Non-Linear Least-Squares Minimization and Curve-Fitting for Python

Release 0.9.6

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CONTENTS

Lmfit provides a high-level interface to non-linear optimization and curve fitting problems for Python. It builds on and extends many of the optimization methods of scipy.optimize. Initially inspired by (and named for) extending the Levenberg-Marquardt method from scipy.optimize.leastsq, lmfit now provides a number of useful enhancements to optimization and data fitting problems, including:

- Using `Parameter` objects instead of plain floats as variables. A `Parameter` has a value that can be varied during the fit or kept at a fixed value. It can have upper and/or lower bounds. A Parameter can even have a value that is constrained by an algebraic expression of other Parameter values. As a Python object, a Parameter can also have attributes such as a standard error, after a fit that can estimate uncertainties.
- Ease of changing fitting algorithms. Once a fitting model is set up, one can change the fitting algorithm used to find the optimal solution without changing the objective function.
- Improved estimation of confidence intervals. While scipy.optimize.leastsq will automatically calculate uncertainties and correlations from the covariance matrix, the accuracy of these estimates is sometimes questionable. To help address this, lmfit has functions to explicitly explore parameter space and determine confidence levels even for the most difficult cases.
- Improved curve-fitting with the `Model` class. This extends the capabilities of scipy.optimize.curve_fit, allowing you to turn a function that models your data into a Python class that helps you parametrize and fit data with that model.
- Many *built-in models* for common lineshapes are included and ready to use.

The lmfit package is Free software, using an Open Source license. The software and this document are works in progress. If you are interested in participating in this effort please use the lmfit github repository.

CHAPTER

ONE

GETTING STARTED WITH NON-LINEAR LEAST-SQUARES FITTING

The lmfit package provides simple tools to help you build complex fitting models for non-linear least-squares problems and apply these models to real data. This section gives an overview of the concepts and describes how to set up and perform simple fits. Some basic knowledge of Python, NumPy, and modeling data are assumed – this is not a tutorial on why or how to perform a minimization or fit data, but is rather aimed at explaining how to use lmfit to do these things.

In order to do a non-linear least-squares fit of a model to data or for any other optimization problem, the main task is to write an *objective function* that takes the values of the fitting variables and calculates either a scalar value to be minimized or an array of values that are to be minimized, typically in the least-squares sense. For many data fitting processes, the latter approach is used, and the objective function should return an array of (data-model), perhaps scaled by some weighting factor such as the inverse of the uncertainty in the data. For such a problem, the chi-square (χ^2) statistic is often defined as:

$$\chi^2 = \sum_i^N \frac{[y_i^{\rm meas} - y_i^{\rm model}({\bf v})]^2}{\epsilon_i^2}$$

where $y_i^{\rm meas}$ is the set of measured data, $y_i^{\rm model}({\bf v})$ is the model calculation, ${\bf v}$ is the set of variables in the model to be optimized in the fit, and ϵ_i is the estimated uncertainty in the data.

In a traditional non-linear fit, one writes an objective function that takes the variable values and calculates the residual array $y_i^{\rm meas} - y_i^{\rm model}({\bf v})$, or the residual array scaled by the data uncertainties, $[y_i^{\rm meas} - y_i^{\rm model}({\bf v})]/\epsilon_i$, or some other weighting factor.

As a simple concrete example, one might want to model data with a decaying sine wave, and so write an objective function like this:

```
def residual(vars, x, data, eps_data):
    amp = vars[0]
    phaseshift = vars[1]
    freq = vars[2]
    decay = vars[3]

    model = amp * sin(x * freq  + phaseshift) * exp(-x*x*decay)

    return (data-model)/eps_data
```

To perform the minimization with `scipy.optimize`, one would do this:

```
from scipy.optimize import leastsq
vars = [10.0, 0.2, 3.0, 0.007]
out = leastsq(residual, vars, args=(x, data, eps_data))
```

Though it is wonderful to be able to use Python for such optimization problems, and the scipy library is robust and easy to use, the approach here is not terribly different from how one would do the same fit in C or Fortran. There are several practical challenges to using this approach, including:

1. The user has to keep track of the order of the variables, and their meaning – vars[0] is the amplitude, vars[2] is the frequency, and so on, although there is no intrinsic meaning to this order.
2. If the user wants to fix a particular variable (*not* vary it in the fit), the residual function has to be altered to have fewer variables, and have the corresponding constant value passed in some other way. While reasonable for simple cases, this quickly becomes a significant work for more complex models, and greatly complicates modeling for people not intimately familiar with the details of the fitting code.
3. There is no simple, robust way to put bounds on values for the variables, or enforce mathematical relationships between the variables. In fact, the optimization methods that do provide bounds, require bounds to be set for all variables with separate arrays that are in the same arbitrary order as variable values. Again, this is acceptable for small or one-off cases, but becomes painful if the fitting model needs to change.

These shortcomings are due to the use of traditional arrays to hold the variables, which matches closely the implementation of the underlying Fortran code, but does not fit very well with Python's rich selection of objects and data structures. The key concept in lmfit is to define and use `Parameter` objects instead of plain floating point numbers as the variables for the fit. Using `Parameter` objects (or the closely related `Parameters` – a dictionary of `Parameter` objects), allows one to:

1. forget about the order of variables and refer to Parameters by meaningful names.
2. place bounds on Parameters as attributes, without worrying about preserving the order of arrays for variables and boundaries.
3. fix Parameters, without having to rewrite the objective function.
4. place algebraic constraints on Parameters.

To illustrate the value of this approach, we can rewrite the above example for the decaying sine wave as:

```
from lmfit import minimize, Parameters

def residual(params, x, data, eps_data):
    amp = params['amp']
    pshift = params['phase']
    freq = params['frequency']
    decay = params['decay']

    model = amp * sin(x * freq  + pshift) * exp(-x*x*decay)

    return (data-model)/eps_data

params = Parameters()
params.add('amp', value=10)
params.add('decay', value=0.007)
params.add('phase', value=0.2)
params.add('frequency', value=3.0)

out = minimize(residual, params, args=(x, data, eps_data))
```

At first look, we simply replaced a list of values with a dictionary, accessed by name – not a huge improvement. But each of the named `Parameter` in the `Parameters` object holds additional attributes to modify the value during the fit. For example, Parameters can be fixed or bounded. This can be done during definition:

```
params = Parameters()
params.add('amp', value=10, vary=False)
params.add('decay', value=0.007, min=0.0)
params.add('phase', value=0.2)
params.add('frequency', value=3.0, max=10)
```

where `vary=False` will prevent the value from changing in the fit, and `min=0.0` will set a lower bound on that parameter's value. It can also be done later by setting the corresponding attributes after they have been created:

```
params['amp'].vary = False
params['decay'].min = 0.10
```

Importantly, our objective function remains unchanged. This means the objective function can simply express the parameterized phenomenon to be modeled, and is separate from the choice of parameters to be varied in the fit.

The *params* object can be copied and modified to make many user-level changes to the model and fitting process. Of course, most of the information about how your data is modeled goes into the objective function, but the approach here allows some external control; that is, control by the **user** performing the fit, instead of by the author of the objective function.

Finally, in addition to the `Parameters` approach to fitting data, lmfit allows switching optimization methods without changing the objective function, provides tools for generating fitting reports, and provides a better determination of Parameters confidence levels.

CHAPTER

TWO

DOWNLOADING AND INSTALLATION

2.1 Prerequisites

The lmfit package requires Python, NumPy, and SciPy.

Lmfit works with Python versions 2.7, 3.3, 3.4, 3.5, and 3.6. Support for Python 2.6 ended with lmfit version 0.9.4. Scipy version 0.15 or higher is required, with 0.17 or higher recommended to be able to use the latest optimization features. NumPy version 1.5.1 or higher is required.

In order to run the test suite, either the nose or pytest package is required. Some functionality of lmfit requires the emcee package, some functionality will make use of the pandas, Jupyter or matplotlib packages if available. We highly recommend each of these packages.

2.2 Downloads

The latest stable version of lmfit is 0.9.6 is available from PyPi.

2.3 Installation

With `pip` now widely avaliable, you can install lmfit with:

```
pip install lmfit
```

Alternatively, you can download the source kit, unpack it and install with:

```
python setup.py install
```

For Anaconda Python, lmfit is not an official package, but several Anaconda channels provide it, allowing installation with (for example):

```
conda install -c conda-forge lmfit
```

2.4 Development Version

To get the latest development version, use:

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

and install using:

```
python setup.py install
```

2.5 Testing

A battery of tests scripts that can be run with either the nose or pytest testing framework is distributed with lmfit in the `tests` folder. These are automatically run as part of the development process. For any release or any master branch from the git repository, running `pytest` or `nosetests` should run all of these tests to completion without errors or failures.

Many of the examples in this documentation are distributed with lmfit in the `examples` folder, and should also run for you. Some of these examples assume matplotlib has been installed and is working correctly.

2.6 Acknowledgements


```
Many people have contributed to lmfit.  The attribution of credit in a project such as
this is very difficult to get perfect, and there are no doubt important contributions
missing or under-represented here.  Please consider this file as part of the␣
↪documentation
that may have bugs that need fixing.

Some of the largest and most important contributions (approximately in order of
contribution in size to the existing code) are from:

  Matthew Newville wrote the original version and maintains the project.

  Till Stensitzki wrote the improved estimates of confidence intervals, and␣
↪contributed
  many tests, bug fixes, and documentation.

  A. R. J. Nelson added differential_evolution, emcee, and greatly improved the code,
  docstrings, and overall project.

  Daniel B. Allan wrote much of the high level Model code, and many improvements to␣
↪the
  testing and documentation.

  Antonino Ingargiola wrote much of the high level Model code and has provided many␣
↪bug
  fixes and improvements.

  Renee Otten wrote the brute force method, and has improved the code  and␣
↪documentation
  in many places.

  Michal Rawlik added plotting capabilities for Models.

  J. J. Helmus wrote the MINUT bounds for leastsq, originally in leastsqbounds.py, and
  ported to lmfit.

  E. O. Le Bigot wrote the uncertainties package, a version of which is used by lmfit.
```

```
Additional patches, bug fixes, and suggestions have come from Christoph Deil, Francois
Boulogne, Thomas Caswell, Colin Brosseau, nmearl, Gustavo Pasquevich, Clemens␣
↪Prescher,
LiCode, Ben Gamari, Yoav Roam, Alexander Stark, Alexandre Beelen, and many others.

The lmfit code obviously depends on, and owes a very large debt to the code in
scipy.optimize.  Several discussions on the scipy-user and lmfit mailing lists have␣
↪also
led to improvements in this code.
```

2.7 License

The LMFIT-py code is distribution under the following license:

CHAPTER

THREE

GETTING HELP

If you have questions, comments, or suggestions for LMFIT, please use the mailing list. This provides an on-line conversation that is and archived well and can be searched well with standard web searches. If you find a bug in the code or documentation, use GitHub Issues to submit a report. If you have an idea for how to solve the problem and are familiar with Python and GitHub, submitting a GitHub Pull Request would be greatly appreciated.

If you are unsure whether to use the mailing list or the Issue tracker, please start a conversation on the mailing list. That is, the problem you're having may or may not be due to a bug. If it is due to a bug, creating an Issue from the conversation is easy. If it is not a bug, the problem will be discussed and then the Issue will be closed. While one *can* search through closed Issues on github, these are not so easily searched, and the conversation is not easily useful to others later. Starting the conversation on the mailing list with "How do I do this?" or "Why didn't this work?" instead of "This should work and doesn't" is generally preferred, and will better help others with similar questions. Of course, there is not always an obvious way to decide if something is a Question or an Issue, and we will try our best to engage in all discussions.

CHAPTER

FOUR

FREQUENTLY ASKED QUESTIONS

A list of common questions.

4.1 What's the best way to ask for help or submit a bug report?

See *Getting Help*.

4.2 Why did my script break when upgrading from lmfit 0.8.3 to 0.9.0?

See *Version 0.9.0 Release Notes*

4.3 I get import errors from IPython

If you see something like:

```
from IPython.html.widgets import Dropdown

ImportError: No module named 'widgets'
```

then you need to install the `ipywidgets` package, try: `pip install ipywidgets`.

