr`) or `rmarkdown::render`, or using the RStudio editor.

Other types of document and frameworks that combine a programming and authoring languages are Sweave files (with Rnw extension, that combine LaTeX and R), Jupyter/IPython for python, R and other languages, orgmode ...

2 R Markdown

R Markdown is an authoring format that enables easy creation of dynamic documents, presentations, and reports from R. It combines the core syntax of markdown (an easy-to-write plain text format) with embedded R code chunks. R Markdown documents are fully *reproducible* (they can be automatically regenerated whenever underlying R code or data changes).

This document describes R Markdown v2 based on knitr and pandoc, the workhorse that converts markdown to html and many other formats. We will focus the generation of reports such this document in html and pdf, although other formats and type of documents are available.

Note that PDF output requires a full installation of TeX and that pandoc is a third party application that needs to be installed outside of R unless you use RStudio, which bundles all necessary R packages and pandoc.

> **Tip**
>
> We would also like to warn against using MS Word as output document, as this breaks the support for reproducibility. The final, compiled document should be used for rendering only (which is implicit for html of pdf files); editing should be performed on the original documents, i.e the Rmd file.

2.1 Installation

You can install the the required package from CRAN as follows:

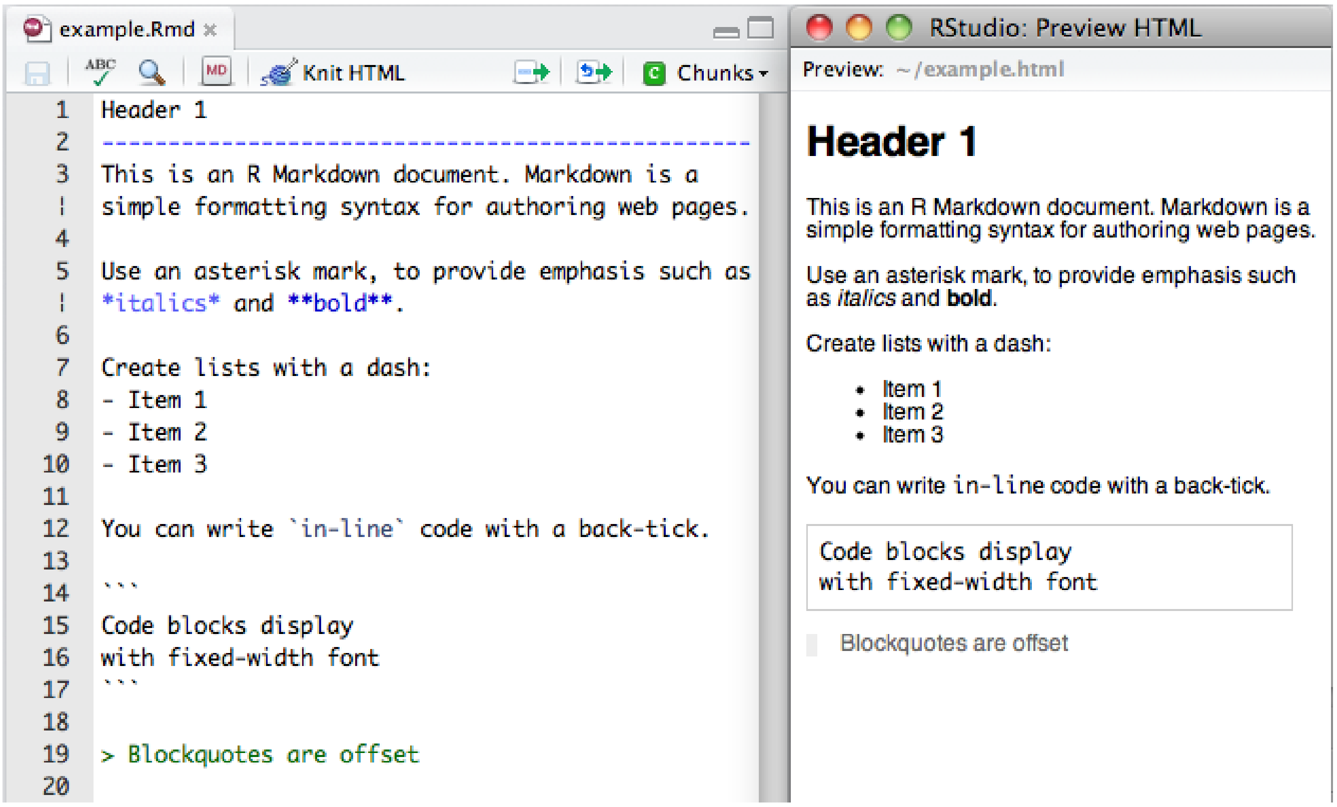
```
install.packages("knitr")
install.packages("rmarkdown")
```

