lmfit documentation

Release 0.1

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The lmfit Python package provides a simple, flexible interface to non-linear least-squares fitting. LMFIT uses the Levenburg-Marquardt from MINPACK-1 as implemented in scipy.optimize.leastsq. While that function provides the core numerical routine for non-linear least-squares minimization, the lmfit packaage adds a few simple conveniences.

For any least-squares minimization, the programmer must provide a function that takes a set of values for the variables in the fit, and produces the residual function to be minimized in the least-squares sense.

The lmfit package allows models to be written in terms of Parameters, which are extensions of simple numerical variables with the following properties:

- Parameters can be fixed or floated in the fit.
- Parameters can be bounded with a minimum and/or maximum value.
- Parameters can be written as simple mathematical expressions of other Parameters. These values will be re-evaluated at each step in the fit, so that the expression is statisfied. This gives a simple but flexible approach to constraining fit variables.

The main advantage to using Parameters instead of fit variables is that the model function does not have to be rewritten for a change in what is varied or what constraints are placed on the fit. The programmer can write a fairly general model, and allow a user of the model to change what is varied and what constraints are placed on the model.

In addition, lmfit calculates are reports the estimated uncertainties and correlation between fitted variables.

CHAPTER

ONE

DOWNLOADING AND INSTALLATION

1.1 Prerequisites

This package requires Python, Numpy, and Scipy. Extensive testing on version compatibility has not yet been done. I have not yet tested with Python 3.

1.2 Downloads

The latest stable version ....

1.3 Development Version

To get the latest development version, use:

```
git clone http://github.com/newville/lmfit-py.git
```

1.4 Installation

Installation from source on any platform is:

```
python setup.py install
```

1.5 License

BSD.

CHAPTER

TWO

NON-LINEAR LEAST-SQUARES FITTING WITH LMFIT-PY

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A simple example ...

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