4.4 How can I fit multi-dimensional data?

The fitting routines accept data arrays that are one dimensional and double precision. So you need to convert the data and model (or the value returned by the objective function) to be one dimensional. A simple way to do this is to use numpy.ndarray.flatten, for example:

```
def residual(params, x, data=None):
    ....
    resid = calculate_multidim_residual()
    return resid.flatten()
```

4.5 How can I fit multiple data sets?

As above, the fitting routines accept data arrays that are one dimensional and double precision. So you need to convert the sets of data and models (or the value returned by the objective function) to be one dimensional. A simple way to do this is to use numpy.concatenate. As an example, here is a residual function to simultaneously fit two lines to two different arrays. As a bonus, the two lines share the 'offset' parameter:

```
import numpy as np
def fit_function(params, x=None, dat1=None, dat2=None):
    model1 = params['offset'] + x * params['slope1']
    model2 = params['offset'] + x * params['slope2']

    resid1 = dat1 - model1
    resid2 = dat2 - model2
    return np.concatenate((resid1, resid2))
```

4.6 How can I fit complex data?

As with working with multi-dimensional data, you need to convert your data and model (or the value returned by the objective function) to be double precision floating point numbers. The simplest approach is to use numpy.ndarray.view, perhaps like:

```
import numpy as np
def residual(params, x, data=None):
     ....
     resid = calculate_complex_residual()
     return resid.view(np.float)
```

4.7 Can I constrain values to have integer values?

Basically, no. None of the minimizers in lmfit support integer programming. They all (I think) assume that they can make a very small change to a floating point value for a parameters value and see a change in the value to be minimized.

4.8 How should I cite LMFIT?

See http://dx.doi.org/10.5281/zenodo.11813

CHAPTER

FIVE

PARAMETER AND PARAMETERS

This chapter describes the *Parameter* object, which is a key concept of lmfit.

A *Parameter* is the quantity to be optimized in all minimization problems, replacing the plain floating point number used in the optimization routines from `scipy.optimize`. A *Parameter* has a value that can either be varied in the fit or held at a fixed value, and can have upper and/or lower bounds placed on the value. It can even have a value that is constrained by an algebraic expression of other Parameter values. Since *Parameter* objects live outside the core optimization routines, they can be used in **all** optimization routines from `scipy.optimize`. By using *Parameter* objects instead of plain variables, the objective function does not have to be modified to reflect every change of what is varied in the fit, or whether bounds can be applied. This simplifies the writing of models, allowing general models that describe the phenomenon and gives the user more flexibility in using and testing variations of that model.

Whereas a *Parameter* expands on an individual floating point variable, the optimization methods actually still need an ordered group of floating point variables. In the `scipy.optimize` routines this is required to be a one-dimensional numpy.ndarray. In lmfit, this one-dimensional array is replaced by a *Parameters* object, which works as an ordered dictionary of *Parameter* objects with a few additional features and methods. That is, while the concept of a *Parameter* is central to lmfit, one normally creates and interacts with a *Parameters* instance that contains many *Parameter* objects. For example, the objective functions you write for lmfit will take an instance of *Parameters* as its first argument. A table of parameter values, bounds and other attributes can be printed using *Parameters.pretty_print()*.

5.1 The Parameter class

class Parameter(*name=None*, *value=None*, *vary=True*, *min=-inf*, *max=inf*, *expr=None*, *brute_step=None*, *user_data=None*)

A Parameter is an object that can be varied in a fit, or one of the controlling variables in a model. It is a central component of lmfit, and all minimization and modeling methods use Parameter objects.

A Parameter has a *name* attribute, and a scalar floating point *value*. It also has a *vary* attribute that describes whether the value should be varied during the minimization. Finite bounds can be placed on the Parameter's value by setting its *min* and/or *max* attributes. A Parameter can also have its value determined by a mathematical expression of other Parameter values held in the *expr* attrribute. Additional attributes include *brute_step* used as the step size in a brute-force minimization, and *user_data* reserved exclusively for user's need.

After a minimization, a Parameter may also gain other attributes, including *stderr* holding the estimated standard error in the Parameter's value, and *correl*, a dictionary of correlation values with other Parameters used in the minimization.

Parameters

- **name** (*str, optional*) – Name of the Parameter.
- **value** (*float, optional*) – Numerical Parameter value.
- **vary** (*bool, optional*) – Whether the Parameter is varied during a fit (default is True).

- **min** (*float, optional*) – Lower bound for value (default is *-numpy.inf*, no lower bound).
- **max** (*float, optional*) – Upper bound for value (default is *numpy.inf*, no upper bound).
- **expr** (*str, optional*) – Mathematical expression used to constrain the value during the fit.
- **brute_step** (*float, optional*) – Step size for grid points in the *brute* method.
- **user_data** (*optional*) – User-definable extra attribute used for a Parameter.

stderr

float – The estimated standard error for the best-fit value.

correl

dict – A dictionary of the correlation with the other fitted Parameters of the form:

```
`{'decay': 0.404, 'phase': -0.020, 'frequency': 0.102}`
```

See *Bounds Implementation* for details on the math used to implement the bounds with `min` and `max`.

The `expr` attribute can contain a mathematical expression that will be used to compute the value for the Parameter at each step in the fit. See *Using Mathematical Constraints* for more details and examples of this feature.

set (*value=None*, *vary=None*, *min=None*, *max=None*, *expr=None*, *brute_step=None*)

Set or update Parameter attributes.

Parameters

- **value** (*float, optional*) – Numerical Parameter value.
- **vary** (*bool, optional*) – Whether the Parameter is varied during a fit.
- **min** (*float, optional*) – Lower bound for value. To remove a lower bound you must use *-numpy.inf*.
- **max** (*float, optional*) – Upper bound for value. To remove an upper bound you must use *numpy.inf*.
- **expr** (*str, optional*) – Mathematical expression used to constrain the value during the fit. To remove a constraint you must supply an empty string.
- **brute_step** (*float, optional*) – Step size for grid points in the *brute* method. To remove the step size you must use `0`.

Notes

Each argument to *set()* has a default value of *None*, which will leave the current value for the attribute unchanged. Thus, to lift a lower or upper bound, passing in *None* will not work. Instead, you must set these to *-numpy.inf* or *numpy.inf*, as with:

```
par.set(min=None)        # leaves lower bound unchanged
par.set(min=-numpy.inf)  # removes lower bound
```

Similarly, to clear an expression, pass a blank string, (not `None`!) as with:

```
par.set(expr=None)  # leaves expression unchanged
par.set(expr='')    # removes expression
```

Explicitly setting a value or setting *vary=True* will also clear the expression.

Finally, to clear the brute_step size, pass 0, not None:

```
par.set(brute_step=None)   # leaves brute_step unchanged
par.set(brute_step=0)      # removes brute_step
```

5.2 The Parameters class

class Parameters(*asteval=None*, **args*, ***kwds*)

An ordered dictionary of all the Parameter objects required to specify a fit model. All minimization and Model fitting routines in lmfit will use exactly one Parameters object, typically given as the first argument to the objective function.

All keys of a Parameters() instance must be strings and valid Python symbol names, so that the name must match `[a-z_][a-z0-9_]*` and cannot be a Python reserved word.

All values of a Parameters() instance must be Parameter objects.

A Parameters() instance includes an asteval interpreter used for evaluation of constrained Parameters.

Parameters() support copying and pickling, and have methods to convert to and from serializations using json strings.

Parameters

- **asteval** (`asteval.Interpreter`, optional) – Instance of the asteval Interpreter to use for constraint expressions. If None, a new interpreter will be created.
- ***args** (*optional*) – Arguments.
- ****kwds** (*optional*) – Keyword arguments.

add(*name*, *value=None*, *vary=True*, *min=-inf*, *max=inf*, *expr=None*, *brute_step=None*)

Add a Parameter.

Parameters

- **name** (*str*) – Name of parameter. Must match `[a-z_][a-z0-9_]*` and cannot be a Python reserved word.
- **value** (*float, optional*) – Numerical Parameter value, typically the *initial value*.
- **vary** (*bool, optional*) – Whether the Parameter is varied during a fit (default is True).
- **min** (*float, optional*) – Lower bound for value (default is *-numpy.inf*, no lower bound).
- **max** (*float, optional*) – Upper bound for value (default is *numpy.inf*, no upper bound).
- **expr** (*str, optional*) – Mathematical expression used to constrain the value during the fit.
- **brute_step** (*float, optional*) – Step size for grid points in the *brute* method.

Examples

```
>>> params = Parameters()
>>> params.add('xvar', value=0.50, min=0, max=1)
>>> params.add('yvar', expr='1.0 - xvar')
```

which is equivalent to:

```
>>> params = Parameters()
>>> params['xvar'] = Parameter(name='xvar', value=0.50, min=0, max=1)
>>> params['yvar'] = Parameter(name='yvar', expr='1.0 - xvar')
```

add_many (**parlist*)

Add many parameters, using a sequence of tuples.

Parameters parlist (sequence of `tuple` or *Parameter*) – A sequence of tuples, or a sequence of *Parameter* instances. If it is a sequence of tuples, then each tuple must contain at least the name. The order in each tuple must be *(name, value, vary, min, max, expr, brute_step)*.

Examples

```
>>>  params = Parameters()
# add with tuples: (NAME VALUE VARY MIN  MAX  EXPR  BRUTE_STEP)
>>> params.add_many(('amp',   10, True, None, None, None, None),
...                 ('cen',    4, True,  0.0, None, None, None),
...                 ('wid',    1, False, None, None, None, None),
...                 ('frac', 0.5))
# add a sequence of Parameters
>>> f = Parameter('par_f', 100)
>>> g = Parameter('par_g',  2.)
>>> params.add_many(f, g)
```

pretty_print (*oneline=False, colwidth=8, precision=4, fmt='g', columns=['value', 'min', 'max', 'stderr', 'vary', 'expr', 'brute_step']*)

Pretty-print of parameters data.

Parameters

- **oneline** (*bool, optional*) – If True prints a one-line parameters representation (default is False).
- **colwidth** (*int, optional*) – Column width for all columns specified in `columns`.
- **precision** (*int, optional*) – Number of digits to be printed after floating point.
- **fmt** (*{'g', 'e', 'f'}, optional*) – Single-character numeric formatter. Valid values are: 'f' floating point, 'g' floating point and exponential, or 'e' exponential.
- **columns** (`list` of `str`, optional) – List of *Parameter* attribute names to print.

valuesdict ()

Return an ordered dictionary of parameter values.

Returns An ordered dictionary of `name:value` pairs for each Parameter.

Return type OrderedDict

dumps (***kws*)

Represent Parameters as a JSON string.

Parameters ****kws** (*optional*) – Keyword arguments that are passed to *json.dumps()*.

Returns JSON string representation of Parameters.

Return type str

See also:

dump(), *loads()*, *load()*, `json.dumps()`

dump (*fp*, ***kws*)

Write JSON representation of Parameters to a file-like object.

Parameters

- **fp** (*file-like object*) – An open and `.write()`-supporting file-like object.
- ****kws** (*optional*) – Keyword arguments that are passed to *dumps()*.

Returns Return value from *fp.write()*. None for Python 2.7 and the number of characters written in Python 3.

Return type None or int

See also:

dump(), *load()*, `json.dump()`

loads (*s*, ***kws*)

Load Parameters from a JSON string.

Parameters ****kws** (*optional*) – Keyword arguments that are passed to *json.loads()*.

Returns Updated Parameters from the JSON string.

Return type *Parameters*

Notes

Current Parameters will be cleared before loading the data from the JSON string.

See also:

dump(), *dumps()*, *load()*, `json.loads()`

load (*fp*, ***kws*)

Load JSON representation of Parameters from a file-like object.

Parameters

- **fp** (*file-like object*) – An open and `.read()`-supporting file-like object.
- ****kws** (*optional*) – Keyword arguments that are passed to *loads()*.

Returns Updated Parameters loaded from *fp*.

Return type *Parameters*

See also:

dump(), *loads()*, `json.load()`

5.3 Simple Example

A basic example making use of *Parameters* and the *minimize()* function (discussed in the next chapter) might look like this:

```
#!/usr/bin/env python
#<examples/doc_basic.py>
from lmfit import minimize, Minimizer, Parameters, Parameter, report_fit
import numpy as np

# create data to be fitted
x = np.linspace(0, 15, 301)
data = (5. * np.sin(2 * x - 0.1) * np.exp(-x*x*0.025) +
        np.random.normal(size=len(x), scale=0.2) )

# define objective function: returns the array to be minimized
def fcn2min(params, x, data):
    """ model decaying sine wave, subtract data"""
    amp = params['amp']
    shift = params['shift']
    omega = params['omega']
    decay = params['decay']
    model = amp * np.sin(x * omega + shift) * np.exp(-x*x*decay)
    return model - data

# create a set of Parameters
params = Parameters()
params.add('amp',   value= 10,  min=0)
params.add('decay', value= 0.1)
params.add('shift', value= 0.0, min=-np.pi/2., max=np.pi/2)
params.add('omega', value= 3.0)


# do fit, here with leastsq model
minner = Minimizer(fcn2min, params, fcn_args=(x, data))
result = minner.minimize()

# calculate final result
final = data + result.residual

# write error report
report_fit(result)

# try to plot results
try:
    import pylab
    pylab.plot(x, data, 'k+')
    pylab.plot(x, final, 'r')
    pylab.show()
except:
    pass

#<end of examples/doc_basic.py>
```

Here, the objective function explicitly unpacks each Parameter value. This can be simplified using the *Parameters* `valuesdict()` method, which would make the objective function `fcn2min` above look like:

```
def fcn2min(params, x, data):
    """ model decaying sine wave, subtract data"""
    v = params.valuesdict()

    model = v['amp'] * np.sin(x * v['omega'] + v['shift']) * np.exp(-x*x*v['decay'])
    return model - data
```

The results are identical, and the difference is a stylistic choice.