These packages are pre-installed with RStudio.

2.2 Markdown basics

The figure below, taken from the RStudio markdown (v2) tutorial illustrates basic markdown syntax and its output using RStudio.

- Section headers can be defined using ====== or ----- (level 1 and 2 respectively) or one or multiple # (for level 1, 2, ... respectively).
- Italic and bold fonts are defined using one to two * around the text.
- Bullet lists items start with a -.
- In-line code and verbatim expression are surrounded by back ticks ‘.
- Code blocks start and end with three back ticks.
- Starting a line with > offsets the text.



```
Header 1
--------------------------------------------------
This is an R Markdown document. Markdown is a
simple formatting syntax for authoring web pages.

Use an asterisk mark, to provide emphasis such as
*italics* and **bold**.

Create lists with a dash:
- Item 1
- Item 2
- Item 3

You can write `in-line` code with a back-tick.

```
Code blocks display
with fixed-width font
```


> Blockquotes are offset

```

**Header 1**

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2.3 File header

R Markdown version 2 uses an *optional* header to define, among other things, the title, author and output formats of the R Markdown document. Below, we want to use `html` as final format; replace with `pdf_document` to produce a pdf report.

```
---
title: "Title comes here"
author: "Your name"
date: "12 June 2015"
output: html_document
---
```

2.4 From `Rmd` to `html` (or `pdf`)

If you are using RStudio, the simplest way to generate your final output is to open your `Rmd` file and click the `Knit HTML` (or `Knit PDF`, ...) button.

From R, you can use the `knitr::knit2html` or `rmarkdown::render` functions and give the `Rmd` source file as input.

1. Both options will first use the `knitr::knit` function to *weave* the document and generate the markdown `md` file that includes the code outputs.
2. The rendering of the final output document will be done using `markdown::markdownToHTML` (in case of `knitr::knit2html`), or the more recent `rmarkdown::render`.

```
library("knitr")
knit2html("my_rr_document.Rmd")
```

```r
library("rmarkdown")
render("my_rr_document.Rmd") ## default output is html
render("my_rr_document.Rmd", output_format = "html_document")
```

For pdf outputs using knitr

```r
knit2pdf("my_rr_document.Rmd")
```

or rmakdown

```r
library("rmarkdown")
render("my_rr_document.Rmd", output_format = "pdf_document")
```

And, to render all output formats defined in the header

```r
render("my_rr_document.Rmd", output_format = "all")
```

Exercise: Experiment with R markdown and the features described so far. To create your starting document, create a new R Markdown file using the RStudio menu or copy/paste the template below.

```
---
title: "Title comes here"
author: "Your name"
date: "12 June 2015"
output: html_document
---

This is an `R` Markdown document. Markdown is a simple formatting syntax
for authoring HTML, PDF, and MS Word documents. For more details on
using `R` Markdown see <http://rmarkdown.rstudio.com>.

When you click the **Knit** button a document will be generated that
includes both content as well as the output of any embedded `R` code
chunks within the document. You can embed an `R` code chunk like this:
```

