Scientific Programming with R

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Literate Programming

From the web page describing his book /Literate Programming/, Donald E Knuth writes:
"Literate programming is a methodology that combines a programming language with a documentation language, thereby making programs more robust, more portable, more easily maintained, and arguably more fun to write than programs that are written only in a high-level language. The main idea is to treat a program as a piece of literature, addressed to human beings rather than to a computer. The program is also viewed as a hypertext document, rather like the World Wide Web. (Indeed, I used the word WEB for this purpose long before CERN grabbed it!) ..."

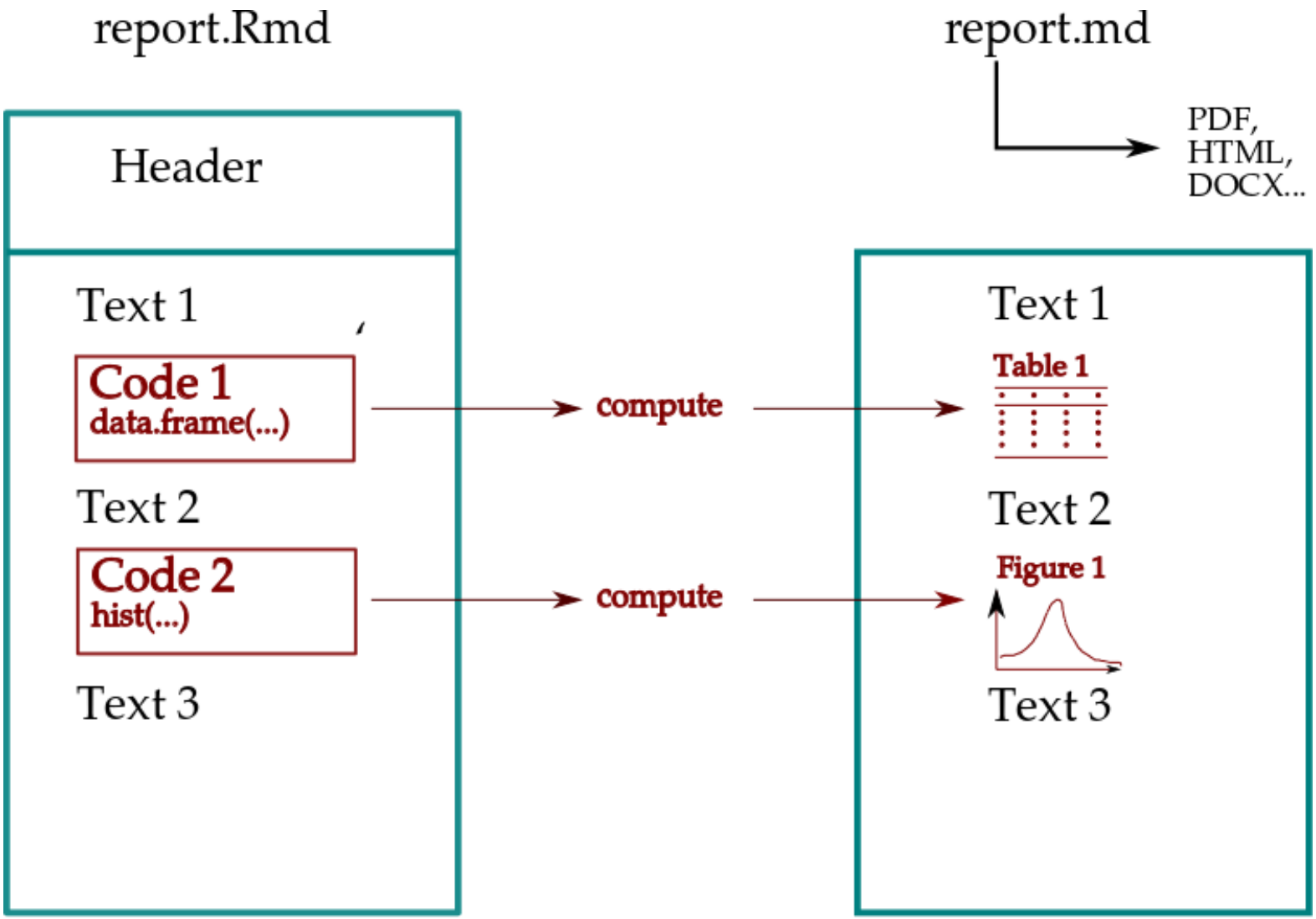
http://www-cs-faculty.stanford.edu/~uno/lp.html

Tangling and Weaving

CWEB: system for documenting C, C++, Java:

```
CTANGLE
      converts a source file foo.w to a
      compilable program file foo.c;
CWEAVE
      converts a source file foo.w to a
      prettily-printable and
      cross-indexed document file foo.tex.
```

Tangling and weaving



What is reproducible research (RR)?

