Literate programming with `rmarkdown` (and `quarto`)

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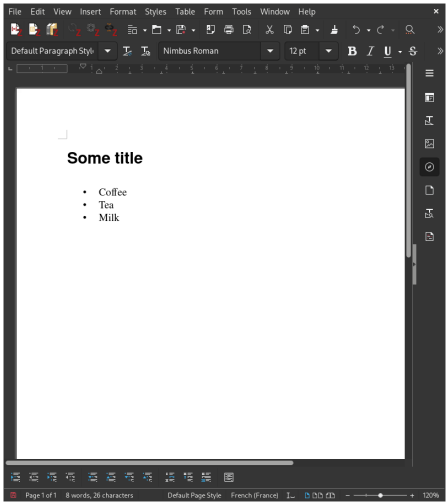
Document creation

(Microsoft) Office

- Non-free editing software
- Proprietary format
- Visual editing
- Non-uniform rendering



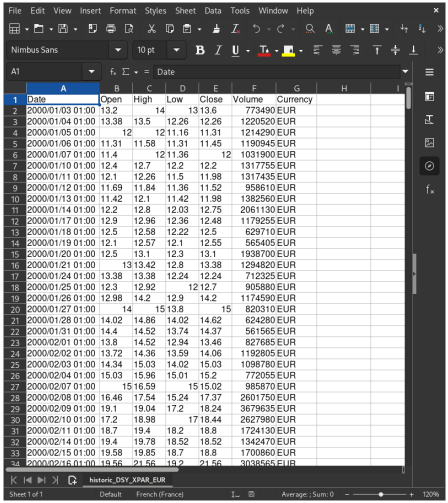
Beyond the document creation

General drawbacks

- Sharing and collaboration
- Version control
- GitHub / GitLab integration

Prone to errors

- Zeeberg et al. (2004)
- McCullough and Wilson (2005)
- McCullough and Heiser (2008)
- Fetzer and Graeber (2020)



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3	2000/01/04 01:00	13.38	13.5	12.26	12.26	1220520	EUR	
4	2000/01/05 01:00	12	12	11.16	11.31	1214290	EUR	
5	2000/01/06 01:00	11.31	11.58	11.31	11.45	1190945	EUR	
6	2000/01/07 01:00	11.4	12	11.36	12	1031900	EUR	
7	2000/01/10 01:00	12.4	12.7	12.2	12.2	1317755	EUR	
8	2000/01/11 01:00	12.1	12.26	11.5	11.98	1317435	EUR	
9	2000/01/12 01:00	11.69	11.84	11.36	11.52	958610	EUR	
10	2000/01/13 01:00	11.42	12.1	11.42	11.98	1382560	EUR	
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14	2000/01/19 01:00	12.1	12.57	12.1	12.55	565405	EUR	
15	2000/01/20 01:00	12.5	13.1	12.3	13.1	1938700	EUR	
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17	2000/01/24 01:00	13.38	13.38	12.24	12.24	712325	EUR	
18	2000/01/25 01:00	12.3	12.92	12	12.7	905880	EUR	
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20	2000/01/27 01:00	14	15	13.8	15	820310	EUR	
21	2000/01/28 01:00	14.02	14.86	14.02	14.62	624280	EUR	
22	2000/01/31 01:00	14.4	14.52	13.74	14.37	561565	EUR	
23	2000/02/01 01:00	13.8	14.52	12.94	13.46	827685	EUR	
24	2000/02/02 01:00	13.72	14.36	13.59	14.06	1192805	EUR	
25	2000/02/03 01:00	14.34	15.03	14.02	15.03	1098780	EUR	
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30	2000/02/10 01:00	17.2	18.98	17	18.44	2627980	EUR	
31	2000/02/11 01:00	18.7	19.4	18.2	18.8	1724130	EUR	
32	2000/02/14 01:00	19.4	19.78	18.52	18.52	1342470	EUR	
33	2000/02/15 01:00	19.58	19.85	18.7	18.8	1700860	EUR	
34	2000/02/16 01:00	19.56	21.56	19.2	21.56	3036565	EUR	

Now

WTP QUALITY ESTIMATES IN COMMUTE MODE CHOICE: ISSUES OF PERFORMANCE COMPARISON UNDER SAMPLE SIZE AND BALANCE IMPACTS.