2.5 More markdown syntax

2.5.1 Emphasis

You can use * or _ to format *italic* and **bold** text.

```
*italic*   **bold**

_italic_   __bold__
```

2.5.2 Headers

```
## Header 2

### Header 3
```

2.5.3 Lists

Unordered List:

```
* Item 1
* Item 2
    + Item 2a
    + Item 2b
```

Ordered List:

```
1. Item 1
2. Item 2
3. Item 3
    + Item 3a
    + Item 3b
```

2.5.4 Links

To use links, enclose the link text in `[]` and the the actual link in `()`: `[my link](http://linkurl.com)` or use a plain http address:

http://example.com

```
[linked phrase](http://example.com)
```

2.5.5 Images

To add a static figure to the document, use the link syntax and precede it by `!`: `![image text](./fig/myfig.png)`.

Image source can be on-line or local files.

```
![alt text](http://example.com/logo.png)


![alt text](figures/img.png)
```

2.5.6 Block quotes

A friend once said:

> It's always better to give than to receive.

```
A friend once said:

> It's always better to give than to receive.
```

2.5.7 Plain code

Plain code blocks are displayed in a fixed-width font but not evaluated (see below for evaluation of code blocks), use 3 back ticks (see figure above)

```
This text is displayed verbatim / preformatted
```

We can also define `in-line` code using single back ticks.

```
We can also define `in-line` code using single back ticks.
```

2.5.8 Horizontal Rule / Page Break

Three or more asterisks or dashes:

```
******

------
```

2.5.9 Tables

There is a simple markdown syntax to produce adequately formatted tables:

First Header	Second Header
Content Cell	Content Cell
Content Cell	Content Cell
Content Cell	Content Cell

which is produced with

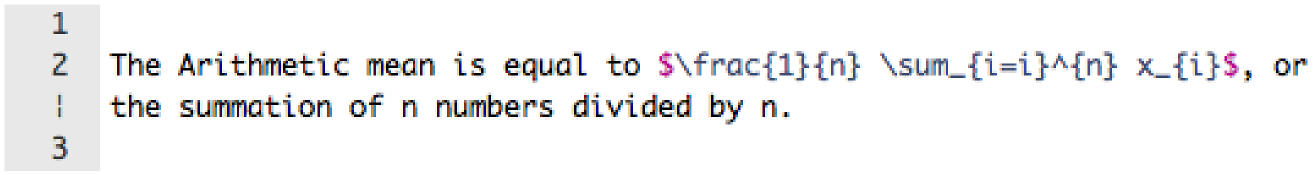
```
First Header  | Second Header
------------- | -------------
Content Cell  | Content Cell
Content Cell  | Content Cell
Content Cell  | Content Cell
```

2.5.10 Embedding Equations

You can embed LaTeX or MathML equations in R Markdown files using the following syntax:

- `$equation$` for inline equations (note there must not be white space adjacent to the $ delimiters)
- `$$ equation $$` for display equations
- `<math>...</math>` for MathML equations.

For example:



```

The Arithmetic mean is equal to $\frac{1}{n} \sum_{i=i}^{n} x_{i}$, or the summation of n numbers divided by n.

