Collaborative Data Science Practices

Will Beasley 2019-02-24

Contents

1	Pre	requisites	7			
2	Arc	hitecture Principles	9			
	2.1	Encapsulation	9			
	2.2	Leverage team member's strenghts & avoid weaknesses	9			
	2.3	Scales	9			
	2.4	Consistency	9			
3	Pro	totypical File	11			
	3.1	Clear Memory	11			
	3.2	Load Sources	11			
	3.3	Load Packages	11			
	3.4	Declare Globals	11			
	3.5	Load Data	11			
	3.6	Tweak Data	11			
	3.7	(Unique Content)	11			
	3.8	Verify Values	11			
	3.9	Specify Output Columns	11			
	3.10	Save to Disk or Database	11			
4	Prototypical Repository 1					
	4.1	Analysis	13			
	4.2	Data Public	13			
	4.3	Data Unshared	13			
	4.4	Documentation	13			
	4.5	Manipulation	13			
	4.6	Stitched Output	13			
	4.7	Utility	13			

4 CONTENTS

5	Dat	a at Rest	15			
	5.1	Data States	15			
	5.2	Data Containers	15			
6	Patt	terns	17			
	6.1	Ellis	17			
	6.2	Arch	19			
	6.3	Ferry	19			
	6.4	Scribe	19			
	6.5	Analysis	19			
	6.6	Presentation -Static	19			
	6.7	Presentation -Interactive	19			
	6.8	Metadata	19			
7	Seci	urity & Private Data	21			
	7.1	File-level permissions	21			
	7.2	Database permissions	21			
	7.3	Public & Private Repositories	21			
8	Aut	omation	23			
	8.1	Flow File in R	23			
	8.2	Makefile	23			
	8.3	SSIS	23			
	8.4	cron Jobs & Task Scheduler	23			
	8.5	Sink Log Files	23			
9	Scaling Up					
	9.1	Data Storage	25			
	9.2	Data Processing	25			
10	Para	allel Collaboration	27			
	10.1	Social Contract	27			
	10.2	Code Reviews	27			
	10.3	Remote	27			
	10.4	Loose Notes	27			

CONTENTS 5

11 Do	cumentation	29
11.1	Team-wide	29
11.2	Project-specific	29
11.3	Dataset Origin & Structure	29
11.4	Issues & Tasks	29
11.5	Flow Diagrams	29
11.6	Setting up new machine	29
12 Sty	le Guide	31
12.1	ggplot2	31
13 Pul	olishing Results	33
13.1	To Other Analysts	33
13.2	To Researchers & Content Experts	33
13.3	To Technical-Phobic Audiences	33
14 Tes	ting, Validation, & Defensive Programming	35
14.1	Testing Functions	35
14.2	Defensive Programming	35
14.3	Validator	35
15 Tro	ubleshooting and Debugging	37
15.1	Finding Help	37
15.2	Debugging	37
16 Est	ablishing Workstation	39
16.1	Required Installation	39
16.2	Recommended Installation	39
16.3	Optional Installation	39
16.4	Asset Locations	39
17 Cor	nsiderations when Selecting Tools	41
17.1	General	41
17.2	Languages	41
17.3	R Packages	41
17.4	Database	41
18 Gro	owing a Team	43
18.1	Recruiting	43
18.2	Training to Data Science	43
18.3	Bridges Outside the Team	43

6 CONTENTS

A	Git & GitHub	45		
В	sentations 47			
	B.1 CDW	47		
	B.2 REDCap	47		
	B.3 GitHub	47		
	B.4 Architectures	47		
\mathbf{C}	Scratch Pad of Loose Ideas	49		
	C.1 Chapters & Sections to Form	49		
D	Introduction	51		

Prerequisites

This is a *sample* book written in **Markdown**. You can use anything that Pandoc's Markdown supports, e.g., a math equation $a^2 + b^2 = c^2$.

The **bookdown** package can be installed from CRAN or Github:

```
install.packages("bookdown")
# or the development version
# devtools::install_github("rstudio/bookdown")
```

Remember each Rmd file contains one and only one chapter, and a chapter is defined by the first-level heading #.

