Name and Affiliation:

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Title:

Reproducible research in computational sciences: A use case for uncertainty quantification using Jupyter notebooks

Abstract:

Reproducible research is gaining attention as a crucial aspect of open science in recent years, emphasizing the core idea that the results of research should be reproducible and replicable by everyone given the original dataset, code, and software. This becomes even more important in computational sciences, where researchers can claim a wide range of different output without providing enough details for reproducibility. In this field, the need for reproducible research comes from a common belief that “never believe anything unless you can run it”.

Making computational research partially or fully transparent will increase its outreach. One way to achieve this is making the developed tools and models available as open-source codes, but meanwhile, as a better approach, the building blocks of the research can be published in a reproducible manner. Doing this helps other researchers to know the techniques used internally in research projects. One of the best approaches in this regard for scientific computing and data science research projects is taking advantage of Jupyter environments, in which researchers can provide a full representation of their work being enriched by extra descriptions. Additionally, the interactive nature of Jupyter notebooks makes it easy to convert the reproducible research works into valuable educational materials.

In this presentation, an example use case shows how Jupyter notebooks facilitate the process of model calibration and parameter estimation, which is an inevitable aspect of computational modeling projects, especially the ones dealing with the phenomena in life and natural sciences (like the models we develop in our research lab on tissue engineering processes, such as neotissue growth, engineered organs, and biodegradable implants). Jupyter increases the transparency of the whole process, especially for the people who are not deeply into the field, and at the same time, makes it easier to fine-tune the output to obtain more accurate results. The example use case is a practical implementation of a parameter estimation process, which can be easily adapted and modified for any specific application. We will have a look at how Jupyter provides a unified environment for understanding, building, running, post-processing, and optimizing such a process. A proof-of-concept implementation can be found at https://nbviewer.jupyter.org/github/mbarzegary/educational-bayesian/blob/master/src/CrashCourseOnParameterEstimation.ipynb.

Bio:

Mojtaba Barzegari is a PhD researcher at KU Leuven in the field of computational biomedical engineering. His research is mainly focused on developing mathematical models and high-performance numerical simulations of tissue engineering systems. He uses solely open-source packages and frameworks in his research, and beside technical advantages, this enables him to contribute more efficiently in open science communities. He also shares his work via reproducible science disciplines (https://mbarzegary.github.io), one important part of which is a collection of Jupyter notebooks with Python and C++ kernels.

Contribution format: 300 seconds presentation