

Mojtaba Barzegari, Liesbet Geris

Title:

Jupyter for uncertainty quantification and parameter estimation of computational models

Brief summary:

This short talk will explore how Jupyter notebooks facilitate the process of parameter estimation, an inevitable part of many mathematical modeling and computational projects. 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.

Outline:

Parameter estimation and uncertainty quantification are inevitable aspects of computational modeling projects, especially the ones that deal with ordinary differential equations (ODE) or partial differential equation (PDE) models. For real-world applications, these equations contain some coefficients that cannot be obtained directly from published scientific materials or experimental studies. In parameter estimation, we calibrate our model to act similar to available experimental data, and then, this calibrated model can be used to simulate other scenarios that haven't been tested yet in the experiments. Similarly, uncertainty quantification deals with controlling the sensitivity of the model to the value of these parameters.

Despite its simplicity, building a parameter estimation or uncertainty quantification is difficult-to-understand and difficult-to-implement for researchers in relevant fields. The problem is although it is relatively simple to describe the process visually, implementing it for a practical application becomes challenging in its early stages.

In this talk, we will have a look at how Jupyter provides a unified environment for understanding, building, running, post-processing, and optimizing such a process by providing a practical implementation of a parameter estimation process using a Bayesian optimization approach. The example can be found at <https://github.com/mbarzegary/educational-bayesian/blob/master/HowToConstructInverseProblems.ipynb>.

Affiliation:

Biomechanics Section, Department of Mechanical Engineering, KU Leuven, Leuven, Belgium