KnitR + LaTeX → paper

Tools for Reproducible Research

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This lecture is about how to create reproducible manuscripts, for journal articles. KnitR with R Markdown is great for informal reports. KnitR with AsciiDoc is great for somewhat fancier reports. There are a number of efforts, especially with Pandoc, to use R Markdown for journal articles. But if you want fine control over the appearance of a document, it's hard to beat LaTeX, and so I'm just going to focus on that.

I can't hope to explain LaTeX properly in just this one lecture. My goals are to give the general gist, indicate resources and options, and show how to use KnitR with LaTeX.

I also want to discuss some more general strategies for ensuring that the results described in a journal article are fully reproducible.

LaTeX

```
\documentclass[12pt]{article}

\usepackage{graphicx}

\title{An example document}
\author{Karl Broman}

\begin{document}

\maketitle
\thispagestyle{empty}

\section{A section}

This is a simple example of a \LaTeX\/ document for an article.
Here's some in-line math: $y = \beta_0 + \beta_1 x + \epsilon$.

And here's a display equation:

$$ \hat{\beta} = (X'X)^{-1} X'y $$

\end{document}
```


LaTeX is like html or Markdown: plain text with special codes to indicate how things are to appear.

A LaTeX document always starts with `\documentclass`, then a bunch of overall controlling information. The actual document is between `\begin{document}` and `\end{document}`.

`\usepackage{}` is like `library()` in R.

Ideally, you focus on semantics rather than style: define the `\title{}` and `\author{}` and use `\maketitle` to have them included in the document, and indicate sections and subsections with `\section{}` and `\subsection{}`.

For some reason, `\thispagestyle{empty}` ("don't show page number on this page") needs to be placed after `\maketitle`.

A key feature of LaTeX is the mathematics typesetting. There's no better system. And your LaTeX skills can be immediately transferred to your Markdown documents, with MathJax.

What I actually do

```
\documentclass[12pt]{article}

\setlength{\headheight}{10pt}
\setlength{\headsep}{15pt}
\setlength{\topmargin}{-25pt}
\setlength{\topskip}{0in}
\setlength{\textheight}{8.7in}
\setlength{\footskip}{0.3in}
\setlength{\oddsidemargin}{0.0in}
\setlength{\evensidemargin}{0.0in}
\setlength{\textwidth}{6.5in}

\begin{document}
\begin{center}
\textbf{\large An example document}

\vspace{10mm}
Karl Broman
\end{center}

\vspace{30mm}
\textbf{\sffamily A section}
```


In reality, for a paper, I don't use `\maketitle` or `\section`, but rather just muck about, hard-coding the placement of things.

But mine is not the recommended approach. If, for some reason, you need to change the style, it's easier if your document is defined in terms of semantics.

Why LaTeX?

- Fine control of document appearance
- Transparency of how that was achieved
- Version control (diff/merge)
- Typesetting equations
- Markdown's not quite ready, or sufficiently rich

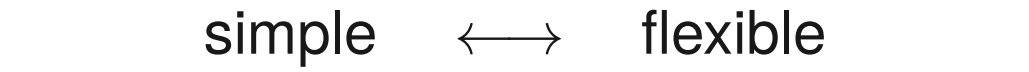
It's a lot of work to learn LaTeX, so we need to be clear about why we'd want to devote the effort to it.

For reproducible research, we need some sort of code-based document system (i.e., not Word!), and LaTeX gives you the most fine-grained control, if you need it. Ultimately, I hope, Markdown will be sufficient, but for now, we often need LaTeX.

The code-based control makes what you're trying to do transparent. And you should treat LaTeX like code: write clearly and simply, and comment the tricky bits.

This sort of document also has the advantage of easy treatment of `diff` and `merge` in a version control system like git.

The real power of LaTeX is in the typesetting of mathematical equations. And what you learn on that aspect can be transferred to your Markdown documents, using MathJax. (But I already said that, didn't I?)




```
\centerline{\Large simple \quad $\longleftrightarrow$ \quad flexible}
```


LaTeX sits at the right of the simple-to-flexible spectrum.

Modify your desires to match the defaults.

Focus your compulsive behavior on things that matter.

I've said this before, but I like to repeat it.

Focus on the text and the figures before worrying too much about fine details of how they appear on the page.

And consider which is more important: a manuscript, web page, blog, grant, course slides, course handout, report to collaborator, scientific poster.