CHAPTER SIX

PERFORMING FITS AND ANALYZING OUTPUTS

As shown in the previous chapter, a simple fit can be performed with the `minimize()` function. For more sophisticated modeling, the `Minimizer` class can be used to gain a bit more control, especially when using complicated constraints or comparing results from related fits.

6.1 The `minimize()` function

The `minimize()` function is a wrapper around `Minimizer` for running an optimization problem. It takes an objective function (the function that calculates the array to be minimized), a `Parameters` object, and several optional arguments. See *Writing a Fitting Function* for details on writing the objective.

`minimize`(*fcn*, *params*, *method='leastsq'*, *args=None*, *kws=None*, *scale_covar=True*, *iter_cb=None*, *reduce_fcn=None*, ***fit_kws*)

Perform a fit of a set of parameters by minimizing an objective (or cost) function using one one of the several available methods.

The minimize function takes a objective function to be minimized, a dictionary (`Parameters`) containing the model parameters, and several optional arguments.

Parameters

- **`fcn`** (`callable`) – Objective function to be minimized. When method is *leastsq* or *least_squares*, the objective function should return an array of residuals (difference between model and data) to be minimized in a least-squares sense. With the scalar methods the objective function can either return the residuals array or a single scalar value. The function must have the signature: *fcn(params, *args, **kws)*
- **`params`** (`Parameters`) – Contains the Parameters for the model.
- **`method`** (`str, optional`) – Name of the fitting method to use. Valid values are:
  - *'leastsq'*: Levenberg-Marquardt (default)
  - *'least_squares'*: Least-Squares minimization, using Trust Region Reflective method by default
  - *'differential_evolution'*: differential evolution
  - *'brute'*: brute force method
  - '*nelder*': Nelder-Mead
  - *'lbfgsb'*: L-BFGS-B
  - *'powell'*: Powell
  - *'cg'*: Conjugate-Gradient

  - *'newton'*: Newton-Congugate-Gradient
  - *'cobyla'*: Cobyla
  - *'tnc'*: Truncate Newton
  - *'trust-ncg'*: Trust Newton-Congugate-Gradient
  - *'dogleg'*: Dogleg
  - *'slsqp'*: Sequential Linear Squares Programming

  In most cases, these methods wrap and use the method of the same name from *scipy.optimize*, or use *scipy.optimize.minimize* with the same *method* argument. Thus '*leastsq*' will use *scipy.optimize.leastsq*, while '*powell*' will use *scipy.optimize.minimizer(...., method='powell')*

  For more details on the fitting methods please refer to the SciPy docs.

- **args** (`tuple, optional`) – Positional arguments to pass to *fcn*.
- **kws** (`dict, optional`) – Keyword arguments to pass to *fcn*.
- **iter_cb** (`callable, optional`) – Function to be called at each fit iteration. This function should have the signature *iter_cb(params, iter, resid, *args, **kws)*, where where *params* will have the current parameter values, *iter* the iteration, *resid* the current residual array, and **args* and ***kws* as passed to the objective function.
- **scale_covar** (`bool, optional`) – Whether to automatically scale the covariance matrix (*leastsq* only).
- **reduce_fcn** (`str or callable, optional`) – Function to convert a residual array to a scalar value for the scalar minimizers. See notes in *Minimizer*.
- ****fit_kws** (`dict, optional`) – Options to pass to the minimizer being used.

Returns Object containing the optimized parameter and several goodness-of-fit statistics.

Return type `MinimizerResult`

Changed in version 0.9.0: Return value changed to `MinimizerResult`.

Notes

The objective function should return the value to be minimized. For the Levenberg-Marquardt algorithm from leastsq(), this returned value must be an array, with a length greater than or equal to the number of fitting variables in the model. For the other methods, the return value can either be a scalar or an array. If an array is returned, the sum of squares of the array will be sent to the underlying fitting method, effectively doing a least-squares optimization of the return values.

A common use for *args* and *kws* would be to pass in other data needed to calculate the residual, including such things as the data array, dependent variable, uncertainties in the data, and other data structures for the model calculation.

On output, *params* will be unchanged. The best-fit values, and where appropriate, estimated uncertainties and correlations, will all be contained in the returned `MinimizerResult`. See *MinimizerResult – the optimization result* for further details.

This function is simply a wrapper around `Minimizer` and is equivalent to:

```
fitter = Minimizer(fcn, params, fcn_args=args, fcn_kws=kws,
                   iter_cb=iter_cb, scale_covar=scale_covar, **fit_kws)
fitter.minimize(method=method)
```

6.2 Writing a Fitting Function

An important component of a fit is writing a function to be minimized – the *objective function*. Since this function will be called by other routines, there are fairly stringent requirements for its call signature and return value. In principle, your function can be any Python callable, but it must look like this:

func(params, *args, **kws):

Calculate objective residual to be minimized from parameters.

Parameters

- **params** (*Parameters*) – Parameters.
- **args** – Positional arguments. Must match `args` argument to `minimize()`.
- **kws** – Keyword arguments. Must match `kws` argument to `minimize()`.

Returns Residual array (generally data-model) to be minimized in the least-squares sense.

Return type numpy.ndarray. The length of this array cannot change between calls.

A common use for the positional and keyword arguments would be to pass in other data needed to calculate the residual, including things as the data array, dependent variable, uncertainties in the data, and other data structures for the model calculation.

The objective function should return the value to be minimized. For the Levenberg-Marquardt algorithm from `leastsq()`, this returned value **must** be an array, with a length greater than or equal to the number of fitting variables in the model. For the other methods, the return value can either be a scalar or an array. If an array is returned, the sum of squares of the array will be sent to the underlying fitting method, effectively doing a least-squares optimization of the return values.

Since the function will be passed in a dictionary of `Parameters`, it is advisable to unpack these to get numerical values at the top of the function. A simple way to do this is with `Parameters.valuesdict()`, as shown below:

```
def residual(pars, x, data=None, eps=None):
    # unpack parameters:
    #  extract .value attribute for each parameter
    parvals = pars.valuesdict()
    period = parvals['period']
    shift = parvals['shift']
    decay = parvals['decay']

    if abs(shift) > pi/2:
        shift = shift - sign(shift)*pi

    if abs(period) < 1.e-10:
        period = sign(period)*1.e-10

    model = parvals['amp'] * sin(shift + x/period) * exp(-x*x*decay*decay)

    if data is None:
        return model
    if eps is None:
        return (model - data)
    return (model - data)/eps
```

In this example, *x* is a positional (required) argument, while the *data* array is actually optional (so that the function returns the model calculation if the data is neglected). Also note that the model calculation will divide *x* by the value of the `period` Parameter. It might be wise to ensure this parameter cannot be 0. It would be possible to use the bounds on the `Parameter` to do this:

```
params['period'] = Parameter(value=2, min=1.e-10)
```

but putting this directly in the function with:

```
if abs(period) < 1.e-10:
    period = sign(period)*1.e-10
```

is also a reasonable approach. Similarly, one could place bounds on the `decay` parameter to take values only between `-pi/2` and `pi/2`.

6.3 Choosing Different Fitting Methods

By default, the Levenberg-Marquardt algorithm is used for fitting. While often criticized, including the fact it finds a *local* minima, this approach has some distinct advantages. These include being fast, and well-behaved for most curve-fitting needs, and making it easy to estimate uncertainties for and correlations between pairs of fit variables, as discussed in *MinimizerResult – the optimization result*.

Alternative algorithms can also be used by providing the `method` keyword to the `minimize()` function or `Minimizer.minimize()` class as listed in the *Table of Supported Fitting Methods*.

Table of Supported Fitting Methods:

Fitting Method	`method` arg to `minimize()` or `Minimizer.minimize()`
Levenberg-Marquardt	`leastsq` or `least_squares`
Nelder-Mead	`nelder`
L-BFGS-B	`lbfgsb`
Powell	`powell`
Conjugate Gradient	`cg`
Newton-CG	`newton`
COBYLA	`cobyla`
Truncated Newton	`tnc`
Dogleg	`dogleg`
Sequential Linear Squares Programming	`slsqp`
Differential Evolution	`differential_evolution`
Brute force method	`brute`

Note: The objective function for the Levenberg-Marquardt method **must** return an array, with more elements than variables. All other methods can return either a scalar value or an array.

Warning: Much of this documentation assumes that the Levenberg-Marquardt method is used. Many of the fit statistics and estimates for uncertainties in parameters discussed in *MinimizerResult – the optimization result* are done only for this method.

6.4 `MinimizerResult` – the optimization result

New in version 0.9.0.

An optimization with `minimize()` or `Minimizer.minimize()` will return a `MinimizerResult` object. This is an otherwise plain container object (that is, with no methods of its own) that simply holds the results of the minimization. These results will include several pieces of informational data such as status and error messages, fit statistics, and the updated parameters themselves.

Importantly, the parameters passed in to `Minimizer.minimize()` will be not be changed. To to find the best-fit values, uncertainties and so on for each parameter, one must use the `MinimizerResult.params` attribute. For example, to print the fitted values, bounds and other parameters attributes in a well formatted text tables you can execute:

```
result.params.pretty_print()
```

with *results* being a *MinimizerResult* object. Note that the method `pretty_print()` accepts several arguments for customizing the output (e.g., column width, numeric format, etcetera).

class MinimizerResult(***kws*)

The results of a minimization.

Minimization results include data such as status and error messages, fit statistics, and the updated (i.e., best-fit) parameters themselves in the `params` attribute.

The list of (possible) *MinimizerResult* attributes is given below:

params
: `Parameters` – The best-fit parameters resulting from the fit.

status
: *int* – Termination status of the optimizer. Its value depends on the underlying solver. Refer to *message* for details.

var_names
: *list* – Ordered list of variable parameter names used in optimization, and useful for understanding the values in `init_vals` and `covar`.

covar
: *numpy.ndarray* – Covariance matrix from minimization (*leastsq* only), with rows and columns corresponding to `var_names`.

init_vals
: *list* – List of initial values for variable parameters using `var_names`.

init_values
: *dict* – Dictionary of initial values for variable parameters.

nfev
: *int* – Number of function evaluations.

success
: *bool* – True if the fit succeeded, otherwise False.

errorbars
: *bool* – True if uncertainties were estimated, otherwise False.

message
: *str* – Message about fit success.

ier
: *int* – Integer error value from scipy.optimize.leastsq (*leastsq* only).

lmdif_message
str – Message from scipy.optimize.leastsq (*leastsq* only).

nvarys
int – Number of variables in fit: $N_{\rm varys}$.

ndata
int – Number of data points: N.

nfree
int – Degrees of freedom in fit: $N - N_{\rm varys}$.

residual
numpy.ndarray – Residual array $\rm Resid_i$. Return value of the objective function when using the best-fit values of the parameters.

chisqr
float – Chi-square: $\chi^2 = \sum_i^N [{\rm Resid}_i]^2$.

redchi
float – Reduced chi-square: $\chi^2_{\nu}= {\chi^2} / {(N - N_{\rm varys})}$.

aic
float – Akaike Information Criterion statistic: $N \ln(\chi^2/N) + 2 N_{\rm varys}$.

bic
float – Bayesian Information Criterion statistic: $N \ln(\chi^2/N) + \ln(N) N_{\rm varys}$.

flatchain
pandas.DataFrame – A flatchain view of the sampling chain from the *emcee* method.

show_candidates()
Pretty_print() representation of candidates from the *brute* method.

6.4.1 Goodness-of-Fit Statistics

Table of Fit Results: These values, including the standard Goodness-of-Fit statistics, are all attributes of the *MinimizerResult* object returned by *minimize()* or *Minimizer.minimize()*.

Attribute Name	Description / Formula
nfev	number of function evaluations
nvarys	number of variables in fit $N_{\rm varys}$
ndata	number of data points: N
nfree	degrees of freedom in fit: $N - N_{\rm varys}$
residual	residual array, returned by the objective function: $\{\rm Resid_i\}$
chisqr	chi-square: $\chi^2 = \sum_i^N [{\rm Resid}_i]^2$
redchi	reduced chi-square: $\chi^2_{\nu}= {\chi^2} / {(N - N_{\rm varys})}$
aic	Akaike Information Criterion statistic (see below)
bic	Bayesian Information Criterion statistic (see below)
var_names	ordered list of variable parameter names used for init_vals and covar
covar	covariance matrix (with rows/columns using var_names)
init_vals	list of initial values for variable parameters

Note that the calculation of chi-square and reduced chi-square assume that the returned residual function is scaled properly to the uncertainties in the data. For these statistics to be meaningful, the person writing the function to be minimized **must** scale them properly.

