Making research reproducible using literate programming
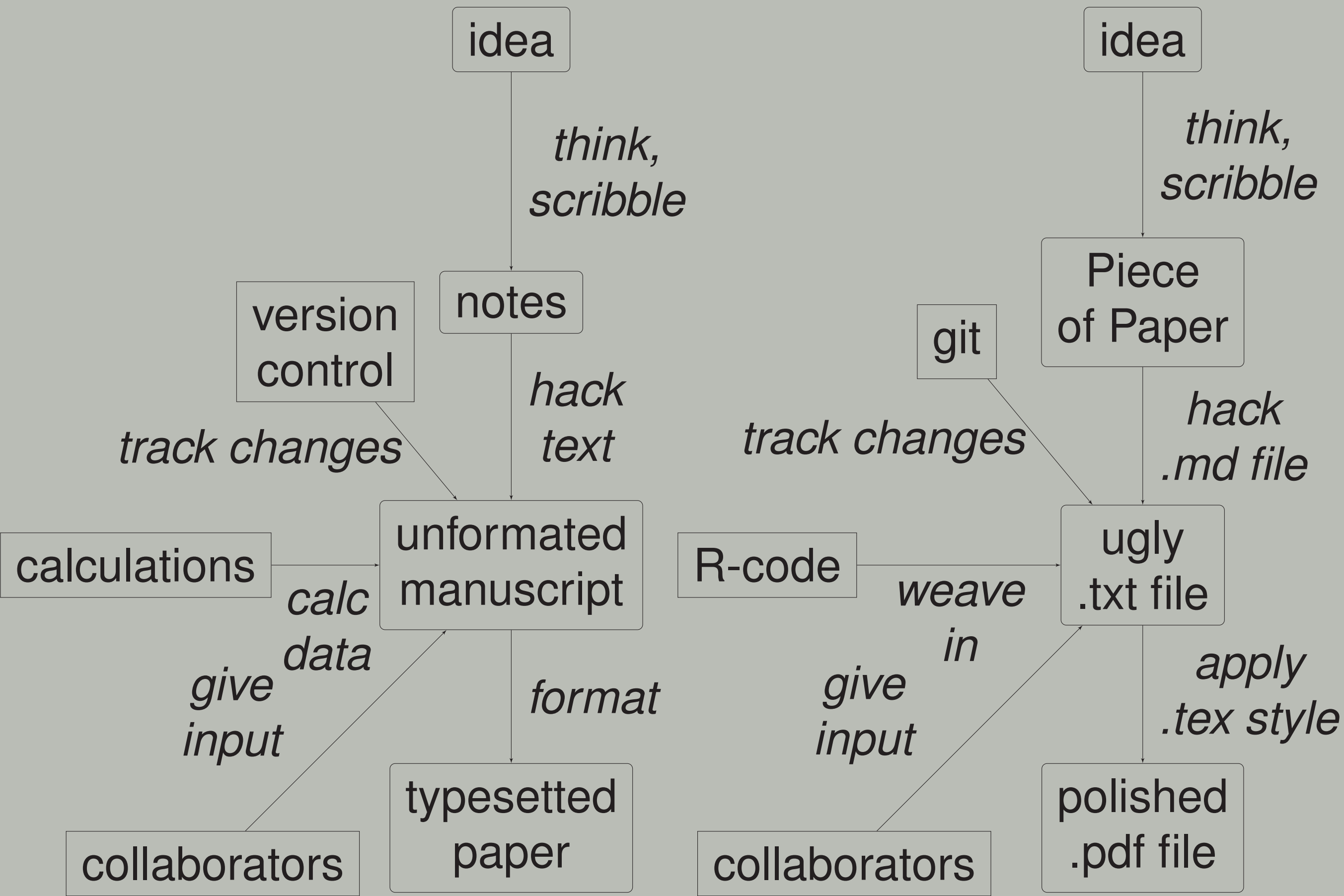
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Reproducibility: What and why?

There is an increasing concern about the reliability of research results [3]. ~~Precisely,~~ it has been found that many published results cannot be replicated [2]. In parts, this can be due to the fact that it is often hardly possible for independent researchers to confirm the results of a research paper. Thus, making research more reproducible seems a pressing need [3]. Here, we present some "recipe" for making (your) research paper more reproducible using literate programming. Literate programming refers to weaving programming code (ie., statistical calculations) with the paper text, ie., the normal text of a paper.

Workflow for reproducible paper writing

idea — think, scribble — notes

version control — track changes — unformated manuscript

calculations — calc data — give input — collaborators

format — typesetted paper

idea — think, scribble — Piece of Paper

git — track changes — hack .md file

R-code — weave in — ugly .txt file

give input — collaborators

apply .tex style — polished .pdf file

The *diagram* shows the workflow *in theory*. The *right* diagram exemplifies useful tools for each step.

Requirements to reproducible paper writing

Some (subjective) criteria ~~to tools helping~~ *to help with* writing scientific papers reproducibly.

