

Notes

packrat

Reproducible package management for R. Makes your R projects reproducible by making them

- **isolated**: installing other packages won't break your project
- **portable**: easy to share, even cross platform
- **reproducible**: because it records the exact versions of the packages your project depends on

Each project has its own package library.

Funny story: so I've known about packrat for a few years now. I've known what it does, and it made all the sense in the world. And yet I didn't use it. God knows what my problem is, but it was only last month, when I bought a new laptop, installed a new and different OS than my previous one and wanted to start working on a project I was working on in the spring, when it suddenly didn't work anymore. It was a big project with dozens of interconnected files and several dozen packages, and it was now broken. Now, I had already returned my old laptop to my employer so I had no way of recreating the package environment that I had there. And no easy way of figuring out which of the packages was the offending package that had been updated in the meantime.

And it made me realise how incredibly lucky I had been that the client—this was a consulting gig—the client was able to run the code on their systems without any problems, presumably because they had the same outdated libraries installed as I had had on my old laptop. I was terribly lucky, but I learned my lesson anyway. So from then on I use packrat, actually preparing this talk was the first time I used it on a new project.

But I wanted to bring up this story also to demonstrate that it is often a slog, this reproducibility stuff. It's upfront work, and it's easy to put it off. Although in the end it turned out that packrat is ridiculously easy to setup, it is literally just one line of code, and if you're initializing it on an existing large project you'll have time to make yourself a quick cup of tea while it creates the snapshot of the working library environment, but I was quite embarrassed once I realised I could have been doing this for years.. Instead I had to first have it go wrong and have the code break, before I came to my senses and started using this tool. It's normal, it's human. But it's also stupid. So don't be stupid like I was, it's a lot less painful to get on the reproducibility bandwagon of your own accord than learning the hard way.

how to cite software

(Jackson 2012)

- Which software should be cited?
 - Critical and/or novel contribution.
 - sometimes the licence requires you cite it
- How should it be cited?
 - find your citation style's examples
 - do not use cite associated papers instead!
 - if there is a DOI, use it!
- Where should you cite it?
 - if cannot cite in references then footnotes are second best option
 - or methods section or appendix or supplementary materials, as long as it is there!

One way or another it is highly likely that software played an important role in you producing your research. This contribution should be acknowledged. Now this doesn't mean you have to make sure everyone knows you used Microsoft Word to write your paper, a good rule of thumb is to ask yourself if the software contributed critically to your research and/or if it provided something novel. This is the recommendation of the British

Software sustainability insititute. If this feels a bit ambiguous, I would suggest you err on the side of citing rather than not.

For example you might think it silly to acknowledge that you used Microsoft Excel to do your analysis, but that is only if you thing it the software is faultless and your analysis would have produced the exact same results in any spreadhseet programme. But that may not be true. Excel—not to pick on any specific programme—but it has a bunch of quirks that are specific to it, you might even call them bugs. And they could very well affect your analysis, which counts as having a critical contribtution.

For example Excel treats 1900 as a leap year. This is due to some historical reasons, to make it compatible with IBM's Lotus-1-2-3 if you're old enough to remember it. Anyway, Microsoft aknowledges that this means "The WEEKDAY function returns incorrect values for dates before March 1, 1900. Because most users do not use dates before March 1, 1900, this problem is rare."

Well, perhaps most users don't but I'm sure with this group of people that is not unheard of... There are other bugs as well, for example the 2007 version had a bug that incorrectly reported the product of 12 pairs of numbers. I think 77.1 times 850 was reported as 100,000 instead of correctly as 65 thousand and something. It would be incredibly unlikely that that error affected your research, but if it did, you can bet that it's impact would be quite critical, so again, I would definitely go so far as to cite even the spreadsheet programme you used.

But more generally you should cite any software that impacts upon the results, includes numerical modelling or simulations, any algorithmic evaluations or research using software that does some form of automated analysis e.g. image analysis or optical character recognition.

Sometimes the decision is made for you, because the licence for the software, that you have of course carefully read, so you know this, but sometimes the licence explicitly requires you cite it.

How should software be cited?

All the main citation styles have examples of how to cite software. For example MLA suggests:

"SPSS Student Version 11.0." Prentice Hall, 2001.

And you should be able to look up examples for your prefered style. Whatever you choose though, make sure you include the version of the software. The idea is for you to be transparent about how your results were produced and allow someone else to replicate them, and software versions could play a role here.