After a fit using using the `leastsq()` method has completed successfully, standard errors for the fitted variables and correlations between pairs of fitted variables are automatically calculated from the covariance matrix. The standard

error (estimated 1σ error-bar) goes into the `stderr` attribute of the Parameter. The correlations with all other variables will be put into the `correl` attribute of the Parameter – a dictionary with keys for all other Parameters and values of the corresponding correlation.

In some cases, it may not be possible to estimate the errors and correlations. For example, if a variable actually has no practical effect on the fit, it will likely cause the covariance matrix to be singular, making standard errors impossible to estimate. Placing bounds on varied Parameters makes it more likely that errors cannot be estimated, as being near the maximum or minimum value makes the covariance matrix singular. In these cases, the `errorbars` attribute of the fit result (*`Minimizer`* object) will be `False`.

6.4.2 Akaike and Bayesian Information Criteria

The *`MinimizerResult`* includes the traditional chi-square and reduced chi-square statistics:

$$\begin{aligned}\chi^2 &= \sum_i^N r_i^2 \\ \chi^2_\nu &= = \chi^2/(N - N_{\rm varys})\end{aligned}$$

where r is the residual array returned by the objective function (likely to be `(data-model)/uncertainty` for data modeling usages), N is the number of data points (`ndata`), and $N_{\rm varys}$ is number of variable parameters.

Also included are the Akaike Information Criterion, and Bayesian Information Criterion statistics, held in the `aic` and `bic` attributes, respectively. These give slightly different measures of the relative quality for a fit, trying to balance quality of fit with the number of variable parameters used in the fit. These are calculated as:

$$\begin{aligned}{\rm aic} &= N \ln(\chi^2/N) + 2 N_{\rm varys} \\ {\rm bic} &= N \ln(\chi^2/N) + \ln(N) N_{\rm varys}\end{aligned}$$

When comparing fits with different numbers of varying parameters, one typically selects the model with lowest reduced chi-square, Akaike information criterion, and/or Bayesian information criterion. Generally, the Bayesian information criterion is considered the most conservative of these statistics.

6.5 Using a Iteration Callback Function

An iteration callback function is a function to be called at each iteration, just after the objective function is called. The iteration callback allows user-supplied code to be run at each iteration, and can be used to abort a fit.

`iter_cb(params, iter, resid, *args, **kws):`
User-supplied function to be run at each iteration.

Parameters

- **`params`** (*`Parameters`*) – Parameters.
- **`iter`** (*`int`*) – Iteration number.
- **`resid`** (*`numpy.ndarray`*) – Residual array.
- **`args`** – Positional arguments. Must match `args` argument to *`minimize()`*
- **`kws`** – Keyword arguments. Must match `kws` argument to *`minimize()`*

Returns Residual array (generally data-model) to be minimized in the least-squares sense.

Return type None for normal behavior, any value like True to abort the fit.

Normally, the iteration callback would have no return value or return `None`. To abort a fit, have this function return a value that is `True` (including any non-zero integer). The fit will also abort if any exception is raised in the iteration callback. When a fit is aborted this way, the parameters will have the values from the last iteration. The fit statistics are not likely to be meaningful, and uncertainties will not be computed.

6.6 Using the `Minimizer` class

For full control of the fitting process, you will want to create a *`Minimizer`* object.

class **`Minimizer`**(*userfcn*, *params*, *fcn_args=None*, *fcn_kws=None*, *iter_cb=None*, *scale_covar=True*, *nan_policy='raise'*, *reduce_fcn=None*, ***kws*)

A general minimizer for curve fitting and optimization.

Parameters

- **`userfcn`** (*`callable`*) – Objective function that returns the residual (difference between model and data) to be minimized in a least-squares sense. This function must have the signature:

```
userfcn(params, *fcn_args, **fcn_kws)
```

- **`params`** (*`Parameters`*) – Contains the Parameters for the model.
- **`fcn_args`** (*`tuple, optional`*) – Positional arguments to pass to *userfcn*.
- **`fcn_kws`** (*`dict, optional`*) – Keyword arguments to pass to *userfcn*.
- **`iter_cb`** (*`callable, optional`*) – Function to be called at each fit iteration. This function should have the signature:

```
iter_cb(params, iter, resid, *fcn_args, **fcn_kws)
```

  where *params* will have the current parameter values, *iter* the iteration, *resid* the current residual array, and **fcn_args* and ***fcn_kws* are passed to the objective function.

- **`scale_covar`** (*`bool, optional`*) – Whether to automatically scale the covariance matrix (*leastsq* only).
- **`nan_policy`** (*`str, optional`*) – Specifies action if *userfcn* (or a Jacobian) returns NaN values. One of:
  - 'raise' : a *ValueError* is raised
  - 'propagate' : the values returned from *userfcn* are un-altered
  - 'omit' : non-finite values are filtered
- **`reduce_fcn`** (*`str or callable, optional`*) – Function to convert a residual array to a scalar value for the scalar minimizers. Optional values are (where *r* is the residual array):
  - None : sum of squares of residual [default]

    = (r*r).sum()
  - 'negentropy' : neg entropy, using normal distribution

    = rho*log(rho).sum()', where rho = exp(-r*r/2)/(sqrt(2*pi))
  - 'neglogcauchy': neg log likelihood, using Cauchy distribution

    = -log(1/(pi*(1+r*r))).sum()

  - callable : must take one argument (*r*) and return a float.
- ****kws** (*dict, optional*) – Options to pass to the minimizer being used.

Notes

The objective function should return the value to be minimized. For the Levenberg-Marquardt algorithm from `leastsq()` or `least_squares()`, this returned value must be an array, with a length greater than or equal to the number of fitting variables in the model. For the other methods, the return value can either be a scalar or an array. If an array is returned, the sum of squares of the array will be sent to the underlying fitting method, effectively doing a least-squares optimization of the return values. If the objective function returns non-finite values then a *ValueError* will be raised because the underlying solvers cannot deal with them.

A common use for the *fcn_args* and *fcn_kws* would be to pass in other data needed to calculate the residual, including such things as the data array, dependent variable, uncertainties in the data, and other data structures for the model calculation.

The Minimizer object has a few public methods:

`Minimizer.`**`minimize`**(*method='leastsq'*, *params=None*, ***kws*)

Perform the minimization.

Parameters

- **method** (*str, optional*) – Name of the fitting method to use. Valid values are:
  - *'leastsq'*: Levenberg-Marquardt (default)
  - *'least_squares'*: Least-Squares minimization, using Trust Region Reflective method by default
  - *'differential_evolution'*: differential evolution
  - *'brute'*: brute force method
  - '*nelder*': Nelder-Mead
  - *'lbfgsb'*: L-BFGS-B
  - *'powell'*: Powell
  - *'cg'*: Conjugate-Gradient
  - *'newton'*: Newton-CG
  - *'cobyla'*: Cobyla
  - *'tnc'*: Truncate Newton
  - *'trust-ncg'*: Trust Newton-CGn
  - *'dogleg'*: Dogleg
  - *'slsqp'*: Sequential Linear Squares Programming

  In most cases, these methods wrap and use the method with the same name from *scipy.optimize*, or use *scipy.optimize.minimize* with the same *method* argument. Thus '*leastsq*' will use *scipy.optimize.leastsq*, while '*powell*' will use *scipy.optimize.minimizer(...., method='powell')*

  For more details on the fitting methods please refer to the SciPy docs.
- **params** (*Parameters*, optional) – Parameters of the model to use as starting values.

- `**kws` (*optional*) – Additional arguments are passed to the underlying minimization method.

Returns Object containing the optimized parameter and several goodness-of-fit statistics.

Return type `MinimizerResult`

Changed in version 0.9.0: Return value changed to `MinimizerResult`.

`Minimizer.`**`leastsq`**(*params=None*, ***kws*)

Use Levenberg-Marquardt minimization to perform a fit.

It assumes that the input Parameters have been initialized, and a function to minimize has been properly set up. When possible, this calculates the estimated uncertainties and variable correlations from the covariance matrix.

This method calls scipy.optimize.leastsq. By default, numerical derivatives are used, and the following arguments are set:

`leastsq()` arg	Default Value	Description
xtol	1.e-7	Relative error in the approximate solution
ftol	1.e-7	Relative error in the desired sum of squares
maxfev	2000*(nvar+1)	Maximum number of function calls (nvar= # of variables)
Dfun	None	Function to call for Jacobian calculation

Parameters

- **`params`** (`Parameters`, optional) – Parameters to use as starting point.
- **`**kws`** (`dict, optional`) – Minimizer options to pass to scipy.optimize.leastsq.

Returns Object containing the optimized parameter and several goodness-of-fit statistics.

Return type `MinimizerResult`

Changed in version 0.9.0: Return value changed to `MinimizerResult`.

`Minimizer.`**`least_squares`**(*params=None*, ***kws*)

Use the *least_squares* (new in scipy 0.17) to perform a fit.

It assumes that the input Parameters have been initialized, and a function to minimize has been properly set up. When possible, this calculates the estimated uncertainties and variable correlations from the covariance matrix.

This method wraps scipy.optimize.least_squares, which has inbuilt support for bounds and robust loss functions.

Parameters

- **`params`** (`Parameters`, optional) – Parameters to use as starting point.
- **`**kws`** (`dict, optional`) – Minimizer options to pass to scipy.optimize.least_squares.

Returns Object containing the optimized parameter and several goodness-of-fit statistics.

Return type `MinimizerResult`

Changed in version 0.9.0: Return value changed to `MinimizerResult`.

`Minimizer.`**`scalar_minimize`**(*method='Nelder-Mead'*, *params=None*, ***kws*)

Scalar minimization using scipy.optimize.minimize.

Perform fit with any of the scalar minimization algorithms supported by scipy.optimize.minimize. Default argument values are:

`scalar_minimize()` arg	Default Value	Description
method	`Nelder-Mead`	fitting method
tol	1.e-7	fitting and parameter tolerance
hess	None	Hessian of objective function

Parameters

- **method** (*str, optional*) – Name of the fitting method to use. One of:
  - 'Nelder-Mead' (default)
  - 'L-BFGS-B'
  - 'Powell'
  - 'CG'
  - 'Newton-CG'
  - 'COBYLA'
  - 'TNC'
  - 'trust-ncg'
  - 'dogleg'
  - 'SLSQP'
  - 'differential_evolution'
- **params** (*Parameters*, optional) – Parameters to use as starting point.
- ****kws** (*dict, optional*) – Minimizer options pass to scipy.optimize.minimize.

Returns Object containing the optimized parameter and several goodness-of-fit statistics.

Return type *MinimizerResult*

Changed in version 0.9.0: Return value changed to *MinimizerResult*.

Notes

If the objective function returns a NumPy array instead of the expected scalar, the sum of squares of the array will be used.

Note that bounds and constraints can be set on Parameters for any of these methods, so are not supported separately for those designed to use bounds. However, if you use the differential_evolution method you must specify finite (min, max) for each varying Parameter.

`Minimizer.`**`prepare_fit`**(*params=None*)

Prepare parameters for fitting.

Prepares and initializes model and Parameters for subsequent fitting. This routine prepares the conversion of `Parameters` into fit variables, organizes parameter bounds, and parses, "compiles" and checks constrain expressions. The method also creates and returns a new instance of a *MinimizerResult* object that contains the copy of the Parameters that will actually be varied in the fit.

Parameters **params** (*Parameters*, optional) – Contains the Parameters for the model; if None, then the Parameters used to initialize the Minimizer object are used.

Returns

Return type *MinimizerResult*

Notes

This method is called directly by the fitting methods, and it is generally not necessary to call this function explicitly.

Changed in version 0.9.0: Return value changed to `MinimizerResult`.

`Minimizer.brute(params=None, Ns=20, keep=50)`

Use the *brute* method to find the global minimum of a function.

The following parameters are passed to scipy.optimize.brute and cannot be changed:

`brute()` arg	Value	Description
full_output	1	Return the evaluation grid and the objective function's values on it.
finish	None	No "polishing" function is to be used after the grid search.
disp	False	Do not print convergence messages (when finish is not None).

It assumes that the input Parameters have been initialized, and a function to minimize has been properly set up.

Parameters

- **params** (`Parameters` object, optional) – Contains the Parameters for the model. If None, then the Parameters used to initialize the Minimizer object are used.
- **Ns** (`int, optional`) – Number of grid points along the axes, if not otherwise specified (see Notes).
- **keep** (`int, optional`) – Number of best candidates from the brute force method that are stored in the `candidates` attribute. If 'all', then all grid points from scipy.optimize.brute are stored as candidates.