To compile this example to PDF, you need XeLaTeX. You are recommended to install TinyTeX (which includes XeLaTeX): https://yihui.name/tinytex/.

Architecture Principles

2.1 Encapsulation

2.2 Leverage team member's strenghts & avoid weaknesses

- 1. Focused code files
- 2. Metadata for content experts

2.3 Scales

- 1. Single source & single analysis
- 2. Multiple sources & multiple analyses

2.4 Consistency

- 1. Across Files {#consistency-files}
- 2. Across Languages
- 3. Across Projects

Prototypical File

As stated before, in Consistency Files, using a consistent file structure can (a) improve the quality of the code because the structure has been proven over time to facilitate good practices and (b) allow your intentions to be more clear to teammates because they are familiar with the order and intentions of the chunks.

We use the term "chunk" for a section of code because it corresponds with knitr terminology (Xie, 2015), and in many cases, the chunk of our R file connects to a knitr Rmd file.

- 3.1 Clear Memory
- 3.2 Load Sources
- 3.3 Load Packages
- 3.4 Declare Globals
- 3.5 Load Data
- 3.6 Tweak Data
- 3.7 (Unique Content)
- 3.8 Verify Values
- 3.9 Specify Output Columns
- 3.10 Save to Disk or Database

Prototypical Repository

https://github.com/wibeasley/RAnalysisSkeleton

4.1 Analysis

4.2 Data Public

- 1. Raw
- 2. Derived
- 3. Metadata
- 4. Database
- 5. Original
- 4.3 Data Unshared
- 4.4 Documentation
- 4.5 Manipulation
- 4.6 Stitched Output
- 4.7 Utility

Data at Rest

5.1 Data States

- 1. Raw
- 2. Derived
 - 1. Project-wide File on Repo
 - 2. Project-wide File on Protected File Server
 - 3. User-specific File on Protected File Server
 - 4. Project-wide Database
- 3. Original

5.2 Data Containers

- 1. csv
- 2. rds
- 3. SQLite
- 4. Central Enterprise database
- 5. Central REDCap database
- 6. Containers to avoid for raw/input
 - 1. Proprietary like xlsx, sas7bdat

Patterns

6.1 Ellis

6.1.1 Purpose

To incorporate outside data source into your system safely.

6.1.2 Philosophy

- Without data immigration, all warehouses are useless. Embrace the power of fresh information in a way that is:
 - repeatable when the datasource is updated (and you have to refresh your warehouse)
 - similar to other Ellis lanes (that are designed for other data sources) so you don't have to learn/remember an entirely new pattern. (Like Rubiks cube instructions.)

6.1.3 Guidelines

- Take small bites.
 - Like all software development, don't tackle all the complexity the first time. Start by processing only the important columns before incorporating move.
 - Use only the variables you need in the short-term, especially for new projects. As everyone knows, the variables from the upstream source can change. Don't spend effort writing code for variables you won't need for a few months/years; they'll likely change before you need them.
 - After a row passes through the verify-values chunk, you're accountable for any failures it causes in your warehouse. All analysts know that external data is messy, so don't be surprised. Sometimes I'll spend an hour writing an Ellis for 6 columns.
- Narrowly define each Ellis lane. One code file should strive to (a) consume only one CSV and (b) produce only one table. Exceptions include:
 - 1. if multiple input files are related, and really belong together (e.g., one CSV per month, or one CSV per clinic). This scenario is pretty common.
 - 2. if the CSV should legitimately produce two different tables after munging. This happens infrequently, such as one warehouse table needs to be wide, and another long.

6.1.4 Examples

- https://github.com/wibeasley/RAnalysisSkeleton/blob/master/manipulation/te-ellis.R
- https://github.com/wibeasley/RAnalysisSkeleton/blob/master/manipulation/
- https://github.com/OuhscBbmc/usnavy-billets/blob/master/manipulation/survey-ellis.R

6.1.5 Elements

1. Clear memory In scripting languages like R (unlike compiled languages like Java), it's easy for old variables to hang around. Explicitly clear them before you run the file again.

```
rm(list=ls(all=TRUE)) #Clear the memory of variables from previous run. This is not called by knit
```

2. Load Sources In R, a source()d file is run to execute its code. We prefer that a sourced file only load variables (like function definitions), instead of do real operations like read a dataset or perform a calculation. There are many times that you want a function to be available to multiple files in a repo; there are two approaches we like. The first is collecting those common functions into a single file (and then sourcing it in the callers). The second is to make the repo a legitimate R package.

