How can we teaching coding to scientists

Matthew Brett

March 15, 2018

Plan of the talk

- why should we teach scientists to code?
- what should we teach them?
- how should we teach them?
- ▶ how can I help?

Why should we teach scientists to code

- ▶ Algorithms are at the heart of science. All scientists need to use and understand algorithms;
- Many branches of science use extensive computation.

Is it reasonable to teach scientists about algorithms?

- understand what algorithms are, how they are implemented as programs on digital devices, and that programs execute by following precise and unambiguous instructions;
- create and debug simple programs;
- use logical reasoning to predict the behaviour of simple programs
- use technology purposefully to create, organise, store, manipulate and retrieve digital content

Does anyone recognize this?

Understanding algorithms

- understand what algorithms are, how they are implemented as programs on digital devices, and that programs execute by following precise and unambiguous instructions;
- create and debug simple programs;
- use logical reasoning to predict the behaviour of simple programs
- use technology purposefully to create, organise, store, manipulate and retrieve digital content

National curriculum key stage 1: ages 5 to 7.

Algorithms for data analysis

It's very common to have the following situation:

- we have some somewhat messy data;
- we have some hypothesis about these data we would like to test;
- the hypothesis can often be formulated as a model.

The combination is - data science, and statistics.

Teaching data science, and all of statistics

Loading data, reviewing data, plotting data:

- Course page at https://matthew-brett.github.io/les-pilot;
- Our notebooks at https: //notebooks.azure.com/matthewbrett/libraries/dev-ac-uk

With thanks and a recommendation for:

- Statistics without the agonizing pain:
- https://www.youtube.com/watch?v=5Dnw46eC-0o

Setup for the demo - running on Azure

- Go to https: //notebooks.azure.com/matthewbrett/libraries/dev-ac-uk;
- ► Clone that site (you'll need a free Microsoft login), and click on the getting_started notebook.

Setup of the demo - running on your laptop

You can also run this on your own machine if you have Python and pip set up:

```
# If you have Anaconda, you will already have these
pip install pandas
pip install jupyter[notebook]
```

Download https://github.com/matthew-brett/dev.ac.uk (via 'Clone or Download' -> 'Download zip').

cd directory_containing_download
unzip dev.ac.uk-master.zip
cd dev.ac.uk-master
jupyter notebook

Code for everyone

We have seen code as a way of:

- expressing operations on data;
- doing (and explaining) statistical inference.

Superficially, this is a course for scientists. But all academic fields are now analyzing data, as are the media. So, how should we teach?

Berkeley Fundamentals of Data Science course

- ▶ All subjects (arts, sciences . . .).
- Written as interactive Jupyter Notebooks.
- ► Textbook at https://www.inferentialthinking.com

Back to the demo

- https://notebooks.azure.com/matthewbrett/libraries/dev-acuk
- Plotting the classics.ipynb.
- ► Literary characters.ipynb.

See the README for the site for the license of these files.

The Berkeley course is substantial

See:

https://www.inferential thinking.com/chapters/16/classification.html

Beyond the basics

- Many academic fields need a lot of computation.
- Computation is often done in a very sloppy and disorganized way.
- It's easy to make errors.
- People usually don't share their analyses.

Easy to make errors in computation

In my own experience, error is ubiquitous in scientific computing, and one needs to work very diligently and energetically to eliminate it. One needs a very clear idea of what has been done in order to know where to look for likely sources of error. I often cannot really be sure what a student or colleague has done from his/her own presentation, and in fact often his/her description does not agree with my own understanding of what has been done, once I look carefully at the scripts.

David L. Donoho (2010) "An invitation to reproducible computational research" *Biostatistics* 11(3) 385

A culture of error

Scientists at Amgen (a drug company) tried to reproduce findings from 53 "landmark" studies.

... when findings could not be reproduced, an attempt was made to contact the original authors, discuss the discrepant findings, exchange reagents and repeat experiments under the authors' direction, occasionally even in the laboratory of the original investigator.

Of 53 studies, only 6 replicated (11%).

Glenn Begley and Lee Ellis (2012) "Raise standards for preclinical cancer research" Nature 483

Improving process

In studies for which findings could be reproduced, authors had paid close attention to controls, reagents, investigator bias and describing the complete data set. For results that could not be reproduced, however, data were not routinely analysed by investigators blinded to the experimental versus control groups. Investigators frequently presented the results of one experiment, such as a single Western-blot analysis. They sometimes said they presented specific experiments that supported their underlying hypothesis, but that were not reflective of the entire data set.

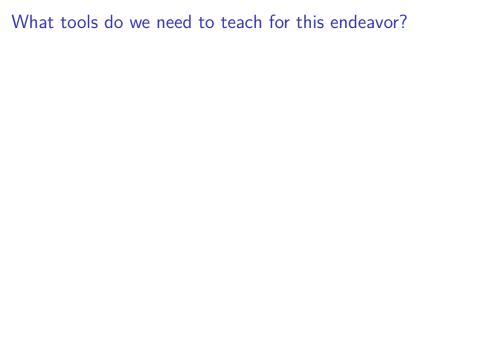
Begley and Ellis (2012).

Sharing analyses

An article about computational science in a scientific publication is **not** the scholarship itself, it is merely **advertising** of the scholarship. The actual scholarship is the complete software development environment and the complete set of instructions which generated the figures.

Jonathan B. Buckheit and David L. Donoho (1995) "Wavelab and reproducible research"

 $http://statweb.stanford.edu/{\sim}wavelab/Wavelab_850/wavelab.pdf$



What tools do we need to teach for this endeavor?

- Unix command line;
- Text editor for everything (including presentations);
- Git for version control;
- A scientific programming language such as Python or R;
- Unit testing, code coverage, continuous integration;
- make / Makefiles;

Can it be taught?

- http://www.jarrodmillman.com/rcsds
- https://github.com/berkeley-stat159

How can I help?

- It's a culture; spread the culture;
- Advocate for open source, serious computing;
- Organize meetups, interest groups, talks;
- Find like-minded lecturers to support you, and for you to support.
- Consider forming or joining a Hacker Within group: http://www.thehackerwithin.org.
- Your message here.

Is this the end?

Yes, it's the end of the talk.