Returns Object containing the parameters from the brute force method. The return values (*x0*, *fval*, *grid*, *Jout*) from scipy.optimize.brute are stored as *brute_<parname>* attributes. The *MinimizerResult* also contains the *candidates* attribute and *show_candidates()* method. The *candidates* attribute contains the parameters and chisqr from the brute force method as a namedtuple, ('Candidate', ['params', 'score']), sorted on the (lowest) chisqr value. To access the values for a particular candidate one can use *result.candidate[#].params* or *result.candidate[#].score*, where a lower # represents a better candidate. The *show_candidates(#)* uses the `pretty_print()` method to show a specific candidate-# or all candidates when no number is specified.

Return type `MinimizerResult`

New in version 0.9.6.

Notes

The `brute()` method evalutes the function at each point of a multidimensional grid of points. The grid points are generated from the parameter ranges using *Ns* and (optional) *brute_step*. The implementation in scipy.optimize.brute requires finite bounds and the *range* is specified as a two-tuple *(min, max)* or slice-object *(min, max, brute_step)*. A slice-object is used directly, whereas a two-tuple is converted to a slice object that interpolates *Ns* points from *min* to *max*, inclusive.

In addition, the `brute()` method in lmfit, handles three other scenarios given below with their respective slice-object:

- **lower bound (`min`) and `brute_step` are specified:** range = (*min*, *min* + *Ns* * *brute_step*, *brute_step*).
- **upper bound (`max`) and `brute_step` are specified:** range = (*max* - *Ns* * *brute_step*, *max*, *brute_step*).
- **numerical value (`value`) and `brute_step` are specified:** range = (*value* - (*Ns*//2) * *brute_step*, *value* + (*Ns*//2) * *brute_step*, *brute_step*).

For more information, check the examples in `examples/lmfit_brute.py`.

`Minimizer.emcee`(*params=None*, *steps=1000*, *nwalkers=100*, *burn=0*, *thin=1*, *ntemps=1*, *pos=None*, *reuse_sampler=False*, *workers=1*, *float_behavior='posterior'*, *is_weighted=True*, *seed=None*)

Bayesian sampling of the posterior distribution using *emcee*.

Bayesian sampling of the posterior distribution for the parameters using the *emcee* Markov Chain Monte Carlo package. The method assumes that the prior is Uniform. You need to have *emcee* installed to use this method.

Parameters

- **params** (*Parameters*, optional) – Parameters to use as starting point. If this is not specified then the Parameters used to initialize the Minimizer object are used.
- **steps** (*int, optional*) – How many samples you would like to draw from the posterior distribution for each of the walkers?
- **nwalkers** (*int, optional*) – Should be set so $nwalkers >> nvarys$, where *nvarys* are the number of parameters being varied during the fit. "Walkers are the members of the ensemble. They are almost like separate Metropolis-Hastings chains but, of course, the proposal distribution for a given walker depends on the positions of all the other walkers in the ensemble." - from the *emcee* webpage.
- **burn** (*int, optional*) – Discard this many samples from the start of the sampling regime.
- **thin** (*int, optional*) – Only accept 1 in every *thin* samples.
- **ntemps** (*int, optional*) – If *ntemps > 1* perform a Parallel Tempering.
- **pos** (*numpy.ndarray, optional*) – Specify the initial positions for the sampler. If *ntemps == 1* then *pos.shape* should be *(nwalkers, nvarys)*. Otherwise, *(ntemps, nwalkers, nvarys)*. You can also initialise using a previous chain that had the same *ntemps*, *nwalkers* and *nvarys*. Note that *nvarys* may be one larger than you expect it to be if your *userfcn* returns an array and *is_weighted is False*.
- **reuse_sampler** (*bool, optional*) – If you have already run *emcee* on a given *Minimizer* object then it possesses an internal `sampler` attribute. You can continue to draw from the same sampler (retaining the chain history) if you set this option to True. Otherwise a new sampler is created. The *nwalkers*, *ntemps*, *pos*, and *params* keywords are ignored with this option. **Important**: the Parameters used to create the sampler must not change in-between calls to *emcee*. Alteration of Parameters would include changed `min`, `max`, `vary` and `expr` attributes. This may happen, for example, if you use an altered Parameters object and call the *minimize* method in-between calls to *emcee*.
- **workers** (*Pool-like or int, optional*) – For parallelization of sampling. It can be any Pool-like object with a map method that follows the same calling sequence as the built-in *map* function. If int is given as the argument, then a multiprocessing-based pool is spawned internally with the corresponding number of parallel processes. 'mpi4py'-based parallelization and 'joblib'-based parallelization pools can also be used here. **Note**: because of multiprocessing overhead it may only be worth parallelising if the objective function is expensive to calculate, or if there are a large number of objective evaluations per step (*ntemps * nwalkers * nvarys*).
- **float_behavior** (*str, optional*) – Specifies meaning of the objective function output if it returns a float. One of:
  - 'posterior' - objective function returns a log-posterior probability
  - 'chi2' - objective function returns χ^2

See Notes for further details.

- **is_weighted** (`bool`, *optional*) – Has your objective function been weighted by measurement uncertainties? If *is_weighted is True* then your objective function is assumed to return residuals that have been divided by the true measurement uncertainty *(data - model) / sigma*. If *is_weighted is False* then the objective function is assumed to return unweighted residuals, *data - model*. In this case *emcee* will employ a positive measurement uncertainty during the sampling. This measurement uncertainty will be present in the output params and output chain with the name *__lnsigma*. A side effect of this is that you cannot use this parameter name yourself. **Important** this parameter only has any effect if your objective function returns an array. If your objective function returns a float, then this parameter is ignored. See Notes for more details.
- **seed** (int or *numpy.random.RandomState*, optional) – If *seed* is an int, a new *numpy.random.RandomState* instance is used, seeded with *seed*. If *seed* is already a *numpy.random.RandomState* instance, then that *numpy.random.RandomState* instance is used. Specify *seed* for repeatable minimizations.

Returns MinimizerResult object containing updated params, statistics, etc. The updated params represent the median (50th percentile) of all the samples, whilst the parameter uncertainties are half of the difference between the 15.87 and 84.13 percentiles. The *MinimizerResult* also contains the `chain`, `flatchain` and `lnprob` attributes. The `chain` and `flatchain` attributes contain the samples and have the shape *(nwalkers, (steps - burn) // thin, nvarys)* or *(ntemps, nwalkers, (steps - burn) // thin, nvarys)*, depending on whether Parallel tempering was used or not. *nvarys* is the number of parameters that are allowed to vary. The `flatchain` attribute is a *pandas.DataFrame* of the flattened chain, *chain.reshape(-1, nvarys)*. To access flattened chain values for a particular parameter use *result.flatchain[parname]*. The `lnprob` attribute contains the log probability for each sample in `chain`. The sample with the highest probability corresponds to the maximum likelihood estimate.

Return type `MinimizerResult`

Notes

This method samples the posterior distribution of the parameters using Markov Chain Monte Carlo. To do so it needs to calculate the log-posterior probability of the model parameters, *F*, given the data, *D*, $\ln p(F_{true}|D)$. This 'posterior probability' is calculated as:

$$\ln p(F_{true}|D) \propto \ln p(D|F_{true}) + \ln p(F_{true})$$

where $\ln p(D|F_{true})$ is the 'log-likelihood' and $\ln p(F_{true})$ is the 'log-prior'. The default log-prior encodes prior information already known about the model. This method assumes that the log-prior probability is *-numpy.inf* (impossible) if the one of the parameters is outside its limits. The log-prior probability term is zero if all the parameters are inside their bounds (known as a uniform prior). The log-likelihood function is given by[1]:

$$\ln p(D|F_{true}) = -\frac{1}{2}\sum_n \left[\frac{(g_n(F_{true}) - D_n)^2}{s_n^2} + \ln(2\pi s_n^2)\right]$$

The first summand in the square brackets represents the residual for a given datapoint (g being the generative model, D_n the data and s_n the standard deviation, or measurement uncertainty, of the datapoint). This term represents χ^2 when summed over all data points. Ideally the objective function used to create *lmfit.Minimizer* should return the log-posterior probability, $\ln p(F_{true}|D)$. However, since the in-built log-prior term is zero, the objective function can also just return the log-likelihood, unless you wish to create a non-uniform prior.

[1] http://dan.iel.fm/emcee/current/user/line/

If a float value is returned by the objective function then this value is assumed by default to be the log-posterior probability, i.e. *float_behavior is 'posterior'*. If your objective function returns χ^2, then you should use a value of *'chi2'* for *float_behavior*. *emcee* will then multiply your χ^2 value by -0.5 to obtain the posterior probability.

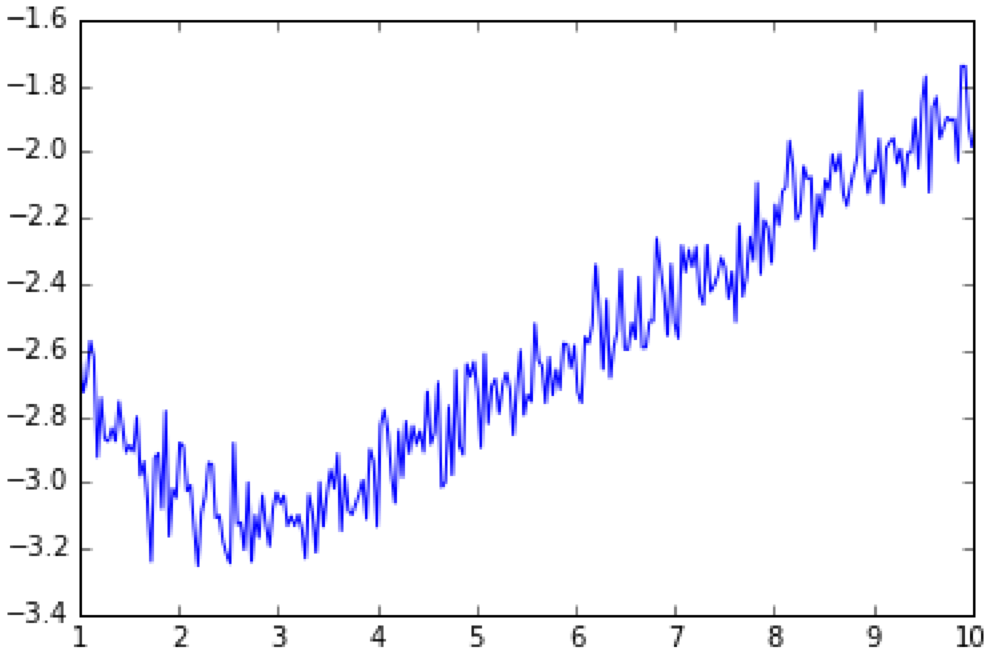
However, the default behaviour of many objective functions is to return a vector of (possibly weighted) residuals. Therefore, if your objective function returns a vector, *res*, then the vector is assumed to contain the residuals. If *is_weighted is True* then your residuals are assumed to be correctly weighted by the standard deviation (measurement uncertainty) of the data points (*res = (data - model) / sigma*) and the log-likelihood (and log-posterior probability) is calculated as: *-0.5 * numpy.sum(res**2)*. This ignores the second summand in the square brackets. Consequently, in order to calculate a fully correct log-posterior probability value your objective function should return a single value. If *is_weighted is False* then the data uncertainty, *s_n*, will be treated as a nuisance parameter and will be marginalized out. This is achieved by employing a strictly positive uncertainty (homoscedasticity) for each data point, $s_n = \exp(\_\_lnsigma)$. *__lnsigma* will be present in *MinimizerResult.params*, as well as *Minimizer.chain*, *nvarys* will also be increased by one.