The first approach is better suited for quick & easy development. The second allows you to add documention and unit tests.

```
# ---- load-sources
source("./manipulation/osdh/ellis/common-ellis.R")
```

3. Load Packages This is another precaution necessary in a scripting language. Determine if the necessary packages are available on the machine. Avoiding attaching packages (with the library() function) when possible. Their functions don't need to be qualified (e.g., dplyr::intersect()) and could cause naming conflicts. Even if you can guarantee they don't conflict with packages now, packages could add new functions in the future that do conflict.

4. **Declare Global Variables and Functions**. This includes defining the expected column names and types of the data sources; use readr::cols_only() (as opposed to readr::cols()) to ignore any new columns that may be been added since the dataset's last refresh.

```
# ---- declare-globals ------
```

5. Load Data Source(s) Read all data (e.g., database table, networked CSV, local lookup table). After this chunk, no new data should be introduced. This is for the sake of reducing human cognition load. Everything below this chunk is derived from these first four chunks.

6.2. ARCH 19

```
# ---- load-data ------
```

6. Tweak Data

```
# ---- tweak-data -----
```

- 7. Body of the Ellis
- 8. Verify

```
# --- verify-values -----
county_month_combo <- paste(ds$county_id, ds$month)
checkmate::assert_character(county_month_combo, pattern ="^\\d{1,2} \\d{2}-\\d{2}$", any.m:</pre>
```

9. **Specify Columns** Define the exact columns and order to upload to the database. Once you import a column into a warehouse that multiple people are using, it's tough to remove it.

```
# --- specify-columns-to-upload -----
```

10. Welcome into your warehouse. Until this chunk, nothing should be persisted.

```
# --- upload-to-db -------
# --- save-to-disk ------
```

- 6.2 Arch
- 6.3 Ferry
- 6.4 Scribe
- 6.5 Analysis
- 6.6 Presentation -Static
- 6.7 Presentation -Interactive
- 6.8 Metadata

Security & Private Data

- 7.1 File-level permissions
- 7.2 Database permissions
- 7.3 Public & Private Repositories

7.3.1 Scrubbing GitHub history

Occassionaly files may be committed to your git repository that need to be removed completely. Not just from the current collections of files (*i.e.*, the branch's head), but from the entire history of the repo.

Scrubbing is require typically when (a) a sensitive file has been accidentally committed and pushed to GitHub, or (b) a huge file has bloated your repository and disrupted productivity.

The two suitable scrubbing approaches both require the command line. The first is the git-filter-branch command within git, and the second is the BFG repo-cleaner. We use the second approach, which is [recommended by GitHub]; it requires 15 minutes to install and configure from scratch, but then is much easier to develop against, and executes much faster.

The bash-centric steps below remove any files from the repo history called 'monster-data.csv' from the 'bloated' repository.

- 1. If the file contains passwords, change them immediately.
- 2. Delete 'monster-data.csv' from your branch and push the commit to GitHub.
- 3. Ask your collaborators to push any outstanding commits to GitHub and delete their local copy of the repo. Once scrubbing is complete, they will re-clone it.
- 4. Download and install the most recent Java JRE from the Oracle site.
- 5. Download the most recent jar file from the BFG site to the home directory.
- 6. Clone a fresh copy of the repository in the user's home directory. The --mirror argument avoids downloading every file, and downloads only the bookkeeping details required for scrubbing.

```
cd ~
git clone --mirror https://github.com/your-org/bloated.git
```

7. Remove all files (in any directory) called 'monster-data.csv'.

```
java -jar bfg-*.jar --delete-files monster-data.csv bloated.git
```

8. Reflog and garbage collect the repo.

```
cd bloated.git
git reflog expire --expire=now --all && git gc --prune=now --aggressive
```

9. Push your local changes to the GitHub server.

```
git push
```

10. Delete the bfg jar from the home directory.

```
cd ~
rm bfg-*.jar
```

- 11. Ask your collaborators to reclone the repo to their local machine. It is important they restart with a fresh copy, so the once-scrubbed file is not reintroduced into the repo's history.
- 12. If the file contains sensitive information, like passwords or PHI, ask GitHub to refresh the cache so the file's history isn't accessible through their website, even if the repo is private.