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Extended abstract

Keywords Willingness to Pay · Mode Choice · Model Performance Comparison · Discrete Choice Modelling · Econometrics · Machine Learning

Word count: 994 words in body, 5975 characters in body, 6910 characters in body (including spaces)

In economics studies one of the wide-spread target metrics is the *Willingness to Pay* (WTP) of individuals for particular attributes of goods or services. In transportation studies popular manifestations of WTP are *Value of Time* (VOT) or *Value of Comfort* (VOC). The WTP elicitation lies at the heart of many various tasks in the transportation mode choice analysis: adoption of emerging sustainable transportation modes (Ilahi et al., 2021), attitudes to resilience and sharing in transportation (Ho et al., 2018; Kang et al., 2021), preferences for emerging services (Ardeshiri et al., 2021; Merkert et al., 2022).

There exist multiple concurrent ways to deduce WTP from the data, most of which rely on the *Random Utility Maximisation* (RUM) framework (McFadden, 1974). With time the number of available models and estimation techniques increases, but many of them are still *RUM-compliant*. Following McFadden (1981) the RUM-compliance translates in the independence of the ranking of the choice probabilities of the alternatives by any monotonically increasing transformation of the utility functions of all elemental alternatives (Brunher and Greene, 2002). The family of RUM-compliant models was recently extended by a number of more advanced models, as the mode choice modelling is on the verge of transition to incorporation of novel *Machine Learning* (ML) based analysis methodologies. The ML or *data driven* methodology focuses on the predictive qualities. In contrast, the econometrics or *theory driven* methodology attempts to decipher the underlying properties of the data. The hypothetico-deductive approach of econometrics allows the production of economic indicators under validity conditions of the model hypotheses, on which ML tools do not depend. The transportation studies and mode choice modelling applications in particular were among the first to attempt the implementation of ML methodology for typically *theory driven* tasks. One can observe a

PDF

- Open-source format
- Software agnostic
- Uniform rendering

Rmarkdown

- Markup editing
- Simple version control
- Code integration
- Data management

Different approaches

What You See Is What You Get

Editing content in a form that is identical to its appearance when displayed as a finished product

Examples

- Microsoft Office
- LibreOffice
- Apache OpenOffice
- GNU TeXmacs

Editing content in a plain text format, where the document contains a set of rules that determine its appearance when displayed a finished product.

Examples

- Groff (Troff, Roff)
- TeX (LaTeX)
- HTML
- XML
- Markdown

Workflow pipeline

Pipeline outline

Requirements

- Possibility to render PDF (and potentially other formats)
- Simple citations management
- Easy syntax
- Integration with other activities
  - Code execution
  - Scripting

Pipeline outline

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- Possibility to render PDF (and potentially other formats)
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  - Scripting

Solutions

- Pandoc conversion + PDF LaTeX engine
- BibTeX support

- Wide variety of supported formats
- Possibility to combine *markdown* with other markup syntax formats (LaTeX, HTML, ...)
- Custom templates support
- Document composition
  - In-document YAML configuration
  - External features

PDF (and other formats) rendering

Pandoc fully-supported formats

- Markdown
- RTF, docx, ODT
- HTML
- EPUB
- Roff
- LaTeX, BibTeX
- OPML
- Jupyter notebooks

Pandoc output formats

- Chunked HTML
- LaTeX Beamer
- Microsoft PowerPoint
- Slidy
- reveal.js
- S5
- OpenDocument XML
- GNU TexInfo