References

6.7 `Minimizer.emcee()` - calculating the posterior probability distribution of parameters

`Minimizer.emcee()` can be used to obtain the posterior probability distribution of parameters, given a set of experimental data. An example problem is a double exponential decay. A small amount of Gaussian noise is also added in:

```
>>> import numpy as np
>>> import lmfit
>>> import matplotlib.pyplot as plt
>>> x = np.linspace(1, 10, 250)
>>> np.random.seed(0)
>>> y = 3.0 * np.exp(-x / 2) - 5.0 * np.exp(-(x - 0.1) / 10.) + 0.1 * np.random.
↪randn(len(x))
>>> plt.plot(x, y)
>>> plt.show()
```

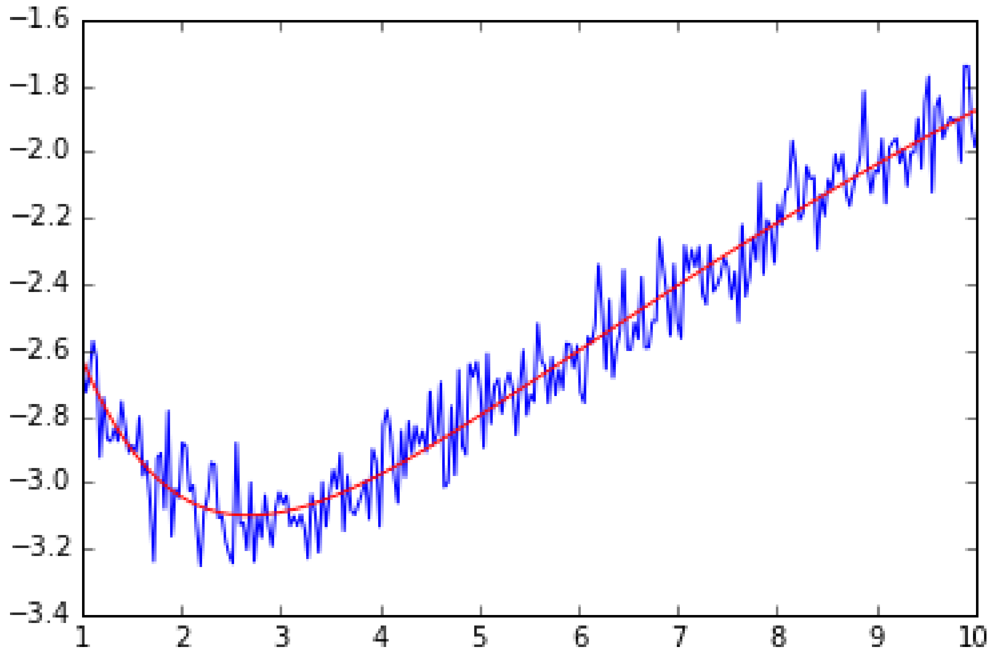


Create a Parameter set for the initial guesses:

```
>>> p = lmfit.Parameters()
>>> p.add_many(('a1', 4.), ('a2', 4.), ('t1', 3.), ('t2', 3., True))

>>> def residual(p):
...     v = p.valuesdict()
...     return v['a1'] * np.exp(-x / v['t1']) + v['a2'] * np.exp(-(x - 0.1) / v['t2
↪']) - y
```

Solving with *minimize()* gives the Maximum Likelihood solution.:

```
>>> mi = lmfit.minimize(residual, p, method='Nelder')
>>> lmfit.printfuncs.report_fit(mi.params, min_correl=0.5)
[[Variables]]
    a1:   2.98623688 (init= 4)
    a2:  -4.33525596 (init= 4)
    t1:   1.30993185 (init= 3)
    t2:   11.8240752 (init= 3)
[[Correlations]] (unreported correlations are <  0.500)
>>> plt.plot(x, y)
>>> plt.plot(x, residual(mi.params) + y, 'r')
>>> plt.show()
```



However, this doesn't give a probability distribution for the parameters. Furthermore, we wish to deal with the data uncertainty. This is called marginalisation of a nuisance parameter. `emcee` requires a function that returns the log-posterior probability. The log-posterior probability is a sum of the log-prior probability and log-likelihood functions. The log-prior probability is assumed to be zero if all the parameters are within their bounds and `-np.inf` if any of the parameters are outside their bounds.

```
>>> # add a noise parameter
>>> mi.params.add('f', value=1, min=0.001, max=2)
```

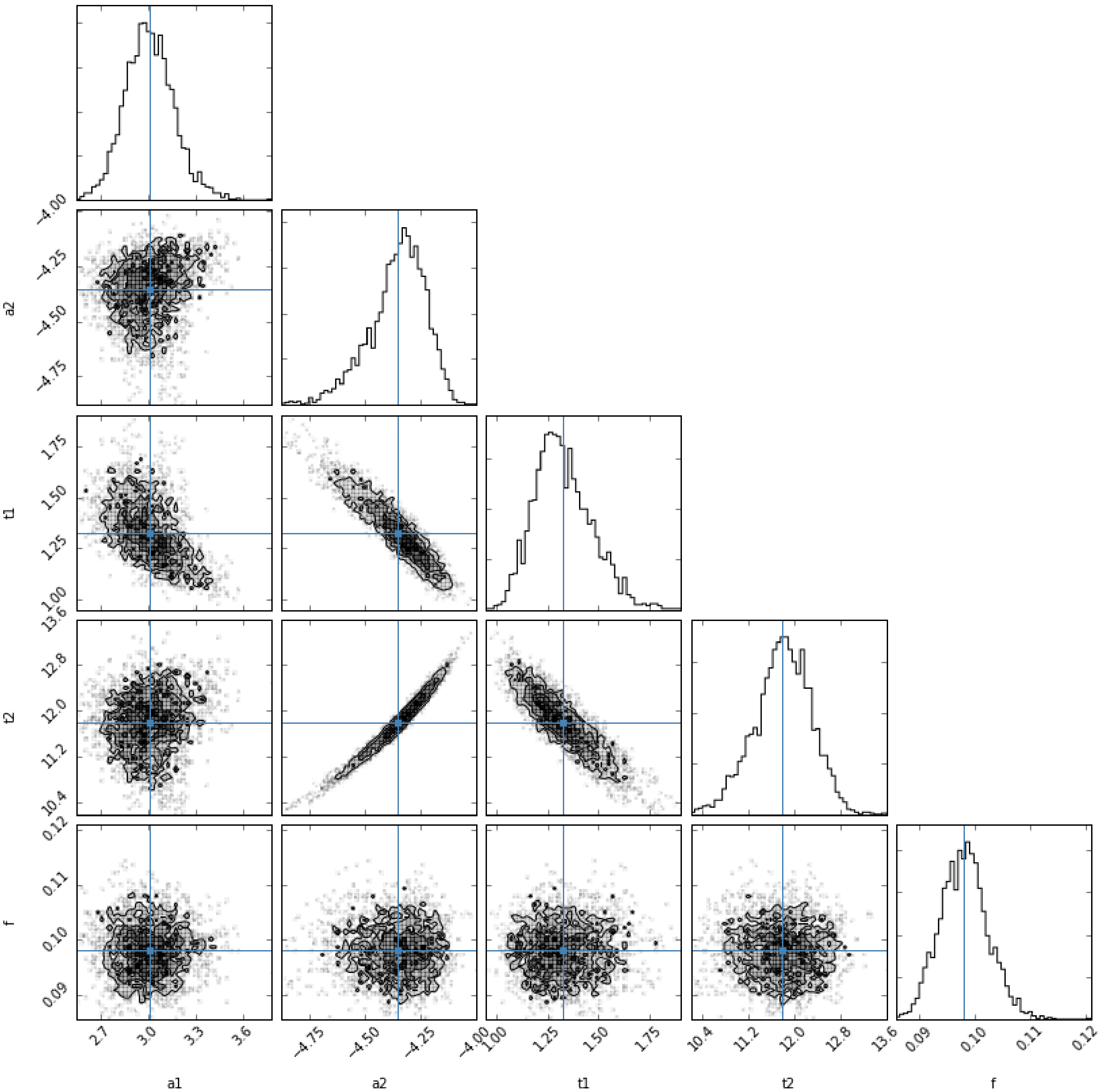
```
>>> # This is the log-likelihood probability for the sampling. We're going to␣
↪estimate the
>>> # size of the uncertainties on the data as well.
>>> def lnprob(p):
...     resid = residual(p)
...     s = p['f']
...     resid *= 1 / s
...     resid *= resid
...     resid += np.log(2 * np.pi * s**2)
...     return -0.5 * np.sum(resid)
```

Now we have to set up the minimizer and do the sampling:

```
>>> mini = lmfit.Minimizer(lnprob, mi.params)
>>> res = mini.emcee(burn=300, steps=600, thin=10, params=mi.params)
```

Lets have a look at those posterior distributions for the parameters. This requires installation of the *corner* package:

```
>>> import corner
>>> corner.corner(res.flatchain, labels=res.var_names, truths=list(res.params.
↪valuesdict().values()))
```



The values reported in the *MinimizerResult* are the medians of the probability distributions and a 1 sigma quantile, estimated as half the difference between the 15.8 and 84.2 percentiles. The median value is not necessarily the same as the Maximum Likelihood Estimate. We'll get that as well. You can see that we recovered the right uncertainty level on the data.:

```
>>> print("median of posterior probability distribution")
>>> print('------------------------------------------')
>>> lmfit.report_fit(res.params)
median of posterior probability distribution
------------------------------------------
[[Variables]]
    a1:   3.00975345 +/- 0.151034 (5.02%) (init= 2.986237)
    a2:  -4.35419204 +/- 0.127505 (2.93%) (init=-4.335256)
    t1:   1.32726415 +/- 0.142995 (10.77%) (init= 1.309932)
    t2:   11.7911935 +/- 0.495583 (4.20%) (init= 11.82408)
```

```
    f:    0.09805494 +/- 0.004256 (4.34%) (init= 1)
[[Correlations]] (unreported correlations are <  0.100)
    C(a2, t2)                    =  0.981
    C(a2, t1)                    = -0.927
    C(t1, t2)                    = -0.880
    C(a1, t1)                    = -0.519
    C(a1, a2)                    =  0.195
    C(a1, t2)                    =  0.146

>>> # find the maximum likelihood solution
>>> highest_prob = np.argmax(res.lnprob)
>>> hp_loc = np.unravel_index(highest_prob, res.lnprob.shape)
>>> mle_soln = res.chain[hp_loc]
>>> for i, par in enumerate(p):
...     p[par].value = mle_soln[i]

>>> print("\nMaximum likelihood Estimation")
>>> print('-----------------------------')
>>> print(p)
Maximum likelihood Estimation
-----------------------------
Parameters([('a1', <Parameter 'a1', 2.9943337359308981, bounds=[-inf:inf]>),
('a2', <Parameter 'a2', -4.3364489105166593, bounds=[-inf:inf]>),
('t1', <Parameter 't1', 1.3124544105342462, bounds=[-inf:inf]>),
('t2', <Parameter 't2', 11.80612160586597, bounds=[-inf:inf]>)])

>>> # Finally lets work out a 1 and 2-sigma error estimate for 't1'
>>> quantiles = np.percentile(res.flatchain['t1'], [2.28, 15.9, 50, 84.2, 97.7])
>>> print("2 sigma spread", 0.5 * (quantiles[-1] - quantiles[0]))
2 sigma spread 0.298878202908
```

6.8 Getting and Printing Fit Reports

fit_report (*inpars*, *modelpars=None*, *show_correl=True*, *min_correl=0.1*, *sort_pars=False*)

Generate a report of the fitting results.

The report contains the best-fit values for the parameters and their uncertainties and correlations.

Parameters

- **inpars** (`Parameters`) – Input Parameters from fit or MinimizerResult returned from a fit.
- **modelpars** (`Parameters, optional`) – Known Model Parameters.
- **show_correl** (`bool, optional`) – Whether to show list of sorted correlations (default is True).
- **min_correl** (`float, optional`) – Smallest correlation in absolute value to show (default is 0.1).
- **sort_pars** (`bool or callable, optional`) – Whether to show parameter names sorted in alphanumerical order. If False (default), then the parameters will be listed in the order they were added to the Parameters dictionary. If callable, then this (one argument) function is used to extract a comparison key from each list element.

Returns Multi-line text of fit report.

Return type string

An example using this to write out a fit report would be:

```
#!/usr/bin/env python
#<examples/doc_withreport.py>

from __future__ import print_function
from lmfit import Parameters, minimize, fit_report
from numpy import random, linspace, pi, exp, sin, sign


p_true = Parameters()
p_true.add('amp', value=14.0)
p_true.add('period', value=5.46)
p_true.add('shift', value=0.123)
p_true.add('decay', value=0.032)

def residual(pars, x, data=None):
    vals = pars.valuesdict()
    amp =  vals['amp']
    per =  vals['period']
    shift = vals['shift']
    decay = vals['decay']

    if abs(shift) > pi/2:
        shift = shift - sign(shift)*pi
    model = amp * sin(shift + x/per) * exp(-x*x*decay*decay)
    if data is None:
        return model
    return (model - data)

n = 1001
xmin = 0.
xmax = 250.0

random.seed(0)

noise = random.normal(scale=0.7215, size=n)
x     = linspace(xmin, xmax, n)
data  = residual(p_true, x) + noise

fit_params = Parameters()
fit_params.add('amp', value=13.0)
fit_params.add('period', value=2)
fit_params.add('shift', value=0.0)
fit_params.add('decay', value=0.02)

out = minimize(residual, fit_params, args=(x,), kws={'data':data})

print(fit_report(out))


#<end of examples/doc_withreport.py>
```

which would write out:

```
[[Fit Statistics]]
    # function evals   = 85
```

```
    # data points      = 1001
    # variables        = 4
    chi-square         = 498.812
    reduced chi-square = 0.500
    Akaike info crit   = -689.223
    Bayesian info crit = -669.587
[[Variables]]
    amp:      13.9121944 +/- 0.141202 (1.01%) (init= 13)
    period:   5.48507044 +/- 0.026664 (0.49%) (init= 2)
    shift:    0.16203676 +/- 0.014056 (8.67%) (init= 0)
    decay:    0.03264538 +/- 0.000380 (1.16%) (init= 0.02)
[[Correlations]] (unreported correlations are <  0.100)
    C(period, shift)             =  0.797
    C(amp, decay)                =  0.582
    C(amp, shift)                = -0.297
    C(amp, period)               = -0.243
    C(shift, decay)              = -0.182
    C(period, decay)             = -0.150
```

CHAPTER

SEVEN

MODELING DATA AND CURVE FITTING

A common use of least-squares minimization is *curve fitting*, where one has a parametrized model function meant to explain some phenomena and wants to adjust the numerical values for the model so that it most closely matches some data. With `scipy`, such problems are typically solved with scipy.optimize.curve_fit, which is a wrapper around scipy.optimize.leastsq. Since lmfit's `minimize()` is also a high-level wrapper around scipy.optimize.leastsq it can be used for curve-fitting problems. While it offers many benefits over scipy.optimize.leastsq, using `minimize()` for many curve-fitting problems still requires more effort than using scipy.optimize.curve_fit.