7.3.1.0.1 Resources

- BFG Repo-Cleaner site
- Additional BFG instructions
- GitHub Sensitive Data Removal Policy

Automation

- 8.1 Flow File in R
- 8.2 Makefile
- 8.3 SSIS
- 8.4 cron Jobs & Task Scheduler
- 8.5 Sink Log Files

Scaling Up

9.1 Data Storage

- 1. Local File vs Conventional Database vs Redshift
- 2. Usage Cases

9.2 Data Processing

- $1. \ \mathrm{R} \ \mathrm{vs} \ \mathrm{SQL}$
- 2. R vs Spark

Parallel Collaboration

10.1 Social Contract

- 1. Issues
- 2. Organized Commits & Coherent Diffs
- 3. Branch & Merge Strategy

10.2 Code Reviews

- 1. Daily Reviews of PRs
- 2. Periodic Reviews of Files

10.3 Remote

1. Headset & sharing screens

10.4 Loose Notes

10.4.1 GitHub

- 1. Review your diffs before committing. Check for things like accidental deletions and debugging code that should be deleted (or at least commented out).
- 2. Keep chatter to a minimum, especially on projects with 3+ people being notified of every issue post.
- 3. When encountering a problem,
 - Take as much ownership as reasonable. Don't merely report there's an error.
 - If you can't figure it out, ask the question and describe it well.
 - what low-level file & line of code threw the error.
 - how you have tried to solve it.
 - If there's a questionable line/chunk of code, trace its origin. Not for the sake of pointing the finger at someone, but for the sake of understanding its origin and history.

10.4.2 Common Code

This involves code/files that multiple people use, like the REDCap arches.

- 1. Run the file before committing it. Run common downstream files too (e.g.), if you make a change to the arch, also run the funnel).
- 2. If an upstream variable name must change, alert people. Post a GitHub issue to announce it. Tell everyone, and search the repo (ctrl+shift+f in RStudio) to alert specific people who might be affected.

Documentation

- 11.1 Team-wide
- 11.2 Project-specific
- 11.3 Dataset Origin & Structure
- 11.4 Issues & Tasks
- 11.5 Flow Diagrams
- 11.6 Setting up new machine

(example)

Style Guide

Using a consistent style across your projects can increase the overhead as your data science team discusses options, decides on a good choice, and develops in compliant code. But like in most themes in this document, the cost is worth the effort. Unforced code errors are reduced when code is consistent, because mistake-prone styles are more apparent.

For the most part, our team follows the tidyverse style. Here are some additional conventions we attempt to follow.

12.1 ggplot2

The expressiveness of ggplot2 allows someone to quickly develop precise scientific graphics. One graph can be specified in many equivalent styles, which increases the opportunity for confusion. We formalized much of this style while writing a textbook for introductory statistics; the 200+ graphs and their code is publically available.

12.1.1 Order of commands

ggplot2 is essentially a collection of functions combined with the + operator. Publication graphs common require at least 20 functions, which means the functions can sometimes be redundant or step on each other toes. The family of functions should follow a consistent order ideally starting with the more important structural functions and ending with the cosmetic functions. Our preference is:

- 1. ggplot2() is the primary function to specify the default dataset and aesthetic mappings. Many arguments can be passed to aes(), and we prefer to follow an order consistent with the scale_*() order below.
- 2. geom_*() creates the *geometric* elements that reperesent the data. Unlike most categories in this list, the order matters. Geoms specified first are drawn first, and therefore can be obscured by subsequent geoms.
- 3. scale_*() describes how a dimension of data (specified in aes()) is translated into a visual element. We specify the dimensions in descending order of (typical) importance: x, y, group, color, fill, size, radius, alpha, shape, linetype.
- 4. coord *()
- 5. facet_*() and label_*()
- 6. theme()
- 7. labs()

12.1.2 Gotchas

Here are some common mistakes we see not-so-infrequently (even sometimes in our own code).