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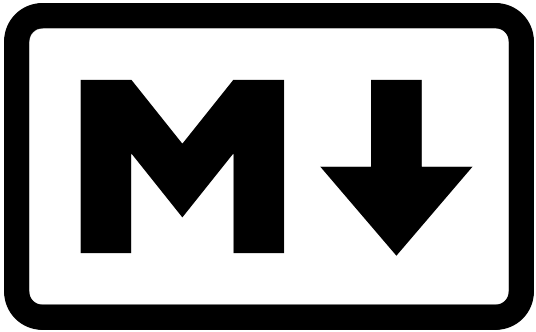
- BibTeX support
- Markdown

Key advantages

- More simple syntax in comparison with pure LaTeX, HTML or Groff
- Best compatibility with Pandoc for conversion into other formats



Easy syntax

LaTeX

```
\begin{itemize}
  \item{Coffee}
  \item{Tea}
  \item{Milk}
\end{itemize}
```

HTML

```
<ul>
  <li>Coffee</li>
  <li>Tea</li>
  <li>Milk</li>
</ul>
```

Markdown

```
- Coffee
- Tea
- Milk
```

Pipeline outline

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Solutions

- Pandoc conversion + PDF LaTeX engine
- BibTeX support
- Markdown
- R
  - knitr

Code execution

knitr

- Executes code inside `.Rmd` document
- Appends the results after the code blocks
- Generates `.md` document

```
'''{r}
x = rnorm(100); y = 1:100
plot(x, y)
'''
```

Pipeline outline

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- Possibility to render PDF (and potentially other formats)
- Simple citations management
- Easy syntax
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Solutions

- Pandoc conversion + PDF LaTeX engine
- BibTeX support
- Markdown
- R
  - knitr
  - rmarkdown

Inside document

- Add `yaml` part

```
---
title: "Some title"
author: J. Doe
params:
  n: 1000
---
```

Inside body

- Call `params` list to retrieve the parameters

```
'''{r}
n = params$n
x = rnorm(n); y = 1:n
plot(x, y)
'''
```

- `knitr` (embedded code execution)
- R front-end to pandoc features
- Support for markdown syntax
- Extended YAML configuration
- Wide variety of preconfigured pandoc templates
- Notebook oriented workflow (alternative to Jupyter)

Potential drawbacks

Different flavours of markdown

- CommonMark
- CriticMarkup
- ExtraMark
- GitHub Markdown
- Pandoc's Markdown
- ...

Dependencies to configure

- Pandoc - `https://pandoc.org/installing.html`
- PDF LaTeX engine - `https://yihui.org/tinytex/`
  (ex: MikTeX, TinyTeX)
- R - `https://www.r-project.org/`

Extensions

- `kable` and `kableExtra` - toolset for `data.frame` display
- `bookdown` - extra features for academic and professional writing (ex: books and manuals)
- `rticles` - preconfigured templates for scientific articles and conferences
- `blogdown` - blog editing with Hugo
- `Python`, `Julia` or `C++` for other code block types support
- `htmlwidgets` - bindings `R` to `JavaScript` libraries.
- `learnr` - interactive tutorials and quizzes
- `shiny` - interactive documents and reports

For further reading

Manuals

- Xie, Dervieux, and Riederer (2020)
- Mailund (2019)

Potential errors

- Li, Liu, and Meng (2021)

Practical part

Dependencies to configure

- Pandoc - `https://pandoc.org/installing.html`
- PDF LaTeX engine - `https://yihui.org/tinytex/` (ex: MikTeX, TinyTeX)
- R - `https://www.r-project.org/`

Getting started

- Run your preferred IDE / editor
- Create a new `test.Rmd` document to experiment with
- Cheat sheets available at `https://www.rstudio.com/resources/cheatsheets/`

At the top of the document the YAML part is placed, which communicates parameters to pandoc and R:

Example

```
---
title: Some title
author: J. Doe
date: March 2023
output:
  pdf_document:
    toc: false
    fig_caption: true
---
```

Basic syntax

- *italics* = `*italics*`
- **bold** = `**bold**`
- hyperlink = `[hyperlink](https://www.rstudio.com)`
- images = `![image description](./path/to/image.png)`
- lists

```
1. list
  * with
  * nested
2. elements
```