You can spend a ton of time trying to get things to look just right. Ideally, you spend that time trying to construct a general solution. Or you can modify your desires to more closely match what you get without any effort.

KnitR + LaTeX → Rnw

```
\documentclass[12pt]{article}

\title{An example Rnw document}
\author{Karl Broman}

\begin{document}
\maketitle

<<load_library, echo=FALSE, results="hide">>=
library(broman) # used for myround()
@

<<example_chunk, out.width="0.8\\textwidth">>=
x <- rnorm(100)
y <- 5*x + rnorm(100)
lm.out <- lm(y ~ x)
plot(x,y)
abline(lm.out$coef)
@

The estimated slope is \Sexpr{myround(lm.out$coef[2], 1)}.
\end{document}
```


KnitR works well with LaTeX.

Most of what you learned about KnitR with R Markdown transfers directly to working with LaTeX.

The main difference is the way in which code chunks are indicated. You use `<<>>=` and `@` for chunks, and `\Sexpr{}` for in-line code.

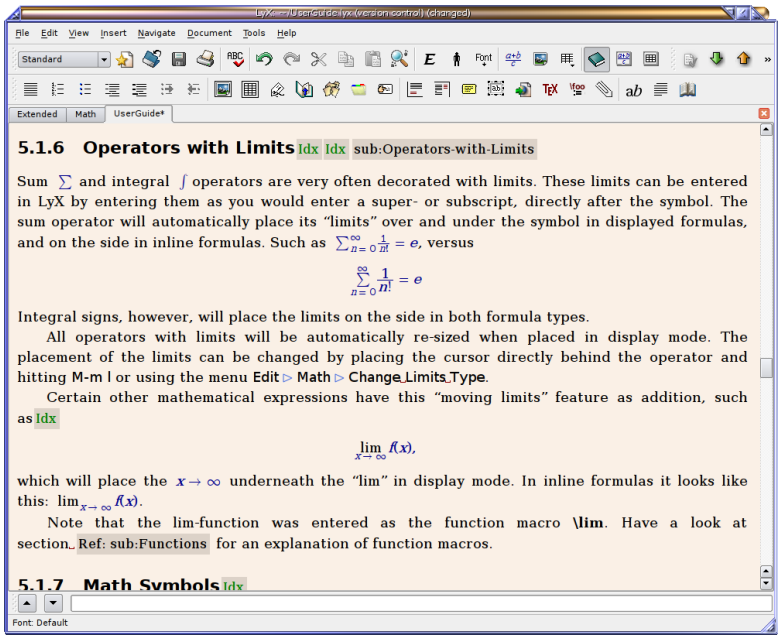
KnitR basically does a search-and-replace for code chunks. Different patterns will be easier, depending on the nature of the surrounding code.

The chunk options are the same. Here, I used `out.width="0.8\textwidth"` to make the figure appear as 80% of the width of the page.

`out.width` and `out.height` need units as in LaTeX (built into `\\textwidth`; otherwise `"in"` or `"cm"` or `"pt"` or whatever).

`fig.width` and `fig.height` are as in R, with implied units.

LyX



lyx.org 8

I create LaTeX documents in emacs. If you want something WYSIWYG, consider LyX. KnitR is built in, and Yihui Xie strongly endorses it. (LyX is not really "WYSIWYG" but rather "WYSIWYM," but that's what you want most, anyway.)

Also

- WriteLaTeX
- Authorea
- ShareLaTeX
- Verbosus

There are a bunch of online tools for creating LaTeX documents, collaboratively.

I have no experience with these, but I've heard good things about WriteLaTeX.

Flavors of LaTeX

- LaTeX
- pdflatex
- xelatex
- lualatex

In addition to regular LaTeX, there's pdflatex (which I mostly use). It has the advantage of being able to include pdf, jpg, and png figures, and produces a PDF file directly.

XeLaTeX and LuaLaTeX are great for fonts and Unicode.

I've not mentioned that behind the scenes is TeX, which is the source of all of this. Believe or not, LaTeX exists because TeX is even harder. PdfLaTeX, XeLaTeX, and LuoLaTeX, really derive from PdfTeX, XeTex, and LuoTex.

Getting help

- Google
- tex.stackexchange.com
- Ask a friend
- Look at others' documents
- Resign yourself to something less-than-ideal

There is a ton of online information about LaTeX. Start with google. It's highly unlikely that you have a completely unique question or problem.