▶ **simple:** The tool should be easy to learn and use (flat learning curve). Life is short.
▶ **beautiful:** The tool should set the text in an eye pleasing way, eg., no holes in block aligned text.
▶ **plain:** The tool should work with plain text files, ~~as they will probably readable in (distant) future~~ *so that they can be readable in the future*. In addition, text file are more compatible with other tools, such as version control.
▶ **versionized:** The tool should ~~should~~ support versionizing (tracking changes), including changes from some more or less helpful collaborators.
▶ **citable:** The tool should be able to manage (scholarly) citations.
▶ **flexible:** The tool should allow for flexible layout, ie., many possibilities for rendering the final, formatted output. This is often in outright contradiction to ~~easyness.~~ *easiness*

Which tools make the researcher happy?

	Word	Latex	Markdown	WebApps
simple	●●●	●	●●	●●
beautiful	●	●●●●	●●●●	●●
plain	●	●●	●●●●	●
versionized	●	●●●	●●●●	●●●
citable	●●●●	●●●	●●●	●●●
flexible	●●●	●●	●	●●
Σ	13	17	18	16

This table compares some (subjective) criteria of what a researcher needs for writing a paper in a reproducible and efficient way. Note: *Word* refers not only to MS Word, but to similar WYSIWYG text processors as well. *WebApps* refer to scholarly writing tools such as *Authorea*. *Markdown* refers to the *Pandoc* dialect (and extensions) of Markdown.
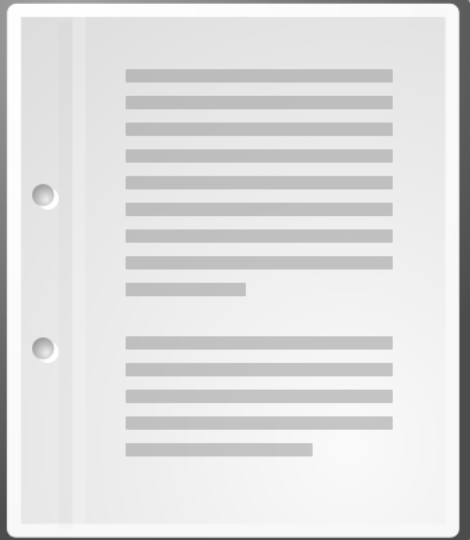
Stating the problem

Figure: 1000 lines of code in your paper

Figure: 20 numbers as results of computations somewhere in your paper

Assume there is ~~not~~ *not a* direct link of your (statistical) computations to the respective number in the text. It will be hard to understand for someone unfamiliar with your work which calculations have yielded some figure in your paper. So confirming that the calculations are valid will be hard.

Software tools for reproducible writing

Logo	Name	Description
	R	Environment for statistical calculations and programming [4]
	R-Studio	IDE for R including features for version control (eg git), and literal programming (Knitr, Pandoc, Markdown)
	Knitr	R-package to "knit" (or "weave") R-code into plain text as a way of functional programming [5]
	Git	version control tool, handles multiples collaborators, tracks changes in text files
PANDOC	**Pandoc**	"swiss army knife" for converting markup text, eg. Markdown → PDF
M↓	**Markdown**	Similar aims as Latex, but you learn it in 5 minutes.

Main commands to turn R+Markup-Text into polished PDF-paper

▶ Weave code in text using **knitr**, giving a R-Markdown (.rmd) (or R-Latex, .rnw) file: "Mean reaction time was `round(mean(rt), 2)` ms". → "Mean reaction time was 433.30 ms".
▶ Knit R-Text-Mixup to pure text plus markup using R-package **knitr**: `knitr(source.rmd)`
▶ Convert Markdown to Latex-PDF with **Pandoc**: `pandoc source.md --output paper.pdf ...`

Conclusion

▶ Note that complex cognitive steps such as creative thinking, drafting a paper outline, writing an argument, debugging code etc. are best dealt with sequentially. Our brain is not so fit for multitasking [1].
▶ A somewhat ideal combinations of tools for efficiently and reproducibly writing papers is: R+RStudio+knitr+markdown+pandoc+git.
▶ Writing in `Markdown` is nice, because little markup clutters the view. Pandoc them compiles the markdown to latex, applying some tex-template of your flavor.
▶ However, `Pandoc` currently does not provide (easily) ~~provides~~ the flexibility to adjust every detail one may think of, in addition changing the default templates is not yet stable ~~(enough for me).~~ *enough (for me).*
▶ Looking forward to the time ~~where~~ *when* you can write in R-Markdown and compile it to Tex easily with all kinds of style-templates.

References

[1] Wesley C Clapp, Michael T Rubens, Jasdeep Sabharwal, and Adam Gazzaley. Deficit in switching between functional brain networks underlies the impact of multitasking on working memory in older adults. *Proceedings of the National Academy of Sciences*, 108(17):7212–7217, apr 2011.
[2] Open Science Collaboration. Estimating the reproducibility of psychological science. *Science*, 349(6251), aug 2015.
[3] Roger Peng. The reproducibility crisis in science: A statistical counterattack. *Significance*, 12(3):30–32, jun 2015.
[4] R Core Team. *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2015.
[5] Yihui Xie. *knitr: A General-Purpose Package for Dynamic Report Generation in R*, 2016.

keine Ahnung, aber muss Aug usw. nicht mit einem Großbuchstaben anfangen?