Inverse Problems and Nonlinear Optimization for Inquiry-based STEM Education Using Open Data Science Tools

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Abstract. Integrating inverse problems and nonlinear optimization using open data science tools in inquiry-based STEM education presents a significant opportunity to bridge theoretical STEM knowledge with real-world applications. Our contribution highlights the limitations of traditional linear least squares (LS) fitting methods and demonstrates using SageMath for real-world, nonlinear problems, such as the fall of a lightweight polystyrene ball, demonstrating a closer alignment of students' work with scientific computing in actual research. This approach not only enhances STEM education by including a wider range of attractive real-world problems but also fosters modeling and problem-solving skills, crucial for future professional careers.

Least squares fitting in real-world STEM problems

One of the strengths of inquiry-based STEM education is promoting strong connections between STEM knowledge, authentic practices, and real-world problems. Such an approach not only enhances student engagement and motivation but also fosters the development of STEM literacy, giving students the competencies required to thrive in future professional careers [1].

An integral part of solving real-world problems, whether through experiments, modeling, or scientific computations, involves fitting data to identify the physical parameters of applied models. Generally, the problem of fitting is an example of so-called *inverse problems* [2], where the goal is to determine either the parameters or the initial, sometimes boundary conditions of the created model so that it best describes the given data.

The most commonly applied mathematical method for fitting data is least squares (LS). However, using LS in STEM education leads to a didactic problem. Typically, in standard software such as Coach, Tracker, Geogebra, or Excel, LS can only fit models that are linear or can be linearized with respect to the fitted parameters. Such a limitation significantly narrows the range of real STEM problems that are both utilizable and inherently appealing for STEM education. *How can this issue be addressed?*

Modern interactive open data science tools offer fast and reliable nonlinear LS procedures for solving these inverse problems. A very promising example is interactive Jupyter notebooks with open Python-based software SageMath, which were currently shaped and developed by an EU Horizon 2020 project (http://opendreamkit.org/; see [3] or our second overview poster contribution "Advanced Modeling, Scientific Computations & Data Analysis with Open SageMath").

A real-world STEM problem illustration using Jupyter SageMath notebooks

To illustrate the didactic problem as well as the power of SageMath, let's briefly examine the modeling results of a standard physical problem: *the fall of a lightweight polystyrene ball* on the Earth's surface. After conducting video measurements (blue dots in Fig. 1), a model without air resistance is overly idealized and does not fit the data at all. Considering quadratic air resistance, $\ddot{y} = g - k\dot{y}^2$ with $k = C\rho S/(2m)$, SageMath can fit the corresponding analytical solution [4]

$$y(t) = y_0 + \frac{v_f^2}{g}\ln\left(\cosh\frac{gt}{v_f} + \frac{v_0}{v_f}\sinh\frac{gt}{v_f}\right), v_f = \sqrt{2mg/(CS\rho)} \tag{1}$$

for $y_0 \neq 0, v_0 \neq 0$, which is not a linearizable problem for standard LS with respect to the parameter C or the initial conditions y_0, v_0. In addition, using the python LMFIT library [5] in SageMath, it's also possible to fit these parameters of the model directly without the need for its analytical solution (1). As you can see, the model (the pink plot in Fig.1, C = 0.636) matches the data meticulously and reasonably in this case.

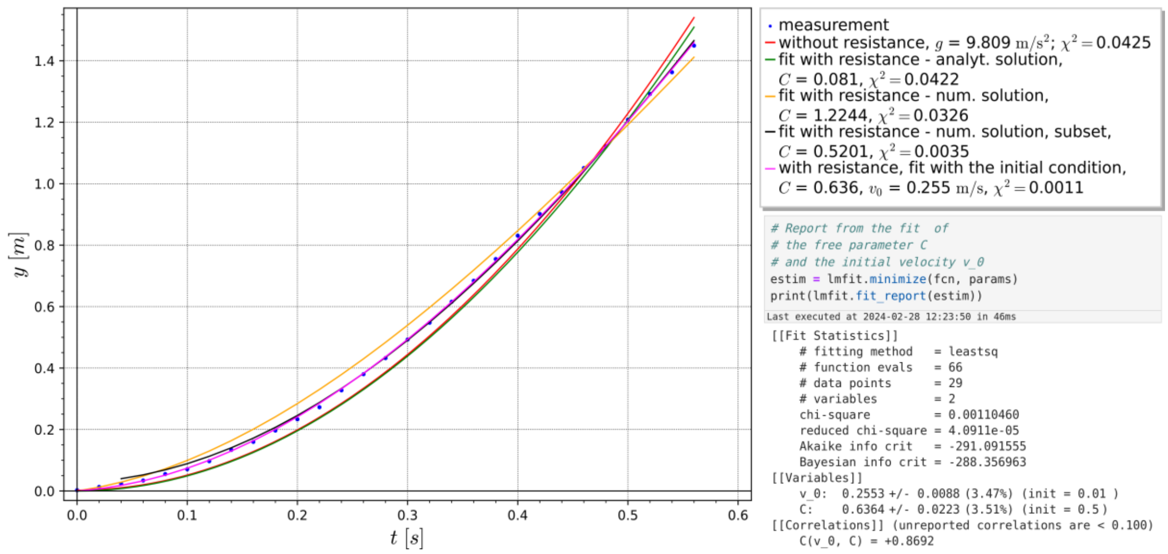

Fig. 1. Results of modeling the fall of a lightweight polystyrene ball in SageMath with the option for the advanced statistical report from fitting with nonlinear least squares if needed.

Further implications and perspectives

Fitting models using nonlinear LS, as in SageMath, enables multiple enhancements of modeling beyond analytical or linear constraints in the spirit of inquiry-based STEM education. This allows including a wider range of attractive real-world inverse problems in STEM education, some of which we will present at the conference as projects or labs in undergraduate courses (e.g., RLC circuits, robotics, or Baumgartner's space jump [6]). Based on our several years of experience [3], we can say this STEM approach really mimics scientific modeling and computing in real science.

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