My last point here is basically that one way to help yourself is by learning to let things go.

Figure captions and floats

```
<<fig_with_caption, fig.cap="Scatterplot of $y$ vs $x$">>=
x <- rnorm(100)
y <- 5*x + rnorm(100)
lm.out <- lm(y ~ x)
plot(x,y)
abline(lm.out$coef)
@
```

```
\begin{figure}[]
\includegraphics{figure/fig_with_caption}

\caption{Scatterplot of $y$ vs $x$\label{fig:fig_with_caption}}
\end{figure}
```


If you use the chunk option `fig.cap`, the figure will get a caption.

But it will also be embedded within a `figure` "environment." (That is, between `\begin{figure}` and `\end{figure}`.)

This makes it a "float." LaTeX decides where it's going to be placed. The placement of floats is the biggest pain in using LaTeX.

The figure also gets a label, from the chunk name. (The `\label{}` bit.) This allows you to cross-reference the figure, to have the figure number determined automatically.

The cross reference would be with `\ref{fig:fig_with_caption}`.

When you use cross references, you need to run LaTeX twice: once to establish where things will sit on the page and how they are numbered, and a second time to insert the cross references.

Tables in LaTeX

```
\begin{tabular}{rrrrr} \hline
& Estimate & Std. Error & t value & Pr($>$$|$t$|$) \\  \hline
(Intercept) & 0.04 & 0.11 &  0.4 & 0.69 \\
      x     & 0.98 & 0.10 & 10.0 & 0.00 \\ \hline
\end{tabular}
```


Tables in LaTeX are a pain, but they offer extremely fine control.

But writing this sort of code (`&` indicates breaks between columns, `\\` indicates the end of a row) reproducibly is hard.

xtable

```
<<generate_and_fit>>=
x <- rnorm(100)
y <- x + rnorm(100)
lm.out <- lm(y ~ x)
@

<<table, results="asis">>=
library(xtable)
xtable(lm.out, digits=c(0,2,2,1,2))
@
```


xtable is a superb R package for producing LaTeX tables. You don't have complete control, but you do have a ton of control. The xtableGallery vignette shows you much of what can be done.

BibTeX for bibliographies

```
%bibliography format
\usepackage[authoryear]{natbib}
\bibpunct{(}{)}{;}{a}{}{,}

A number of investigators have developed methods for identifying
such sample mix-ups \citep{Westra2011, Schadt2012, Lynch2012,
Ekstrom2012}, and a similar approach was applied by
\citet{Baggerly2008, Baggerly2009} in their forensic...

\bibliographystyle{genetics}
\renewcommand*{\refname}{\centerline{\normalsize\sffamily
   \textbf{Literature Cited}}}
\bibliography{samplemixups}
```

```
@article{Baggerly2008,
author = {Baggerly, Keith A. and Coombes, Kevin R.},
journal = {J. Clin. Oncol.},
pages = {1186--1187},
title = {Run batch effects potentially compromise...},
volume = {26},
year = {2008} }
```


References with LaTeX are via BibTeX, which is fabulous once you get used to it. Most software to track references will produce BibTeX files for you.

The formatting of citations and the reference listings, to match what the journal wants, can be painful. But I've figured out how to produce what Genetics wants, and I send all of my papers there.

The first box is the sort of code that would appear in your LaTeX file: the bit at the top goes in the header (before `\begin{document}`). The bit in the middle shows how to cite papers: use `\citep` to get the whole thing in parentheses, and use `\citet` to get a reference like "...applied by Baggerly and Coombes (2008, 2009)..." The last bit in the first box produces the actual list of references.

The second box is the BibTeX format for a particular reference.

When you use BibTeX, you tend to run `pdflatex`, then `bibtex`, and then `pdflatex` a couple of more times.

Organizing analyses

- Directory for the main analysis project

  `~/Projects/Blah`

- Directory for a paper

  `~/Docs/Papers/Blah`

- Paper directory may have an analysis directory

  `~/Docs/Papers/Blah/Analysis`

- Symbolic links to `.RData` files

  `ln -s ~/Projects/Blah/DerivedData/blah.RData .`

- Each part well organized and fully reproducible.
- R Markdown reports documenting different aspects.
- Analysis with the paper may be re-done "properly."

This is how I organize a paper related to a larger project.

Some of the work in the main project may be re-done a bit differently (or cleaner) in the analysis with the paper.

