This lecture is based on slides for a talk I’ve given a whole bunch of times.

Source: https://github.com/kbroman/Talk_ReproRes
These slides, with notes: https://bit.ly/steps2rr
Full slides without notes: https://bit.ly/steps2rr_nonotes

By “reproducible research,” I’m referring to “computational reproducibility,” by which I mean that the data and code for a project are packaged together in a way that they can be handed to someone else, who can rerun the code and get the same results—the same figures and tables. This is surprisingly hard to do, and it’s even more difficult in the context of a collaboration between two or more data analysts.
I'm an applied statistician; my goal is to help people make sense of their data. I have a lot of collaborators, and there's nothing I enjoy more than puzzling over their data. So I write a lot of reports, describing what I've done and what I've learned.

This is an email I got from a collaborator, in response to an analysis report that I had sent him. It's always a bit of a shock to get an email like this: what have I done? Why am I working with the wrong data, and where is the right data?

But what he didn’t know is that by this point in my life, I’d adopted a reproducible workflow. Because I’d set things up carefully, I could just substitute in the newer dataset, type a single command (“make”) to rerun the analyses, and get the revised report.

This is a reproducibility success story. We all make mistakes, but if our projects are reproducible, we can nimbly recover from those mistakes.

There is a second important lesson here: At the start of such reports, I always include a paragraph about our shared goals, along with some brief data summaries. By doing so, he immediately saw that I had an old version of the data. If I hadn’t done so, we might never have discovered my error.
The results in Table 1 don’t seem to correspond to those in Figure 2.

My computational life is not entirely rosy. This is the sort of email that will freak me out.
Where did we get this data file?

Record the provenance of all data or metadata files.
Why did I omit those samples?

I may decide to omit a few samples. Will I record why I omitted those particular samples?
Which image goes with which experiment?

For experimental biologists, it can be tricky to keep track of the vast set of images and experiments they perform.
How did I make that figure?

Sometimes, in the midst of a bout of exploratory data analysis, I’ll create some exciting graph and have a heck of a time reproducing it afterwards.
In what order do I run these scripts?

Sometimes the process of data file manipulation and data cleaning gets spread across a bunch of scripts that need to be executed in a particular order. Will I record this information? Is it obvious what script does what?
“Your script is now giving an error.”

It was working last week. Well, last month, at least.

How easy is it to go back through that script’s history to see when and why it stopped working?
“The attached is similar to the code we used.”

From an email in response to my request for code used for a paper.
Reproducible

vs.

Replicable

Computational work is reproducible if the data and code are organized in a way that they can be handed to someone else, who can rerun the code and get the same results—the same figures and tables. Replicable is more stringent: can someone repeat the experiment and get the same results?

Reproducibility is a minimal standard. That something is reproducible doesn’t imply that it is correct. The code may have bugs. The methods may be poorly behaved. There could be experimental artifacts.

(But reproducibility is probably associated with correctness.)

Note that some scientists say replicable for what I call reproducible, and vice versa.
It was a long, hard process for me to move from my old standard practice to a fully reproducible workflow. In thinking through that process, I wrote down my thoughts on the basic steps to take towards full reproducibility. This forms the basis of what I’ll present here.
A little bit reproducible
is better than not reproducible.

A little bit open
is better than not open.

Strive to make each project
a bit better organized than the last.

While it’s good to strive for full reproducibility, it can be difficult to achieve. But partially reproducible is better than not-at-all reproducible. Similarly, making data and code partially open is better than nothing.

Don’t try to change every aspect of your workflow all at once. Focus on revising one aspect at a time. When you get to the end of a project, you may be dissatisfied with the state of things, but don’t give up. Try to make each project a bit better organized and reproducible than the last.
Organize your project

Your closest collaborator is you six months ago, but you don’t reply to emails.

(paraphrasing Mark Holder)

The first thing to do is to make your project understandable to others (or yourself, later, when you try to figure out what it was that you did).
Segregate all the materials for a project in one directory/folder on your hard drive.

There will be a lot of files. Organize them in a meaningful way.

This is the way I organize a project directory. The key principles are to put everything related to a project in a common directory, but then to separate data from code and separate raw data from processed data.

Write *ReadMe* files to explain what’s what. Make sure they stay current.
This is a folder on my hard drive, for the project that led me to reassess my life.
Choose good names for things

You'll have a lot of files. In addition to organizing them in subfolders, it's important to choose good names for them.