- Gentleman et al (2004) advocate RR:
  Buckheit and Donoho (35), referring to the work and philosophy of Claerbout, state the following principle: "An article about computational science in a scientific publication is not the scholarship itself, it is merely advertising of the scholarship. The actual scholarship is the complete software development environment and that complete set of instructions that generated the figures."

  `http://genomebiology.com/2004/5/10/R80`
- Bioconductor packages are good examples of reproducible research.
- This article is also good background reader for open software development.
- Bioconductor has had a positive impact on genomic data analysis.

The case of the Duke cancer trials

- Technical details (37 mins, Cambridge 2010) http://videolectures.net/cancerbioinformatics2010_baggerly_irrh/
- Wide audience, but rather narrow-sighted: 13-minute video from 60 minutes: https://www.youtube.com/watch?v=W5sZTNPMQRM

Aproaches to reproducible research

1. Makefiles
2. Sweave / knitr
3. Build a package

1. Make and Makefiles

- Make is an automated build system, designed to avoid costly recomputation.
- make examines a Makefile, which contains a set of rules describing dependencies among files.
- A rule is run (i.e the recipes are executed) if the *target* is older than any of its *dependencies* (*prerequisites*).

```
target: prerequisites ...
        recipe
        ...
```

- make works backwards from the target to the prerequisites and compares creation time of files (timestamp).

Example rule

```
res.txt: param1.dat param2.dat
        simulation param1.dat param2.dat > res1.dat
        post-process res1.dat > res.txt
```

We can define the (a) target, (b) dependencies (c) commands to run.

