CMEE Masters: Miniproject Assessment February 14, 2022

Assignment Objectives: To address on a model-fitting problem using computational methods, and produce a written report, all in a coherent, reproducible, modular workflow under version control.

Student's Name: Natasha Ramsden

Overall Miniproject Mark: 92.5%

Overall Project Organization

All directories in place, no clutter.

You have included a comprehensive readme file describing the project, giving clear instructions how to run it, listing languages used (with version numbers) and required packages (with useage descriptions for each), summarising the repo structure and listing key files along with descriptions of each. This is all in keeping with best practise and simplifies the job of getting to grips with the project for a new user.

You could have put the writeup LATEX source files and pdf in a separate directory – this is what you should aim to do for your final dissertation.

Overall a clean and well organised project with thorough documentation. Very good!

The Code

Your choice of coding tools is generally appropriate - having a preferred language is OK. Be open to using Python for computationally intensive work though. You used a minimum of packages in your R which is good - too many packages stunt your development as a programmer and are bad for reproducibility.

Your code is sensibly commented, giving a good at-a-glance sense of what is going on at a given location within your scripts. You could remove blocks of commented code that you have decided not to use in the final workflow, to avoid building up blocks of commented-out code that do not contribute anything to the workflow itself (e.g. ModelFit.R L201-204, L231-234). Your workflow is very nicely subdivided into specific tasks, with relevant functions collected in dedicated scripts and imported into execution scripts to be called as needed. Nice software architecture! Similar approaches will stand you in good stead even with other languages like Python.

Your master script ran with no errors, well done!. Nice touch to redirect script stdout/stderr to log files, though be aware that this means that fatal errors are likely to end the execution of your workflow without any indication on the terminal that this has happened. Not much you can do about this, just have to be conscious of it (and maybe explicitly notify users about the log files!). You successfully fit 5 models (quadratic, cubic, logistic, Baryani and Gompertz) to your data, and compare them using a number of metrics.

Recall that you should write into your workflow commands that will delete all existing output files every time the workflow is run (they should be re-generated afresh).

Your master script printed progress updates to the terminal. This helps the user know what is going at a finer level, and helps troubleshoot should they need to. On account of other terminal output from within your sub-scripts being redirected to logs, the progress updates are not crowded out by other text. Nicely done.

Your project ran in reasonable time (5.5 min), with most of the time spent in model fitting and random sampling of initial parameters. Consider profiling here to see if any straightforward time savings can be found, though it is not a major concern overall.

Overall an excellent project. Cleanly organised, with very adept code structure/architecture, well commented and error-free! Impressive all around.

Marks for the project and computational workflow: 95%

The Report

A well written report with a tight abstract and intro section, commendable attention to details in the methods and analysis, and a mature, thorough and well-reasoned discussion. Extremely strong work.

Title: Concise, specific, outlines key finding.

Abstract: Excellent aside from a rather generic opening sentence. Model objectives and methods clearly stated, and results and conclusions succinctly summarised. (85%)

Intro: Short and sweet. Background expanded nicely with reference to literature. Bacterial growth phases succinctly described and clearly related to mechanistic and phenomenological model classes. This done, study aims are clearly stated, though it would have been nice to briefly name the method by which models were to be compared. (80%)

Methods: All essential elements present. Commendably careful filtering and treatment of the data. Models clearly defined. Model fitting and comparison clearly described, though would have been nice to see the equations for the model comparison metrics. Commendable attention to detail in ensuring that residuals of log and non-log data were correctly transformed before comparison. Extra credit for fitting 5 models, implementing random sampling of initial parameters and going being just AIC for model comparison. Computing tools section present. (95%)

Results: Major results reported with clarity and reference to well constructed plots involving the different model comparison metrics. Nice work performing analyses based on both log and non-log space! Figure and Table text legibly sized, which is nice. (95%)

Discussion: Study goals and key findings summarised. Discussion of mechanistic vs phenomenological model performance in both log and non-log space, with adroit interpretation of the implications of differences between the two, and attention paid to underlying differences between the models/classes of model. Findings are contextualised and discussed with reference to the wider literature. Caveats are explored and improvements suggested. The study concludes with a restatement of the central finding and some final take-away messages. (100%)

(Some specific feedback is in the attached pdf, and we can also discuss more aspects of your write-up in our 1:1 feedback meeting)

Marks for the Report: 90%

Signed: Samraat Pawar & Alexander Kier Christensen

February 14, 2022

Notes on Assessment:

- This written feedback will be discussed in a 1:1 session scheduled after this assessment has been given to you.
- The coursework marking criteria (included in this feedback at bottom) were used for both the computing and report components of the Miniproject Assessment. *In contrast*, Your final dissertation project marks are going to be based pretty much exclusively on the written report and viva (not code). Expect your final dissertation report to be marked more stringently, using the dissertation marking criteria (also included in this report).
- In the written feedback, the markers may have contrasted what you have done with what you should do in your actual dissertation. This does not mean that you were penalized—one of the main goals of the miniproject is to provide feedback useful for your main dissertation. However, there may be cases where what you have done is just really bad practise (for example missing line numbers or abstract), irrespective of whether it is a mini- or main- project report you will be penalized in that case.
- The markers for this assessment are playing the role of somebody trying to understand and use your project organization and workflow from scratch. So it will seem like the feedback is particularly pedantic in places please take it in the right spirit!