- headers = `# Header`
- unnumbered header = `# Header {-}`

Basic syntax

- quotation = `> quotation`
- footnote = `^[footnote]`
- *inlinemaths* = `$inline maths$`
- maths equations

```
$$
X = \frac{1}{\sigma}
$$
```

For full guide see here `https://bookdown.org/yihui/rmarkdown/`

Code integration

Inline code

```
'r x = 10; print(x)'
```

Separate code blocks

````
```{r, include = TRUE}
x = 10
print(x)
```
````

You can get the available engines with the command:

```
names(knitr::knit_engines$get())
```

Using other languages

````
```{python, engine.path = '/usr/bin/python3'}
x = 10
print(x)
```
````

Create a sample template for LaTeX output and a `.Rmd` document:

template.tex

```
\documentclass{article}
$if(encoding)$
\usepackage[$encoding$]{inputenc}
$else$
\usepackage[utf8]{inputenc}
$endif$
\begin{document}
$body$
\end{document}
```

somefile.Rmd

```
---
encoding: utf8
output:
  pdf_document:
    template: template.tex
---

Some text in body.
```

To convert the document one can:

1. Use the integrated features of the IDE
   - `Ctrl + Shift + K` in VS Code
   - `knit` button in RStudio

2. Call the rendering function directly

```
rmarkdown::render(
  "path/to/the/file.Rmd"
)
```

Create a new `test.md` markdown document to experiment with.

test.md

```
---
title: Some title
author: J. Doe
---
Some text in body.
```

Convert it to .tex

```
pandoc test.md -f markdown -o test.tex -t pdf
```

Alternatives

Language specific

- Pmarkdown (seems to have lost support)
- Jmarkdown
- Jupyter (notebooks)

Language agnostic (standalone)

- Quarto
  - Mostly back-compatible with `.Rmd` format
  - Has dedicated extensions for VS Code, Emacs, etc.
  - Specification of `knitr` options in YAML
  - Some packages break

References

References I

Fetzer, Thiemo, and Thomas Graeber. 2020. "Does Contact Tracing Work? Quasi-Experimental Evidence from an Excel Error in England." December 15, 2020. https://doi.org/10.1101/2020.12.10.20247080.

Li, Penghui, Yinxi Liu, and Wei Meng. 2021. "Understanding and Detecting Performance Bugs in Markdown Compilers." In *2021 36th IEEE/ACM International Conference on Automated Software Engineering (ASE)*, 892–904. https://doi.org/10.1109/ASE51524.2021.9678611.

Mailund, Thomas. 2019. *Introducing Markdown and Pandoc: Using Markup Language and Document Converter*. Berkeley, CA: Apress. https://doi.org/10.1007/978-1-4842-5149-2.

McCullough, B. D., and David A. Heiser. 2008. "On the Accuracy of Statistical Procedures in Microsoft Excel 2007." *Computational Statistics & Data Analysis* 52 (10): 4570–78. https://doi.org/10.1016/j.csda.2008.03.004.

McCullough, B. D., and Berry Wilson. 2005. "On the Accuracy of Statistical Procedures in Microsoft Excel 2003." *Computational Statistics & Data Analysis* 49 (4): 1244–52. https://doi.org/10.1016/j.csda.2004.06.016.

References II

Xie, Yihui, Christophe Dervieux, and Emily Riederer. 2020. *R Markdown Cookbook*. New York: Chapman and Hall/CRC. https://doi.org/10.1201/9781003097471.

Zeeberg, Barry R., Joseph Riss, David W. Kane, Kimberly J. Bussey, Edward Uchio, W. Marston Linehan, J. Carl Barrett, and John N. Weinstein. 2004. "Mistaken Identifiers: Gene Name Errors Can Be Introduced Inadvertently When Using Excel in Bioinformatics." *BMC Bioinformatics* 5 (1, 1): 1–6. https://doi.org/10.1186/1471-2105-5-80.