```

2.5.11 Super- and subscripts

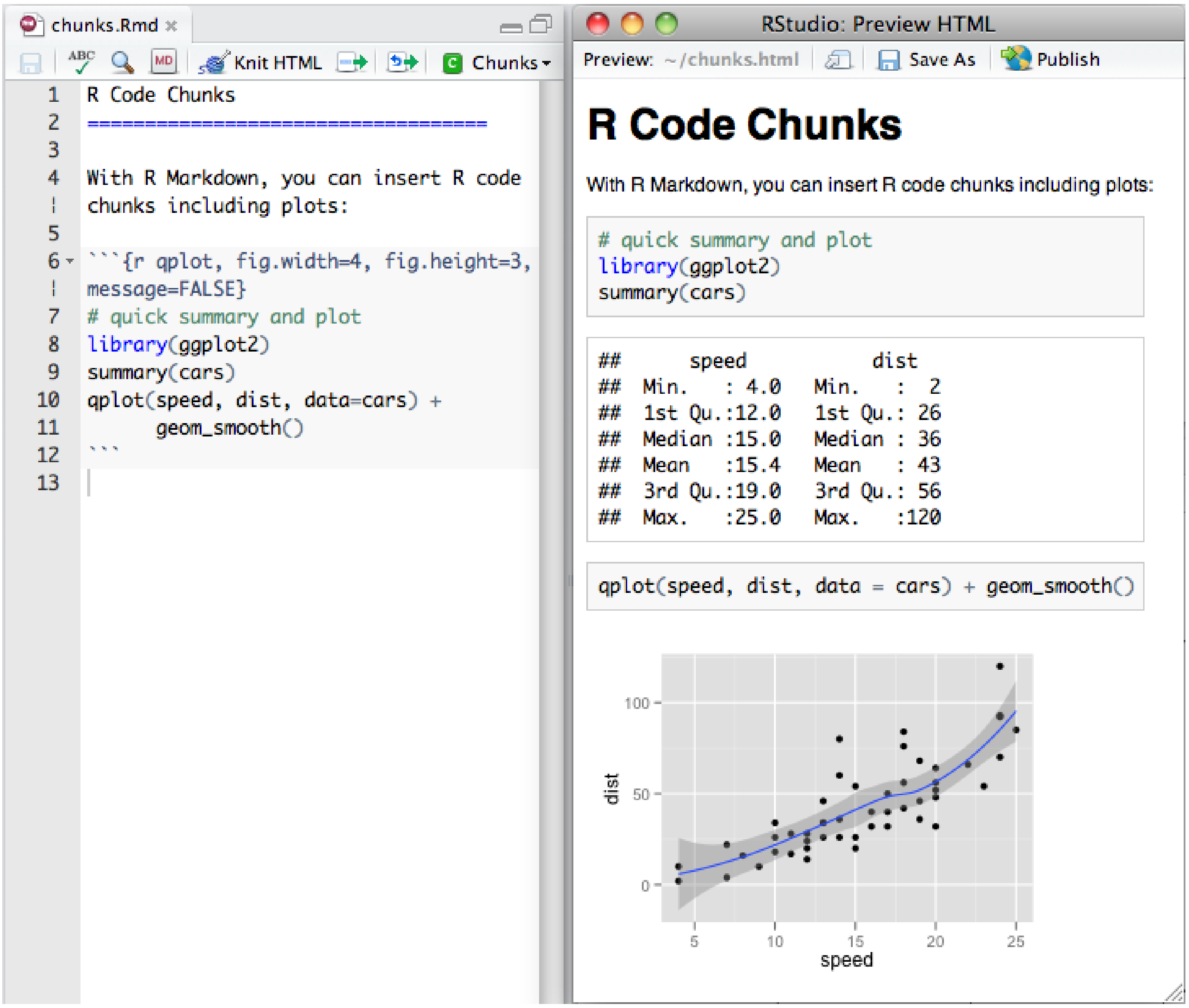
H_2O is a liquid. 2^{10} is 1024.

```
H~2~O is a liquid.  2^10^ is 1024.
```

Exercise: Complement you Rmd file with some new syntax elements.

2.6 R code chunks

To include R code in the R markdown file, the native code chunk syntax is augmented with code chunk tags inside `{r, ...}`, as illustrated below:



~~~
R Code Chunks
=====================================

With R Markdown, you can insert R code
chunks including plots:

```{r qplot, fig.width=4, fig.height=3,
message=FALSE}
# quick summary and plot
library(ggplot2)
summary(cars)
qplot(speed, dist, data=cars) +
      geom_smooth()
```
~~~