These names of these files largely explain their contents, but they’re also left rather disorganized.
Choose good names for things

| fig1.png  | fig5.png |
| fig10.png | fig6.png |
| fig2.png  | fig7.png |
| fig3.png  | fig8.png |
| fig4.png  | fig9.png |

These names are well organized, but you have to remember the order of all of the figures to find the one you want.

And note that, alphabetically, figure 10 ends up between figure 1 and figure 2.
Choose good names for things

► Machine readable
  – No spaces
  – No special characters except _ and -

► Human readable
  – Explain the contents

► Consistent
  – Name similar files in a similar way

► Make use of computer’s sorting
  – pad numbers with 0’s (e.g., 01, 02, ...)
  – start with general grouping, then more specific
  – dates like 2019-05-14

You want the names to be easily to handle in software, which generally means no spaces or special characters except for underscore and hyphen (which are useful for separating words).

But you want the names to explain the files’ contents, so that you don’t have to open the files to figure out what they are.

Consistency is important: if you have a bunch of similar files, you should have some system for naming them.

And make use of the computer’s sort of files, by padding numbers with 0’s (so that 10 appears after 9 rather than before 2) and organizing the files into groups.

Dates should always be written as ‘YYYY-MM-DD’, so that when sorted they are in order by date.
Go with the xkcd format for writing dates, for ease of sorting.
Choose good names for things

Here’s an example to take advantage of the way the computer sorts files: a set of R scripts, which show up in the order they are used.
No “final” in file names

Never include “final” in a file name.
No “final” in file names

This is an actual directory on my computer. If you include final in a file name, there’s a risk that you’ll end up with final_rev, final_rev2, and final_old.

Another problem here is that the files aren’t organized very well.
Choose good names for things

This is the same set of files, renamed. Using clinical and geneexpr brings similar files together.

A lot of files, but less forbidding.
Document your work

▶ What is all of this stuff?
▶ What was your analysis process?

→ ReadMe files

An overall ReadMe file plus an additional such file in each directory.

Well-named files and directories makes everything easier.

Also, keep the documentation current. There’s nothing worse than documentation that is out of date and doesn’t match the contents.
How you organize your data within files can have a big impact on how easy they are to work with.

You can probably figure out what the numbers mean here, particularly if I tell you that there were triplicate measurements under two treatments (1 min or 5 min) of cells that were either normal or mutant and came from mouse strains B6 or BTBR.

But it’s hard to tell a computer program about the data structure here.
Organizing data in spreadsheets

<table>
<thead>
<tr>
<th></th>
<th>A</th>
<th>B</th>
<th>C</th>
<th>D</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>ttt_min</td>
<td></td>
<td>strain</td>
<td>response</td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>B6</td>
<td>normal</td>
<td>146.6</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>B6</td>
<td>normal</td>
<td>138.6</td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>B6</td>
<td>normal</td>
<td>155.6</td>
</tr>
<tr>
<td>5</td>
<td>1</td>
<td>B6</td>
<td>mutant</td>
<td>166</td>
</tr>
<tr>
<td>6</td>
<td>1</td>
<td>B6</td>
<td>mutant</td>
<td>179.3</td>
</tr>
<tr>
<td>7</td>
<td>1</td>
<td>B6</td>
<td>mutant</td>
<td>186.9</td>
</tr>
<tr>
<td>8</td>
<td>1</td>
<td>BTBR</td>
<td>normal</td>
<td>245.7</td>
</tr>
<tr>
<td>9</td>
<td>1</td>
<td>BTBR</td>
<td>normal</td>
<td>240</td>
</tr>
<tr>
<td>10</td>
<td>1</td>
<td>BTBR</td>
<td>normal</td>
<td>243.1</td>
</tr>
<tr>
<td>11</td>
<td>1</td>
<td>BTBR</td>
<td>mutant</td>
<td>177.8</td>
</tr>
<tr>
<td>12</td>
<td>1</td>
<td>BTBR</td>
<td>mutant</td>
<td>171.6</td>
</tr>
<tr>
<td>13</td>
<td>1</td>
<td>BTBR</td>
<td>mutant</td>
<td>188.1</td>
</tr>
<tr>
<td>14</td>
<td>5</td>
<td>B6</td>
<td>normal</td>
<td>333.6</td>
</tr>
<tr>
<td>15</td>
<td>5</td>
<td>B6</td>
<td>normal</td>
<td>353.6</td>
</tr>
</tbody>
</table>

This is the first few rows of a reorganized version of the data, as a rectangle where the rows are individual measurements and the columns are variables.

This is maybe less pretty, but it’s much easier to work with.
Here are some key principles for organizing data in spreadsheets: make a rectangle with a single header row.