Additionally most software developers will have a suggested citation format.

Sometimes it seems more straightforward to cite the associated paper for a programme instead of the software itself. It fits the format we're used to, I guess it's always nicer to cite a person than an institution or company. You should avoid doing that. Always cite the software explicitly. If the associated paper was substatnively useful in your analysis, then by all means cite it as well, additionally, but not instead.

Several reasons for this: not all software has associated journal articles. Also an article is not specific to the version you were using, so does not serve to enhance reproducibility in that way.

Publishers and reviewers might take issue with the citing of software, however that sort of attitude is hopefully becoming a thing of the past. If you were to receive pushback the alternative is always to include the citation information in a footnote or otherwise stated in the methods section. From the point of view of reproducibility, the important thing is the information is accessible to the reader. However from the point of view of the authors, especially if they have mandated citation in the licence, that may be too little.

If the software you are using has a DOI, then use it! Use it even at the expense of a url. Because DOIs are perseistent and urls are not. If you cite the DOI in its url form with the resolver service url as its prefix, for example like this <http://dx.doi.org/NNNN>, then it will work like a link and lead to the source, even if it has moved in the meantime.

If there is no DOI, use urls, even though MLA recommends against it (becuase of breakage). It is still better Examples Software purchased off-the-shelf:

ProductName. Version. ReleaseDate. Publisher. Location.

SuperScience. 1.2. December 2012. ResearchSoftware. Edinburgh, UK.

Software downloaded from the web:

ProductName. Version. ReleaseDate. Publisher. Location. DOIorURL. DownloadDate.

OGSA-DAI REST. 4.2.1. December 2012. OGSA-DAI Project. <http://sourceforge.net/projects/ogsa-dai>. 27/04/2012.

UltimateFFT. 2.4. December 2012. Fred Bloggs, EPCC, The University of Edinburgh, UK. <http://www.epcc.ed.ac.uk/ultimate-fft>. 27/04/2012.

C implementation of Wu's color quantizer. 2. 1991. Xiaolin Wu, Department of Electrical & Computer Engineering, McMaster University, Hamilton, Ontario. <http://www.ece.mcmaster.ca/~xwu/cq.c>. 27/04/2012.

Software checked-out from a public repository:

ProductName. Publisher. URL. CheckoutDate. RepositorySpecificCheckoutInformation.

OGSA-DAI REST. OGSA-DAI Project. <http://sourceforge.net/projects/ogsa-dai>. 27/04/2012. Check-out: [ogsa-dai/branch/ogsadai4.1/](http://sourceforge.net/projects/ogsa-dai), revision 1657.

Software provided by a researcher:

ProductName. Author. Location. ContactDetails. ReceivedDate. BestFFTroutine ever file. Fred Bloggs, EPCC, The University of Edinburgh, UK. Fred.bloggs@epcc.ed.ac.uk. 27/04/2012. (Hong et al. 2015)

additional details

In addition to software there are other environmental variables that should be explicitly stated if they affect the results: " This information may include: operating system, specific packages, sub-routines, queries, files, libraries, scripts, service end-points, configurations, parameters or workflows" "this information should be described in the body of your paper, in the methods section, footnotes, acknowledgements or appendices.

style guide

text

References

Hong, Neil P Chue, Tom Crick, Ian P Gent, Lars Kotthoff, and Kenji Takeda. 2015. "Top Tips to Make Your Research Irreproducible." *arXiv Preprint arXiv:1504.00062*.

Jackson, Mike. 2012. "How to Cite and Describe Software." Software Sustainability Institute; <https://software.ac.uk/how-cite-software>.