1. Call coord_*() to restrict the plotted x/y values, not scale_*() or lims()/xlim()/ylim(). coord_*() zooms in on the axes, so extreme values essentially fall off the page; in contrast, the latter three functions essentially remove the values from the dataset. The distinction does not matter for a simple bivariate scatterplot, but likely will mislead you and the viewer in two common scenarios. First, a call to geom_smooth() (e.g., that overlays a loess regression curve) ignore the extreme values entirely; consequently the summary location will be misplaced and its standard errors too tight. Second, when a line graph or spaghetti plots contains an extreme value, it is sometimes desirable to zoom in on the the primary area of activity; when calling coord_*(), the trend line will leave and return to the plotting panel (which implies points exist which do not fit the page), yet when calling the others, the trend line will appear interrupted, as if the extreme point is a missing value.

Publishing Results

- 13.1 To Other Analysts
- 13.2 To Researchers & Content Experts
- 13.3 To Technical-Phobic Audiences

Testing, Validation, & Defensive Programming

14.1 Testing Functions

14.2 Defensive Programming

1. Throwing errors

14.3 Validator

- 1. Benefits for Analysts
- 2. Benefits for Data Collectors

Troubleshooting and Debugging

15.1 Finding Help

- 1. Within your group (eg, Thomas and REDCap questions)
- 2. Within your university (eg, SCUG)
- 3. Outside (eg, Stack Overflow; GitHub issues)

15.2 Debugging

1. traceback(), browser(), etc

Establishing Workstation

https://github.com/OuhscBbmc/RedcapExamplesAndPatterns/blob/master/DocumentationGlobal/ResourcesInstallation.md

- 16.1 Required Installation
- 16.2 Recommended Installation
- 16.3 Optional Installation
- 16.4 Asset Locations

Considerations when Selecting Tools

17.1 General

17.1.1 The Component's Goal

While disussing the advantages and disadvanages of tools, a colleague once said, "Tidyverse packages don't do anything that I can't already do in Base R, and sometimes it even requires more lines of code". Regardless if I agree, I feel these two points are irrelevant. Sometimes the advantage of a tool isn't to expand existing capabilities, but rather to facilitate development and maintaince for the same capability.

Likewise, I care less about the line count, and more about the readability. I'd prefer to maintain a 20-line chunk that is familiar and readable than a 10-line chunk with dense phrases and unfamiliar functions. The bottleneck for most of our projects is human time, not execution time.

- 17.1.2 Current Skillset of Team
- 17.1.3 Desired Future Skillset of Team
- 17.1.4 Skillset of Audience
- 17.2 Languages
- 17.3 R Packages
- 17.4 Database

Growing a Team

18.1 Recruiting

18.2 Training to Data Science

- 1. Starting with a Researcher
- 2. Starting with a Statistician
- 3. Starting with a DBA
- 4. Starting with a Software Developer

18.3 Bridges Outside the Team

- 1. Monthly User Groups
- 2. Annual Conferences

Appendix A

Git & GitHub

Jenny Bryan and Jim Hester have published a thorough description of using Git from a data scientist's perspective, and we recommend following their guidance. It is consistent with our approach, with a few exceptions noted below. A complementary resource is *Team Geek*, which has insightful advice for the human and collaborative aspects of version control.

Appendix B

Presentations

Here is a collection of presentations by the BBMC and friends that may help demonstrate concepts discussed in the previous chapters.

B.1 CDW

- 1. prairie-outpost-public: Documentation and starter files for OUHSC's Clinical Data Warehouse.
- 2. OUHSC CDW

B.2 REDCap

- 1. REDCap Systems Integration. REDCap Con 2015, Portland, Oregon.
- 2. Literate Programming Patterns and Practices with REDCap REDCap Con 2014, Park City, Utah.
- 3. Interacting with the REDCap API using the REDCapR Package REDCap Con 2014, Park City, Utah.