Never do calculations in your raw data file. If you’re doing analyses or making charts in Excel, do so in a copy of the data file. Every time you open the raw data file, there’s a risk that you’ll mess things up.
“What the heck is ‘FAD_NAD SI 8.3_3.3G’?”

Sometimes the columns in your data files have meaning only to you.

If the data analyst can’t connect to the measurements, they’re just columns of numbers.
Clear metadata is critical for others to be able to understand your data. In particular, make a data dictionary that describes the variables. In addition to a description of each column, I like to have short and longer versions of the names for use in data visualizations, as the column names themselves can be cryptic.

These metadata are data, and so rather than make a Word document describing the data, I personally would prefer to have another data file with the metadata.
Here’s an example data dictionary. You might also include units and information about possible valid values.
The most basic principle for reproducible research is: do everything via code.

Downloading data from the web, converting an Excel file to CSV, renaming columns/variables, omitting bad samples or data points...do all of this with scripts.

You may be tempted to open up a data file and hand-edit. But if you get a revised version of that file, you’ll need to do it again. And it’ll be harder to figure out what it was that you did.

Some things are more cumbersome via code, but in the long run you’ll save time.
I love R Markdown for making reproducible reports that document the full details of my analysis. R Markdown mixes Markdown (for light-weight markup of text) and R code chunks; when processed with knitr, the R code is executed and results inserted into the final document.

With these informal reports, I seek to fully capture the entirety of my data explorations and decisions.

Python people should look at Jupyter notebooks.
Automate the process (GNU Make)

GNU Make is an old (and rather quirky) tool for automating the process of building computer programs. But it’s useful much more broadly, and I find it valuable for automating the full process of data file manipulation, data cleaning, and analysis.

In addition to automating a complex process, it also documents the process, including the dependencies among data files and scripts.
Another important step towards reproducibility is to revise your code to make it more clear.

The single most important step towards clear code is to pull out complex or repeated code as a separate function. This makes your code easier to read and maintain.

Next, combine those functions together into a package or module. It’s surprisingly easy to create an R package (see https://kbroman.org/pkg_primer) and it’s even easier to make a Python module.

When writing functions, try to write them in a somewhat-general way and then pull them out of the project as separate package or module, so that you (and/or others) may reuse them for other purposes.
We all struggle to keep track of versions of things.

Shared drives (like google drive, dropbox, and box) often keep track of past versions, but usually there’s a time limit (like 30 days or a year).

You can make copies of file with a version number appended to the name. You might zip up a directory and include the date in the zipped file.

Formal version control has a number of advantages, including easy of browsing the history or jumping to a particular time point. The ability to merge simultaneous changes from multiple users is a key advantage.

git can be hard to learn; it’s designed for pretty hard-core programmers. But there are growing learning resources, and the long-term payoff is considerable. For collaborative projects, the payoff is immediate.
git has a steep learning curve, but ultimately I think you’ll find it really helpful.

The big selling point is in collaboration: merging changes from collaborators, and keep your work synchronized.

Longer term, there’s great value in having the entire history of changes to your project. If something stops working, you can go back to any point in that history to see when it stopped working and why.

With git, you can also work on new features or analyses without fear of breaking the parts that are currently working well.
Backups

- Multiple places, including off-site
- Automatic

I can’t emphasize enough the importance of backups. And you must have a copy off-site. And if it’s not automatic, it won’t happen.
License your software

Pick a license, any license

– Jeff Atwood

If you don’t pick a license for your software, no one else can use it.

So if you want to distribute your code so that others can reproduce your analyses, you need to pick a license, any license.

I choose between the MIT license and the GPL.

Don’t use the Creative Commons licenses for code. But feel free to use them for other things.
A reproducible workflow is valuable even if you don’t intend to share your work with others.

But if do want to share, it’s best to place things at a third-party site. Ideally one that can be trusted as an archive and that provides DOIs.

Place code at GitHub (or the similar site, BitBucket). The only problem is that it can’t necessarily be trusted to still be there 5 years from now. There’s an easy way to have “releases” archived at zenodo.org automatically, with a DOI. So I recommend that.

For data, it’s probably best to use a domain-specific repository, if there is an appropriate one. Otherwise, general repositories github, figshare, zenodo, or datadryad. Again, github is not ideal because it’s not archival and doesn’t give DOIs.
Summary

1. Organize your project
2. Choose good names for things
3. Document what’s what
4. Organize data as a rectangle
5. Metadata is data
6. Everything with a script
7. Even better: reproducible reports
8. Automate the process (GNU Make)
9. Write modular code (functions and packages)
10. Use version control (git/GitHub)
11. License your software
12. Share your data and code

Summaries are always good.