The `Model` class in lmfit provides a simple and flexible approach to curve-fitting problems. Like scipy.optimize.curve_fit, a `Model` uses a *model function* – a function that is meant to calculate a model for some phenomenon – and then uses that to best match an array of supplied data. Beyond that similarity, its interface is rather different from scipy.optimize.curve_fit, for example in that it uses `Parameters`, but also offers several other important advantages.

In addition to allowing you to turn any model function into a curve-fitting method, lmfit also provides canonical definitions for many known line shapes such as Gaussian or Lorentzian peaks and Exponential decays that are widely used in many scientific domains. These are available in the `models` module that will be discussed in more detail in the next chapter (*Built-in Fitting Models in the models module*). We mention it here as you may want to consult that list before writing your own model. For now, we focus on turning Python functions into high-level fitting models with the `Model` class, and using these to fit data.

7.1 Motivation and simple example: Fit data to Gaussian profile

Let's start with a simple and common example of fitting data to a Gaussian peak. As we will see, there is a buit-in `GaussianModel` class that can help do this, but here we'll build our own. We start with a simple definition of the model function:

```
>>> from numpy import sqrt, pi, exp, linspace, random
>>>
>>> def gaussian(x, amp, cen, wid):
...     return amp * exp(-(x-cen)**2 /wid)
```

We want to use this function to fit to data $y(x)$ represented by the arrays *y* and *x*. With scipy.optimize.curve_fit, this would be:

```
>>> from scipy.optimize import curve_fit
>>>
>>> x = linspace(-10,10, 101)
>>> y = gaussian(x, 2.33, 0.21, 1.51) + random.normal(0, 0.2, len(x))
>>>
>>> init_vals = [1, 0, 1]     # for [amp, cen, wid]
>>> best_vals, covar = curve_fit(gaussian, x, y, p0=init_vals)
>>> print best_vals
```

That is, we create data, make an initial guess of the model values, and run scipy.optimize.curve_fit with the model function, data arrays, and initial guesses. The results returned are the optimal values for the parameters and the covariance matrix. It's simple and useful, but it misses the benefits of lmfit.

With lmfit, we create a `Model` that wraps the *gaussian* model function, which automatically generates the appropriate residual function, and determines the corresponding parameter names from the function signature itself:

```
>>> from lmfit import Model
>>> gmodel = Model(gaussian)
>>> gmodel.param_names
set(['amp', 'wid', 'cen'])
>>> gmodel.independent_vars
['x']
```

As you can see, the Model *gmodel* determined the names of the parameters and the independent variables. By default, the first argument of the function is taken as the independent variable, held in `independent_vars`, and the rest of the functions positional arguments (and, in certain cases, keyword arguments – see below) are used for Parameter names. Thus, for the *gaussian* function above, the independent variable is *x*, and the parameters are named *amp*, *cen*, and *wid*, and – all taken directly from the signature of the model function. As we will see below, you can modify the default assignment of independent variable / arguments and specify yourself what the independent variable is and which function arguments should be identified as parameter names.

The Parameters are *not* created when the model is created. The model knows what the parameters should be named, but not anything about the scale and range of your data. You will normally have to make these parameters and assign initial values and other attributes. To help you do this, each model has a `make_params()` method that will generate parameters with the expected names:

```
>>> params = gmod.make_params()
```

This creates the `Parameters` but does not automaticaly give them initial values since it has no idea what the scale should be. You can set initial values for parameters with keyword arguments to `make_params()`:

```
>>> params = gmod.make_params(cen=5, amp=200, wid=1)
```

or assign them (and other parameter properties) after the `Parameters` class has been created.

A `Model` has several methods associated with it. For example, one can use the `eval()` method to evaluate the model or the `fit()` method to fit data to this model with a `Parameter` object. Both of these methods can take explicit keyword arguments for the parameter values. For example, one could use `eval()` to calculate the predicted function:

```
>>> x = linspace(0, 10, 201)
>>> y = gmod.eval(params, x=x)
```

or with:

```
>>> y = gmod.eval(x=x, cen=6.5, amp=100, wid=2.0)
```

Admittedly, this a slightly long-winded way to calculate a Gaussian function, given that you could have called your *gaussian* function directly. But now that the model is set up, we can use its `fit()` method to fit this model to data, as with:

```
>>> result = gmod.fit(y, params)
```

or with:

```
>>> result = gmod.fit(y, cen=6.5, amp=100, wid=2.0)
```

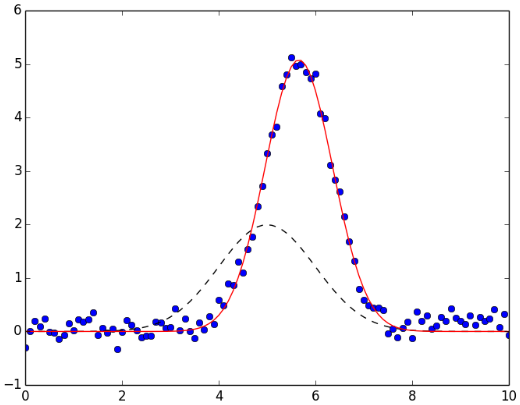
Putting everything together, (included in the `examples` folder with the source code) is:

```
#!/usr/bin/env python
#<examples/doc_model1.py>
from numpy import sqrt, pi, exp, linspace, loadtxt
from lmfit import  Model

import matplotlib.pyplot as plt

data = loadtxt('model1d_gauss.dat')
x = data[:, 0]
y = data[:, 1]

def gaussian(x, amp, cen, wid):
    "1-d gaussian: gaussian(x, amp, cen, wid)"
    return (amp/(sqrt(2*pi)*wid)) * exp(-(x-cen)**2 /(2*wid**2))

gmodel = Model(gaussian)
result = gmodel.fit(y, x=x, amp=5, cen=5, wid=1)

print(result.fit_report())

plt.plot(x, y,         'bo')
plt.plot(x, result.init_fit, 'k--')
plt.plot(x, result.best_fit, 'r-')
plt.show()
#<end examples/doc_model1.py>
```

which is pretty compact and to the point. The returned *result* will be a *ModelResult* object. As we will see below, this has many components, including a `fit_report()` method, which will show:

```
[[Model]]
    Model(gaussian)
[[Fit Statistics]]
    # function evals   = 31
    # data points      = 101
    # variables        = 3
    chi-square         = 3.409
    reduced chi-square = 0.035
    Akaike info crit   = -336.264
    Bayesian info crit = -328.418
[[Variables]]
    amp:   5.07800631 +/- 0.064957 (1.28%) (init= 5)
    cen:   5.65866112 +/- 0.010304 (0.18%) (init= 5)
    wid:   0.97344373 +/- 0.028756 (2.95%) (init= 1)
[[Correlations]] (unreported correlations are <  0.100)
    C(amp, wid)                  = -0.577
```

As the script shows, the result will also have *init_fit* for the fit with the initial parameter values and a *best_fit* for the fit with the best fit parameter values. These can be used to generate the following plot:



which shows the data in blue dots, the best fit as a solid red line, and the initial fit as a dashed black line.

Note that the model fitting was really performed with:

```
gmodel = Model(gaussian)
result = gmodel.fit(y, params, x=x, amp=5, cen=5, wid=1)
```

These lines clearly express that we want to turn the *gaussian* function into a fitting model, and then fit the $y(x)$ data to this model, starting with values of 5 for *amp*, 5 for *cen* and 1 for *wid*. In addition, all the other features of lmfit are included: `Parameters` can have bounds and constraints and the result is a rich object that can be reused to explore the model fit in detail.

7.2 The `Model` class

The `Model` class provides a general way to wrap a pre-defined function as a fitting model.

class **`Model`** (*func*, *independent_vars=None*, *param_names=None*, *missing='none'*, *prefix=''*, *name=None*, ***kws*)

Create a model from a user-supplied model function.

The model function will normally take an independent variable (generally, the first argument) and a series of arguments that are meant to be parameters for the model. It will return an array of data to model some data as for a curve-fitting problem.

Parameters

- **`func`** (*`callable`*) – Function to be wrapped.
- **`independent_vars`** (*`list of str, optional`*) – Arguments to func that are independent variables (default is None).
- **`param_names`** (*`list of str, optional`*) – Names of arguments to func that are to be made into parameters (default is None).
- **`missing`** (*`str, optional`*) – How to handle NaN and missing values in data. One of:
  – 'none' or None : Do not check for null or missing values (default).
  – 'drop' : Drop null or missing observations in data. If pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  – 'raise' : Raise a (more helpful) exception when data contains null or missing values.
- **`prefix`** (*`str, optional`*) – Prefix used for the model.

- **name** (*str, optional*) – Name for the model. When None (default) the name is the same as the model function (*func*).
- ****kws** (*dict, optional*) – Additional keyword arguments to pass to model function.

Notes

1. Parameter names are inferred from the function arguments, and a residual function is automatically constructed.

2. The model function must return an array that will be the same size as the data being modeled.

Examples

The model function will normally take an independent variable (generally, the first argument) and a series of arguments that are meant to be parameters for the model. Thus, a simple peak using a Gaussian defined as:

```
>>> import numpy as np
>>> def gaussian(x, amp, cen, wid):
...     return amp * np.exp(-(x-cen)**2 / wid)
```

can be turned into a Model with:

```
>>> gmodel = Model(gaussian)
```

this will automatically discover the names of the independent variables and parameters:

```
>>> print(gmodel.param_names, gmodel.independent_vars)
['amp', 'cen', 'wid'], ['x']
```

7.2.1 Model class Methods

`Model.`**eval**(*params=None*, ***kwargs*)

Evaluate the model with supplied parameters and keyword arguments.

Parameters

- **params** (*Parameters, optional*) – Parameters to use in Model.
- ****kwargs** (*optional*) – Additional keyword arguments to pass to model function.

Returns Value of model given the parameters and other arguments.

Return type numpy.ndarray

Notes

1. if *params* is None, the values for all parameters are expected to be provided as keyword arguments. If *params* is given, and a keyword argument for a parameter value is also given, the keyword argument will be used.

2. all non-parameter arguments for the model function, **including all the independent variables** will need to be passed in using keyword arguments.

`Model.`**fit**(*data*, *params=None*, *weights=None*, *method='leastsq'*, *iter_cb=None*, *scale_covar=True*, *verbose=False*, *fit_kws=None*, ***kwargs*)

Fit the model to the data using the supplied Parameters.

Parameters

- **data** (*array_like*) – Array of data to be fit.
- **params** (Parameters, *optional*) – Parameters to use in fit (default is None).
- **weights** (array_like of same size as *data*, optional) – Weights to use for the calculation of the fit residual (default is None).
- **method** (*str, optional*) – Name of fitting method to use (default is *'leastsq'*).
- **iter_cb** (*callable, optional*) – Callback function to call at each iteration (default is None).
- **scale_covar** (*bool, optional*) – Whether to automatically scale the covariance matrix when calculating uncertainties (default is True, *leastsq* method only).
- **verbose** (*bool, optional*) – Whether to print a message when a new parameter is added because of a hint (default is True).
- **fit_kws** (*dict, optional*) – Options to pass to the minimizer being used.
- ****kwargs** (*optional*) – Arguments to pass to the model function, possibly overriding params.

Returns

Return type *ModelResult*

Examples

Take *t* to be the independent variable and data to be the curve we will fit. Use keyword arguments to set initial guesses:

```
>>> result = my_model.fit(data, tau=5, N=3, t=t)
```

Or, for more control, pass a Parameters object.

```
>>> result = my_model.fit(data, params, t=t)
```

Keyword arguments override Parameters.

```
>>> result = my_model.fit(data, params, tau=5, t=t)
```

Notes

1. if *params* is None, the values for all parameters are expected to be provided as keyword arguments. If *params* is given, and a keyword argument for a parameter value is also given, the keyword argument will be used.