B.3 GitHub

1. Scientific Collaboration with GitHub. OU Bioinformatics Breakfast Club 2015.

B.4 Architectures

- 1. Linear Pipeline of the R Analysis Skeleton
- 2. Many-to-many Pipeline of the R Analysis Skeleton
- 3. Immunization transfer

illinanization transic

Appendix C

Scratch Pad of Loose Ideas

C.1 Chapters & Sections to Form

- 1. Tools to Consider
 - 1. tidyverse
 - 2. odbc
- 2. ggplot2
 - 1. use factors for explanatory variables when you want to keep the order consistent across graphs. (?)
- 3. styles
 - 1. variable names: within a variable name order from big to small terms (lexigraphical scoping) (?)
- 4. public reports (and dashboards)
 - 1. when developing a report for a external audience (ie, people outside your immediate research team), choose one or two pals who are unfamilar with your aims/methods as an impromptu focus group. Ask them what things need to be redesigned/reframed/reformated/further-explained. (?)
 - 1. plots
 - 2. plot labels/axes
 - 3. variable names
 - 4. units of measurement (eg, proportion vs percentage on the y axis)

Appendix D

Introduction

You can label chapter and section titles using {#label} after them, e.g., we can reference Chapter D. If you do not manually label them, there will be automatic labels anyway, e.g., Chapter 2.

Figures and tables with captions will be placed in figure and table environments, respectively.

```
par(mar = c(4, 4, .1, .1))
plot(pressure, type = 'b', pch = 19)
```

Reference a figure by its code chunk label with the fig: prefix, e.g., see Figure D.1. Similarly, you can reference tables generated from knitr::kable(), e.g., see Table D.1.

```
knitr::kable(
  head(iris, 20), caption = 'Here is a nice table!',
  booktabs = TRUE
)
```

You can write citations, too. For example, we are using the **bookdown** package (Xie, 2018) in this sample book, which was built on top of R Markdown and **knitr** (Xie, 2015).

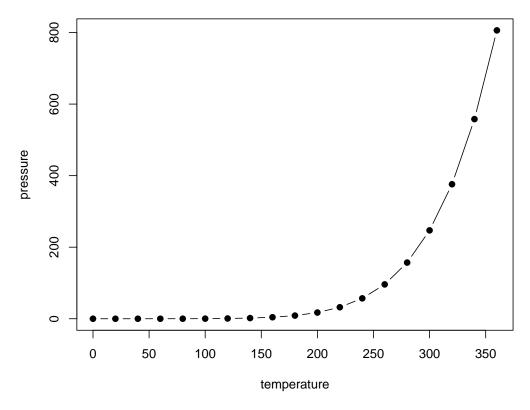


Figure D.1: Here is a nice figure!

Table D.1: Here is a nice table!				
Sepal.Length	Sepal.Width	Petal.Length	Petal.Width	Species
5.1	3.5	1.4	0.2	setosa
4.9	3.0	1.4	0.2	setosa
4.7	3.2	1.3	0.2	setosa
4.6	3.1	1.5	0.2	setosa
5.0	3.6	1.4	0.2	setosa
5.4	3.9	1.7	0.4	setosa
4.6	3.4	1.4	0.3	setosa
5.0	3.4	1.5	0.2	setosa
4.4	2.9	1.4	0.2	setosa
4.9	3.1	1.5	0.1	setosa
5.4	3.7	1.5	0.2	setosa
4.8	3.4	1.6	0.2	setosa
4.8	3.0	1.4	0.1	setosa
4.3	3.0	1.1	0.1	setosa
5.8	4.0	1.2	0.2	setosa
5.7	4.4	1.5	0.4	setosa
5.4	3.9	1.3	0.4	setosa
5.1	3.5	1.4	0.3	setosa
5.7	3.8	1.7	0.3	setosa
5.1	3.8	1.5	0.3	setosa

Bibliography

Xie, Y. (2015). Dynamic Documents with R and knitr. Chapman and Hall/CRC, Boca Raton, Florida, 2nd edition. ISBN 978-1498716963.

Xie, Y. (2018). bookdown: Authoring Books and Technical Documents with R Markdown. R package version 0.9.