Winter School on Reproducible Research

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Last week from Sunday to Friday I was at Dr. Holms hotel (Geilo, Norway), organizing a winter school on reproducible research. The winter school topic was identified by Knut-Andreas Lie, and is a timely and important topic in computational science.

One of the key elements of the scientific method is that scientific findings should be possible to reproduce by others. After all, if it is not possible for others to reproduce the result, how can we have faith that it is not simply pseudo-science?

Most of research today requires the use of computers in some way or another: whether it is to create graphs in Excel from measurements, writing special software for simulation, or simple data processing in Matlab. Unfortunately, it seems that in a large part (most?) of the computational sciences, the aspect of reproducibility has somewhat lost its position and esteem.

To give one example: I believe that there is a lot of non-reproducible research as a paper deadline approaches. A typical workflow to create a graph in such circumstances can be to experiment with a large number of parameters and settings until just the right plot is created. Unfortunately, these parameters and settings are too often forgotten once the paper has been submitted, and the graph is virtually impossible to reproduce, even for its author.

The example above is one of personal reproducibility, and I believe all researchers must be able to reproduce their own findings and conclusions. But there is also the aspect of public reproducibility, in which a published result should be possible for other researchers to reproduce and build upon.

The aim for the winter school was therefore to teach philosophy, workflows, and tools for working reproducibly both personally and publicly. We had four lecturers (including myself), an roughly fourty participants. We started on Sunday evening, and had over thirteen double lectures over the full week.

Fernando Perez gave an excellent introduction to version control (specifically git and github), including hands-on sessions. He also demonstrated IPython, an interactive shell for running python. I was really impressed by the IPython notebook as a tool for working reproducibly (a really cool demo can be seen on http://nbviewer.ipython.org/).

Johan Seland gave an overview of testing and how it fits with the scientific work flow. We had a hands-on session in which we implemented the rules of bowling using test driven development, and we were also given an overview of licensing, intellectual property rights, and how to use the Amazon cloud for reproducible research. I believe all scientific project should have at least a set of simple regression tests to help in development: if the output changes, but you did not mean to, something's wrong.

Rasmus Benestad covered verification and validation, and the concept of agnotology. Verification and validation essentially amounts to checking that we are solving things correctly, and that what we are solving is relevant to the problem. In climate science and meteorology, these are extremely difficult questions to answer.

Finally, I gave some lectures to give an overview of reproducible research, the limits of reproducible research, and to cover some advanced topics (such as floating point and parallel computing).

The full slides and code used during the winter school is available on the winter school webpages,http://www.sintef.no/Projectweb/eVITA/Winter-Schools/2013/Program/.

Further resources:

- ICERM Workshop December 2012, Wiki with supplementary material
- AMP 2011 Workshop