R Code Chunks

With R Markdown, you can insert R code chunks including plots:

```
# quick summary and plot
library(ggplot2)
summary(cars)
```

```
##      speed           dist    
##  Min.   : 4.0   Min.   :  2  
##  1st Qu.:12.0   1st Qu.: 26  
##  Median :15.0   Median : 36  
##  Mean   :15.4   Mean   : 43  
##  3rd Qu.:19.0   3rd Qu.: 56  
##  Max.   :25.0   Max.   :120  
```

```
qplot(speed, dist, data = cars) + geom_smooth()
```

The following code chunk options are available:

- `{r chunkname}` the first unnamed string is used to name the code chunk; useful for following the code execution and debugging.
- `{r, eval=TRUE}` by default the code in the chunk is executed. Alternatively, set `eval=FALSE`.
- `{r, echo=TRUE}` by default, the code is displayed before the output. Use `echo=FALSE` to hide the code chunk content.
- Control if messages, warnings or errors are to be displayed with `{r, message=TRUE, warning=TRUE, error=TRUE}` or `FALSE`.
- Figure dimensions can be controlled with `fig.height` and `fig.width`.
- To avoid wasting time in repeating long calculations over and over again, it is possible to cache specific code chunks specifying `cache=TRUE` in the chunk header.
- To execute in-line code, use `‘ r 1+1‘` (no space in front of the `r`, though).

Tables can easily be printed inside an code chunk. Below, we explicitly create and use a `data.frame`.

```
dfr <- data.frame(name = c("John", "David", "Caroline", "Igor"),
                  id = c(123, 234, 321, 231),
                  gender = c("M", "M", "F", "M"))
dfr
```

```
##       name  id gender
## 1     John 123      M
## 2    David 234      M
## 3 Caroline 321      F
## 4     Igor 231      M
```

Tables produced in R as data frames or matrices can be rendered with the helper function `knitr::kable` and are then displayed accordingly.

```
library("knitr")
kable(dfr)
```

name	id	gender
John	123	M
David	234	M
Caroline	321	F
Igor	231	M

Exercise: Using the `iris` data set, create a reproducible report that documents the data (dimensions, summary statistics, ...) and provides a set of visualisations (a PCA plot, `pairs`, ...). To conclude your report, add a *Session information* section with the output of `sessionInfo()`.

3 Next steps

- Publishing your R markdown documents on the web with RPubs.
- Using R markdown to create package vignettes.
- Source code and R markdown documents versioning using, for example, `git` and GitHub.
- Producing dynamic documents with `shiny` (there will be a dedicated lab on `shiny`).

4 References

- The `knitr` package, including excellent documentation.
- `markdown` and `rmarkdown` packages
- R markdown documentation
- R markdown video

5 Session information

```
## R version 3.2.0 Patched (2015-04-22 r68234)
## Platform: x86_64-unknown-linux-gnu (64-bit)
## Running under: Ubuntu 14.04.2 LTS
##
## locale:
##  [1] LC_CTYPE=en_GB.UTF-8       LC_NUMERIC=C
##  [3] LC_TIME=en_GB.UTF-8        LC_COLLATE=en_GB.UTF-8
##  [5] LC_MONETARY=en_GB.UTF-8    LC_MESSAGES=en_GB.UTF-8
##  [7] LC_PAPER=en_GB.UTF-8       LC_NAME=C
##  [9] LC_ADDRESS=C               LC_TELEPHONE=C
## [11] LC_MEASUREMENT=en_GB.UTF-8 LC_IDENTIFICATION=C
##
## attached base packages:
## [1] stats     graphics  grDevices utils     datasets  base
##
## other attached packages:
## [1] knitr_1.10.5    BiocStyle_1.7.3
##
## loaded via a namespace (and not attached):
##  [1] magrittr_1.5    formatR_1.2     tools_3.2.0     htmltools_0.2.6
##  [5] yaml_2.1.13     stringi_0.4-1   rmarkdown_0.6.1 highr_0.5
##  [9] stringr_1.0.0   digest_0.6.8    evaluate_0.7
```