Reproducibility of mathematical data: practical 6 (Alex Elzenaar, 2/8/22)

Important Warning

We are going to look at real MathRepo pages that were written by people that you know. We have tried to choose examples that are overall good examples of the kinds of things you should try to produce, but that might have one or two flaws. Please be nice and stay constructive in any criticism you come up with.

Have a look at the MathRepo page: https://mathrepo.mis.mpg.de/compday/index.html Don't worry about the mathematics, we are just interested in the practical aspects of reproducibility. It is not important for you to get through everything here unless you find you have a lot of time, it is only important to us that you end up answering the following questions:

- 1. List three things that are good practice which this page does.
- 2. List three things you would change or improve.
- 3. Do you think that there were any particular challenges faced by the authors of this page when they made it?

1 Work out what results you want to reproduce, and find them.

This one is a bit different, since it isn't related to a paper. Think about alternative ways of giving context:- is it clear who the audience for the page is? There are a few subpages, is it clear what they are supposed to contain and how they relate to each other? What kinds of things do you think should be added to the front page?

We will take a look at some of the problems, namely 1, 6, 7, 16, and 19. Check that all of the problems we just listed contain enough information to reproduce what the author did. (That is, they should contain at the very least the problem statement, and some information about how the author solved the problem.)

Get the tools that the authors used. 2

Let us now restrict to problem 16, which uses Mathematica. Can you tell which Mathematica version the authors used? What about the computer operating system which they were running on?

In any case, at this point try to spin up a copy of Mathematica. Here is how to do it from a terminal if you are on a UNIX-like computer (including MacOS X) connected to the MPI network:

```
ssh -Y [your mpi username]@hydra.mis.mpg.de
ssh -Y compsrv
module load mathematica
mathematica
```

3 Modify the tools so that they are in a form which we can actually use.

4 Actually reproducing the results.

Essentially these final steps boil down to trying to reproduce the output given in the subpage, so we want to try to copy and paste each section separately. If you get any errors, try to work out whether it is a typo or error in the code, or perhaps a missing file that you need to put somewhere. If you want help moving a file onto the compute server, please ask for help.

Now, suppose you have managed to run the code without errors. Do the authors give enough information to check that the output is correct (for instance, example output)? Is the format of the information given useful? Could it be improved?