Again, don’t try to change everything at once. Reproducibility can be surprisingly hard and requires a daily commitment. And here I’m just thinking about a project with a single data analyst. A collaboration with multiple analysts is yet harder.
Other considerations

- **Testing**
  
  are you getting the right answers?

- **Software versions**
  
  will your stuff work when dependencies change?

- **Large-scale computations**
  
  computation time + dependence on cluster environment

- **Collaborations**
  
  coordinating who does what and where things live

I’ve focused on issues for small-scale, single-investigator projects, and even with that limited scope, I’ve not covered everything.
Collaboration has a lot of advantages, including for reproducibility efforts.

It can be useful to have a pair of people regularly review each other’s code, but it can be hard to get your busy friends to pay attention to your little project. But if you are working together on a project, you can more naturally build in some code review.

Moreover, you can explicitly test the reproducibility of your analyses, by having your collaborator rerun your work, and vice versa.
Collaboration also has challenges.

Do you have a shared vision for the reproducibility of the project? You’ll no doubt need to make some compromises about how things are done: you can’t both just do things the way you’ve always done them. Careful coordination and regular communication are key.

And then there are the technical challenges of how to share the code and data and make sure your two working projects remain in sync.

In a sense, the reproducibility of a collaborative project is dependent on the weakest link. If one collaborator refuses to fully participate and share their work, the chain is broken.
Challenges

(totally hypothetical)

A collaboration like this will pose many challenges. The following are totally hypothetical. Really.
“Could we meet to talk about the data file structure?”

“No.”

Say the first of many sets of data are set up in a way that is complicated to handle, both in data entry and for analysis. Will your collaborator work with you to refine things? Or will every new data file require a day of work, so that it can be combined with prior data?
It can be hard to keep in sync across groups in a multi-site project. If a problem is discovered and some aspect of data preprocessing needs to be redone, will this get communicated to all analysis teams, so that relevant analyses get rerun as needed?
“Could you write the methods section?”

“But I didn’t do the work, and we don’t have the code that was used.”

Are all teams sharing their work with each other?
“My data analyst has taken a job at Google.”

What happens if a key data analyst leaves the project?
“Could you do these analyses? X said they would, but they’re not responding to my emails.”

Everyone has multiple things going on, and sometimes there is need for rush analyses, say for a grant submission or conference presentation. Is there a shared understanding of who will do what when, and how emergencies can be handled?

The organization of a project often depends on the worst day you spent on it. If you need to do a bunch of stuff last-minute, will you leave the project directory in a mess, or will you clean up after yourself?
Critical for a successful collaboration is that the collaborators have a shared vision for the project. We often maybe think about being in agreement on the approach to publication and co-authorship. But perhaps more difficult is coming to an agreement on data and code sharing (what, where, and when?), on who will do what, on how soon it will be done, and on the ongoing sharing, among collaborators, of detailed methods and results.
Also important is the technology or engineering of sharing. Can the collaborators agree on the project structure, data and metadata formats, and the software environment?

Some groups may use R and some python. This should not pose a problem.

A key issue is how to keep the multiple groups’ work in sync. It is best that this can be done automatically. Experience demonstrates that if synchronization approach requires some manual steps, they will not be done consistently.
Technology for sharing

- **Data**
  - figshare
  - dropbox / box / google drive

- **Code**
  - github / bitbucket

- **Pipeline / workflow**
  - make / drake / snakemake / rake

- **Full environment**
  - docker containers
  - mybinder.org / wholetale.org

I must admit to not being totally confident about what advice to give, regarding the tools to use for sharing data and code among collaborators.

For sharing data, simple options include posting large files on a data repository like figshare, or using cloud drive like dropbox, box, or google drive.

For sharing code, I prefer to use a version control system like git, with github, bitbucket, or a locally-managed equivalent.

For sharing the analysis pipeline or workflow, one can incorporate a system like make (or drake, snakemake, or rake) with the code.

The full software environment could be replicated across teams using docker containers. Binder and Whole Tale are two systems for making this easier.
The most important tool is the mindset, when starting, that the end product will be reproducible.

– Keith Baggerly

So true. Desire for reproducibility is step one.
The second-most important tool is training.

– me

I’ve long felt that the key need, in getting computational scientists to adopt a reproducible workflow, is training. For the most part, all of the software tools are available, but many people haven’t incorporated them into their daily work.
Here’s where you can find me, as well as the slides for this talk.