A complete example

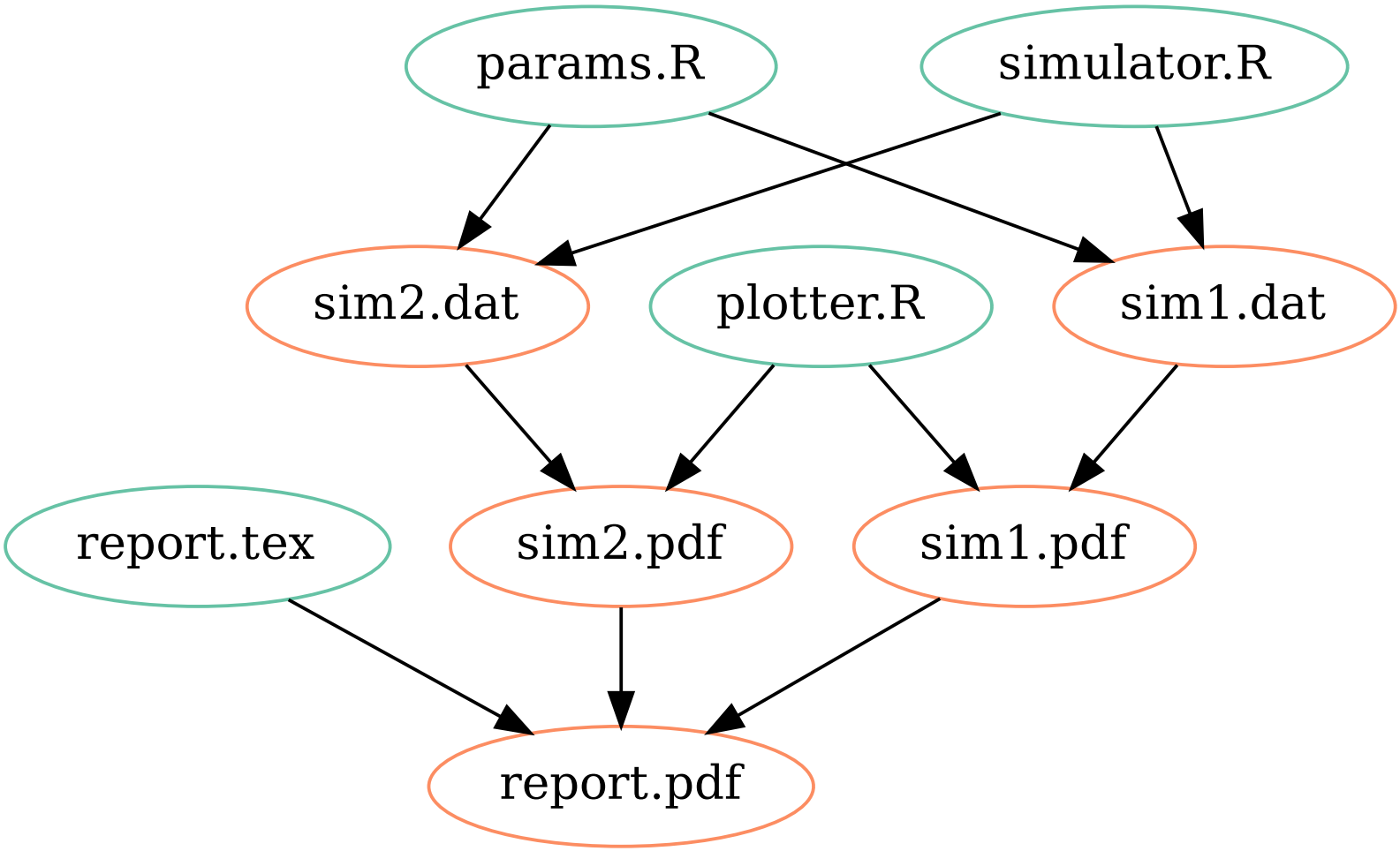
See `rr_make/Makefile`.

```
report.pdf: report.tex sim1.pdf sim2.pdf
	texi2pdf report.tex

sim1.dat: params.R simulator.R
	Rscript simulator.R rnorm > sim1.dat

sim2.dat: params.R simulator.R
	Rscript simulator.R runif > sim2.dat

sim1.pdf: sim1.dat plotter.R
	Rscript plotter.R sim1.dat

sim2.pdf: sim2.dat plotter.R
	Rscript plotter.R sim2.dat


.PHONY: all clean

all: report.pdf

clean:
	rm -f report.pdf report.log report.aux
	rm -f sim1.* sim2*
```

A complete example

See `rr_make/Makefile`.

Graphical representation



Makefile conventions

- PHONY targets: denote actions; ignore filenames with same name. PHONY targets are always run.

```
.PHONY: all clean
all: report.pdf

clean:
        rm -f report.pdf report.log report.aux
        rm -f sim1.* sim2*
```

command	action
make	check first rule
make all	rebuild everything
make clean	remove files that can be rebuilt
touch file	update timestamp, preserving contents

Makefile: next steps

- variables
- implicit rules
- saving space:

```
sim2.dat: params.R simulator.R
        Rscript simulator.R runif > sim2.dat

sim2.dat: simulator.R params.R
        Rscript $< runif > $@
```

- parallel processing `make -j8 jobs`

Further reading

- Managing Projects with GNU Make
  http://oreilly.com/catalog/make3/book/index.csp
- The GNU make manual
  http://www.gnu.org/software/make/manual/make.html
- Tutorial (work in progress) https://github.com/sje30/make-tutorial/blob/master/make-tut.pdf

2. Sweave: literate programming for R

1. Sweave is the system for mixing LaTeX and R code in the same document.
2. Used within R often to create "vignettes" which can be dynamically run.
3. Allows you to write reports where results (tables, graphs) are automatically generated by your R code.

Code chunks

By default we are in 'LaTeX mode', and we switch to code mode by using a code chunk.

```
We can then test the procedure a few
times, using the default number
of darts, 1000:

<<>>=
replicate(9, estimate.pi())
@

... back to latex here.
```

What is markdown?

What is markdown? A light-weight markup language for generating HTML.

```
### Example

Here is some *markup text* with **bold** and a
[link](http://www.rstudio.org).
Maths can be included $x^2 + y^2 = z^2$.
```

Useful also e.g. on github.

A full example

Estimate the value of π using the dartboard method.
https://github.com/lgatto/spr/blob/master/estimate/estimatek.Rnw
shows how to include figures, tables, and caching feature.

What next?

Bookdown.org, vignettes, packages (https://devtools.r-lib.org/).