FitBenchmarking

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Summary

FitBenchmarking is a tool that compares multiple different software packages for non-linear least squares fitting on several problem sets. This project was originally written to benchmark Mantid minimizers (Arnold et al. 2014) for neutron and muon scattering data sets. However, fitting a mathematical model to data is a fundamental task across all scientific disciplines. (At least) three groups of people have an interest in fitting software:

- Scientists, who want to know what is the best algorithm for fitting their model to data they might encounter, on their specific hardware;
- Scientific software developers, who want to know what is the state-of-the-art in fitting algorithms and implementations, what they should recommend as their default solver, and if they should implement a new method in their software; and
- Mathematicians and numerical software developers, who want to understand the types of problems on which current algorithms do not perform well, and to have a route to expose newly developed methods to users.

Representatives of each of these communities have got together to build FitBenchmarking. We hope this tool will help foster fruitful interactions and collaborations across the disciplines.

Statement of need

FitBenchmarking takes data and models from real world applications and data analysis packages, such as Mantid (Arnold et al. 2014), SasView (???) and CUTEst (Gould, Orban, and Toint 2015). It fits the data to the models by casting them as a nonlinear least-squares problem. We fit the data using a range of data fitting and nonlinear optimization software, and present comparisons through a variety of different metrics.

Given data (the crosses in Figure 2) and a model, we find the best parameters for the model by solving a least-squares problem. From Figure 2, it is clear that

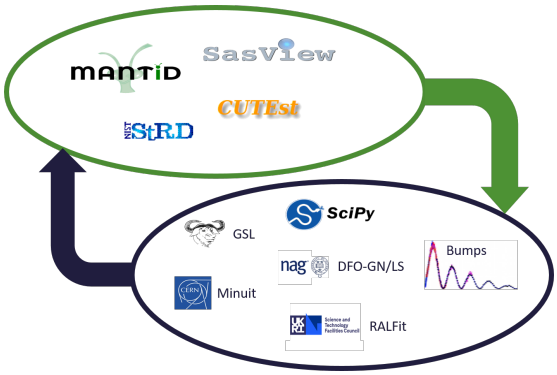

Figure 1: Concept

the solution given by lmsder is better. As the volume of data increases, and we do more and more data analysis algorithmically, it is increasingly important that we have the best algorithm without needing to check it by eye.

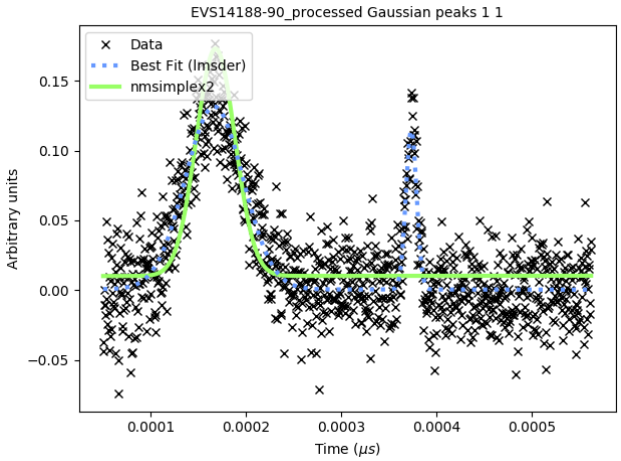

Figure 2: Concept

To enable ease of use, the core modules within `FitBenchmarking` are installed via `pip` with scripts and extra documentation to address the installation of the external packages (for example, `Mantid` or `RALFit` (https://github.com/ralna/RALFit, n.d.)). We've also made it straightforward to add new software and data sets by following the instructions in our `readthedocs` documentation – the software just needs to be callable from `Python`.

FitBenchmarking will help the scientist make an informed choice by comparing runtime and accuracy of all available minimizers, on their specific hardware, on

problems from their science area, which will ensure they are using the most appropriate minimizer.

FitBenchmarking will help the scientific software developer ensure that the most robust and quickest algorithms for the type of data analysis they support are available in their software.

FitBenchmarking will help mathematicians see what the state of the art is, and what kinds of data are problematic. It will give them access to real data, and will give a route for novel methods to quickly make it into production.

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References

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Gould, N., D. Orban, and P. Toint. 2015. "CUTEst : A Constrained Testing Environment with Safe Threads for Mathematical Optimization." *Computational Optimization and Applications* 60 (3): 545–57.

https://github.com/ralna/RALFit. n.d. "RALFit: A Non-Linear Least Squares Solver."