You don't want to re-do all analyses for the paper, but it'd also be nice to have the data and code related to the paper be a bit more self-contained.

And usually when you're sitting down to write the paper, you have better ideas about how to re-do things properly, and so it might be a good idea to go ahead and re-do things.

Ideally, you'd separate out each aspect of the analysis: data manipulation, data cleaning, and different parts of the analysis.

Have an R Markdown document describing each aspect, with the actual manuscript and its figures and tables drawing from the results of those R Markdown documents.

Make every number reproducible.

```
<<define_numbers, echo=FALSE>>=
numbers <- c("one", "two", "three", "four", "five",
             "six", "seven", "eight", "nine", "ten")
cap <- function(vec) paste0(toupper(substr(vec, 1, 1)),
                            substr(vec, 2, nchar(vec)))
Numbers <- cap(numbers)
n <- sample(1:10, 1)
@

Then if I want to talk about a number, like \Sexpr{n}, I can
refer to it by name: \Sexpr{numbers[n]}. And I can start a
sentence with it. \Sexpr{Numbers[n]} grasshoppers walked into a
bar\dots

But be careful about singular vs. plural, and so write
\Sexpr{Numbers[n]} grasshopper\Sexpr{ifelse(n>1, "s", "")}
walked\dots
```


Every statistic, figure and table in your manuscript should be fully reproducible. So when you're citing statistics, use `\Sexpr{}` liberally.

This should inhibit you from writing numbers as words, though the LaTeX code can get a bit ugly.

There's a bit of fanciness here about capitalization and about ensuring that singular or plural nouns are correct. If `\Sexpr{}` produces a character string, it ends up as plain text in your document

I'll use a lot of `myround()` from my R/broman package, too.

Long explanations or descriptions of figures can't be fully reproducible, but the figures themselves and any statistics you mention should be.

Keep the figures separate

```
# simple make file

mypaper.pdf: mypaper.tex Figs/fig1.pdf Figs/fig2.pdf
pdflatex mypaper

Figs/fig1.pdf: R/fig1.R
cd R;R CMD BATCH fig1.R fig1.Rout

Figs/fig2.pdf: R/fig2.R
cd R;R CMD BATCH fig2.R fig2.Rout
```

```
\clearpage
\includegraphics{Figs/fig1.pdf}

\clearpage
\includegraphics{Figs/fig2.pdf}
```


While you could include all code in your `.Rnw` file, I prefer to pull out the code for my figures as separate files, and then write a `Makefile` for the manuscript construction and include them with `\includegraphics`.

The advantage of this is the ability to reuse the figures in talks or whatever. Also, journals will generally want the figures as separate files. Finally, the code for my figures is often incredibly long and ugly, so it's best to separate it out.

Ideally, the code for a figure would be structured as a function and then a function call. Put a bit more effort into the code, so that you can reuse it later for a similar figure with different data. At the very least, you should write the repeated bits as functions.

If your function takes arguments that define the placement of things (padding for text and so forth), then the fine adjustments of the figure appearance would be easier.

Version Control

- Your manuscript is under version control, right?
- Local or private repository for the whole thing
  - including reviewers' reports and my response
  - PDF of submitted and final manuscript
- Snapshot of the final version as a public repository
  - I don't really want to show the whole history

Git is as good for tracking manuscripts and data analyses as it is for tracking code. Use it!

But I don't want to make everything public, and I want to include private stuff in my repository.

I've been using just a local repository, but I'm moving towards having a private repository hosted on BitBucket.

I'll put a snapshot of the final version, and maybe a few final changes, on GitHub.

Word

- With papers led by a collaborator, I'm usually stuck with Word.
- But my analyses and figures are fully reproducible.
- Create an R Markdown document with the detailed results.

Often, you'll be stuck with Word. And you can't reproducibly insert numbers into Word.

So have a separate R Markdown report with the detailed results, including every statistic that will get inserted into Word.

And take control of the figures and ensure that they are reproducible (and respectable).

Teach your collaborators to at least have their figures be reproducible?

Summary

- LaTeX is brilliant for fine control and for equations
- Floating figures and tables can be a pain
- You use KnitR with LaTeX much the same way as you'd used it with Markdown.
- Ensure that every statistic, figure, and table in your paper are fully reproducible.
- Use xtable to make tables.
- Separate out the code for the figures.
- Use version control!

Summaries are helpful.