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FitBenchmarking: a tool for comparing numerical optimization algorithms

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Science often uses mathematics to represent physical process and behaviour. Hence, it is important to know the values of the parameters used within these models. For example, a parameter may relate to the internal magnetic field of a material. Nonlinear least squares fitting is the most common way of determining these parameters, providing both the values and errors, and is an important part of the scientific workflow across the National Facilities. FitBenchmarking (https://fitbenchmarking.github.io/) is an open-source Python package which takes data and models from real world applications and data analysis packages. It fits the model parameters to the data by casting this as a nonlinear least-squares problem, producing several tables and reports as outputs that allow users to compare different optimization algorithms across metrics like runtime, accuracy, and energy usage. This poster will introduce FitBenchmarking and highlight some of our recently added features.

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