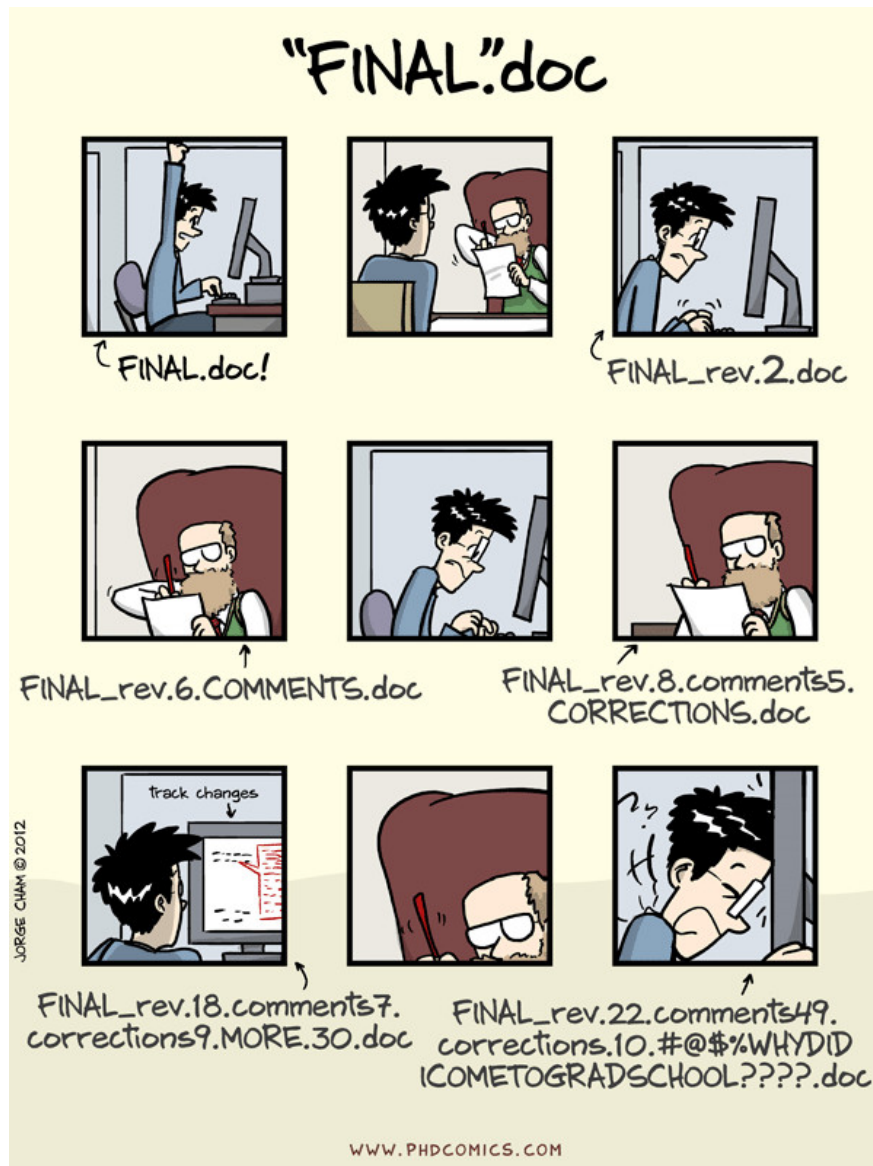


Figure 1: PhD: final.doc [<http://phdcomics.com/comics/archive.php?comid=1531>]

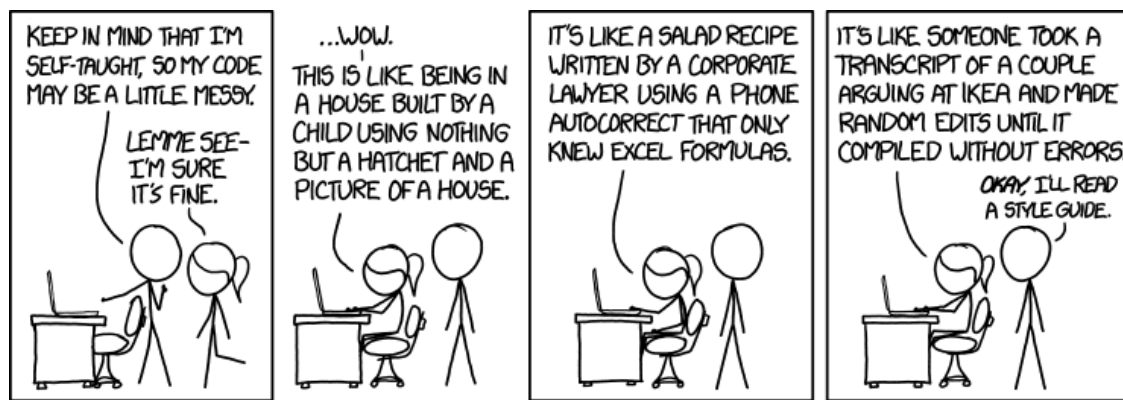


Figure 2: [xkcd: Code Quality [<https://xkcd.com/1513/>]]