2. all non-parameter arguments for the model function, **including all the independent variables** will need to be passed in using keyword arguments.

3. Parameters (however passed in), are copied on input, so the original Parameter objects are unchanged, and the updated values are in the returned *ModelResult*.

`Model.guess`(*data*, ***kws*)

Guess starting values for the parameters of a model.

This is not implemented for all models, but is available for many of the built-in models.

Parameters

- **data** (*array_like*) – Array of data to use to guess parameter values.
- ****kws** (*optional*) – Additional keyword arguments, passed to model function.

Returns params

Return type *Parameters*

Notes

Should be implemented for each model subclass to run self.make_params(), update starting values and return a Parameters object.

Raises `NotImplementedError`

`Model.`**`make_params`**(*verbose=False*, ***kwargs*)

Create a Parameters object for a Model.

Parameters

- **verbose** (*bool, optional*) – Whether to print out messages (default is False).
- ****kwargs** (*optional*) – Parameter names and initial values.

Returns params

Return type *Parameters*

Notes

1. The parameters may or may not have decent initial values for each parameter.
2. This applies any default values or parameter hints that may have been set.

`Model.`**`set_param_hint`**(*name*, ***kwargs*)

Set *hints* to use when creating parameters with *make_params()* for the named parameter.

This is especially convenient for setting initial values. The *name* can include the models *prefix* or not. The hint given can also include optional bounds and constraints `(value, vary, min, max, expr)`, which will be used by make_params() when building default parameters.

Parameters

- **name** (*string*) – Parameter name.
- ****kwargs** (*optional*) – Arbitrary keyword arguments, needs to be a Parameter attribute. Can be any of the following:
  - **value** [float, optional] Numerical Parameter value.
  - **vary** [bool, optional] Whether the Parameter is varied during a fit (default is True).
  - **min** [float, optional] Lower bound for value (default is *-numpy.inf*, no lower bound).
  - **max** [float, optional] Upper bound for value (default is *numpy.inf*, no upper bound).
  - **expr** [str, optional] Mathematical expression used to constrain the value during the fit.

Example

```
>>> model = GaussianModel()
>>> model.set_param_hint('sigma', min=0)
```

See *Using parameter hints*.

`Model.`**`print_param_hints`**`(`*colwidth=8*`)`
Print a nicely aligned text-table of parameter hints.

Parameters **`colwidth`** (*`int, optional`*) – Width of each column, except for first and last columns.

7.2.2 `Model` class Attributes

`func`
The model function used to calculate the model.

`independent_vars`
List of strings for names of the independent variables.

`missing`
Describes what to do for missing values. The choices are:

- None: Do not check for null or missing values (default).
- 'none': Do not check for null or missing values.
- 'drop': Drop null or missing observations in data. If pandas is installed, `pandas.isnull()` is used, otherwise `numpy.isnan()` is used.
- 'raise': Raise a (more helpful) exception when data contains null or missing values.

`name`
Name of the model, used only in the string representation of the model. By default this will be taken from the model function.

`opts`
Extra keyword arguments to pass to model function. Normally this will be determined internally and should not be changed.

`param_hints`
Dictionary of parameter hints. See *Using parameter hints*.

`param_names`
List of strings of parameter names.

`prefix`
Prefix used for name-mangling of parameter names. The default is ''. If a particular *`Model`* has arguments *amplitude*, *center*, and *sigma*, these would become the parameter names. Using a prefix of *'g1_'* would convert these parameter names to *g1_amplitude*, *g1_center*, and *g1_sigma*. This can be essential to avoid name collision in composite models.

7.2.3 Determining parameter names and independent variables for a function

The *`Model`* created from the supplied function *func* will create a *`Parameters`* object, and names are inferred from the function arguments, and a residual function is automatically constructed.

By default, the independent variable is take as the first argument to the function. You can, of course, explicitly set this, and will need to do so if the independent variable is not first in the list, or if there are actually more than one independent variables.

If not specified, Parameters are constructed from all positional arguments and all keyword arguments that have a default value that is numerical, except the independent variable, of course. Importantly, the Parameters can be modified after creation. In fact, you will have to do this because none of the parameters have valid initial values. In addition, one can place bounds and constraints on Parameters, or fix their values.

7.2.4 Explicitly specifying `independent_vars`

As we saw for the Gaussian example above, creating a *Model* from a function is fairly easy. Let's try another one:

```
>>> from lmfit import Model
>>> import numpy as np
>>> def decay(t, tau, N):
...    return N*np.exp(-t/tau)
...
>>> decay_model = Model(decay)
>>> print decay_model.independent_vars
['t']
>>> for pname, par in decay_model.params.items():
...     print pname, par
...
tau <Parameter 'tau', None, bounds=[None:None]>
N <Parameter 'N', None, bounds=[None:None]>
```

Here, *t* is assumed to be the independent variable because it is the first argument to the function. The other function arguments are used to create parameters for the model.

If you want *tau* to be the independent variable in the above example, you can say so:

```
>>> decay_model = Model(decay, independent_vars=['tau'])
>>> print decay_model.independent_vars
['tau']
>>> for pname, par in decay_model.params.items():
...     print pname, par
...
t <Parameter 't', None, bounds=[None:None]>
N <Parameter 'N', None, bounds=[None:None]>
```

You can also supply multiple values for multi-dimensional functions with multiple independent variables. In fact, the meaning of *independent variable* here is simple, and based on how it treats arguments of the function you are modeling:

independent variable A function argument that is not a parameter or otherwise part of the model, and that will be required to be explicitly provided as a keyword argument for each fit with *Model.fit()* or evaluation with *Model.eval()*.

Note that independent variables are not required to be arrays, or even floating point numbers.

7.2.5 Functions with keyword arguments

If the model function had keyword parameters, these would be turned into Parameters if the supplied default value was a valid number (but not None, True, or False).

```
>>> def decay2(t, tau, N=10, check_positive=False):
...     if check_small:
...         arg = abs(t)/max(1.e-9, abs(tau))
...     else:
...         arg = t/tau
...     return N*np.exp(arg)
...
>>> mod = Model(decay2)
>>> for pname, par in mod.params.items():
...     print pname, par
...
t <Parameter 't', None, bounds=[None:None]>
N <Parameter 'N', 10, bounds=[None:None]>
```

Here, even though *N* is a keyword argument to the function, it is turned into a parameter, with the default numerical value as its initial value. By default, it is permitted to be varied in the fit – the 10 is taken as an initial value, not a fixed value. On the other hand, the *check_positive* keyword argument, was not converted to a parameter because it has a boolean default value. In some sense, *check_positive* becomes like an independent variable to the model. However, because it has a default value it is not required to be given for each model evaluation or fit, as independent variables are.

7.2.6 Defining a *prefix* for the Parameters

As we will see in the next chapter when combining models, it is sometimes necessary to decorate the parameter names in the model, but still have them be correctly used in the underlying model function. This would be necessary, for example, if two parameters in a composite model (see *Composite Models : adding (or multiplying) Models* or examples in the next chapter) would have the same name. To avoid this, we can add a *prefix* to the `Model` which will automatically do this mapping for us.

```
>>> def myfunc(x, amplitude=1, center=0, sigma=1):
...
```

```
>>> mod = Model(myfunc, prefix='f1_')
>>> for pname, par in mod.params.items():
...     print pname, par
...
f1_amplitude <Parameter 'f1_amplitude', None, bounds=[None:None]>
f1_center <Parameter 'f1_center', None, bounds=[None:None]>
f1_sigma <Parameter 'f1_sigma', None, bounds=[None:None]>
```

You would refer to these parameters as *f1_amplitude* and so forth, and the model will know to map these to the *amplitude* argument of *myfunc*.

7.2.7 Initializing model parameters

As mentioned above, the parameters created by `Model.make_params()` are generally created with invalid initial values of None. These values **must** be initialized in order for the model to be evaluated or used in a fit. There are four different ways to do this initialization that can be used in any combination:

1. You can supply initial values in the definition of the model function.
2. You can initialize the parameters when creating parameters with `Model.make_params()`.
3. You can give parameter hints with `Model.set_param_hint()`.

4. You can supply initial values for the parameters when you use the `Model.eval()` or `Model.fit()` methods.

Of course these methods can be mixed, allowing you to overwrite initial values at any point in the process of defining and using the model.

Initializing values in the function definition

To supply initial values for parameters in the definition of the model function, you can simply supply a default value:

```
>>> def myfunc(x, a=1, b=0):
>>>     ...
```

instead of using:

```
>>> def myfunc(x, a, b):
>>>     ...
```

This has the advantage of working at the function level – all parameters with keywords can be treated as options. It also means that some default initial value will always be available for the parameter.

Initializing values with `Model.make_params()`

When creating parameters with `Model.make_params()` you can specify initial values. To do this, use keyword arguments for the parameter names and initial values:

```
>>> mod = Model(myfunc)
>>> pars = mod.make_params(a=3, b=0.5)
```

Initializing values by setting parameter hints

After a model has been created, but prior to creating parameters with `Model.make_params()`, you can set parameter hints. These allows you to set not only a default initial value but also to set other parameter attributes controlling bounds, whether it is varied in the fit, or a constraint expression. To set a parameter hint, you can use `Model.set_param_hint()`, as with:

```
>>> mod = Model(myfunc)
>>> mod.set_param_hint('a', value = 1.0)
>>> mod.set_param_hint('b', value = 0.3, min=0, max=1.0)
>>> pars = mod.make_params()
```

Parameter hints are discussed in more detail in section *Using parameter hints*.

Initializing values when using a model

Finally, you can explicitly supply initial values when using a model. That is, as with `Model.make_params()`, you can include values as keyword arguments to either the `Model.eval()` or `Model.fit()` methods:

```
>>> y1 = mod.eval(x=x, a=7.0, b=-2.0)

>>> out = mod.fit(x=x, pars, a=3.0, b=-0.0)
```

These approaches to initialization provide many opportunities for setting initial values for parameters. The methods can be combined, so that you can set parameter hints but then change the initial value explicitly with `Model.fit()`.

7.2.8 Using parameter hints

After a model has been created, you can give it hints for how to create parameters with `Model.make_params()`. This allows you to set not only a default initial value but also to set other parameter attributes controlling bounds, whether it is varied in the fit, or a constraint

expression. To set a parameter hint, you can use `Model.set_param_hint()`, as with:

```
>>> mod = Model(myfunc)
>>> mod.set_param_hint('a', value = 1.0)
>>> mod.set_param_hint('b', value = 0.3, min=0, max=1.0)
```

Parameter hints are stored in a model's `param_hints` attribute, which is simply a nested dictionary:

```
>>> print mod.param_hints
{'a': {'value': 1}, 'b': {'max': 1.0, 'value': 0.3, 'min': 0}}
```

You can change this dictionary directly, or with the `Model.set_param_hint()` method. Either way, these parameter hints are used by `Model.make_params()` when making parameters.

An important feature of parameter hints is that you can force the creation of new parameters with parameter hints. This can be useful to make derived parameters with constraint expressions. For example to get the full-width at half maximum of a Gaussian model, one could use a parameter hint of:

```
>>> mod = Model(gaussian)
>>> mod.set_param_hint('fwhm', expr='2.3548*sigma')
```

7.3 The `ModelResult` class

A `ModelResult` (which had been called *ModelFit* prior to version 0.9) is the object returned by `Model.fit()`. It is a subclass of `Minimizer`, and so contains many of the fit results. Of course, it knows the `Model` and the set of `Parameters` used in the fit, and it has methods to evaluate the model, to fit the data (or re-fit the data with changes to the parameters, or fit with different or modified data) and to print out a report for that fit.

While a `Model` encapsulates your model function, it is fairly abstract and does not contain the parameters or data used in a particular fit. A `ModelResult` *does* contain parameters and data as well as methods to alter and re-do fits. Thus the `Model` is the idealized model while the `ModelResult` is the messier, more complex (but perhaps more useful) object that represents a fit with a set of parameters to data with a model.

A `ModelResult` has several attributes holding values for fit results, and several methods for working with fits. These include statistics inherited from `Minimizer` useful for comparing different models, including *chisqr*, *redchi*, *aic*, and *bic*.

class **`ModelResult`**(*model*, *params*, *data=None*, *weights=None*, *method='leastsq'*, *fcn_args=None*, *fcn_kws=None*, *iter_cb=None*, *scale_covar=True*, ***fit_kws*)

Result from the Model fit.

This has many attributes and methods for viewing and working with the results of a fit using Model. It inherits from Minimizer, so that it can be used to modify and re-run the fit for the Model.

Parameters

- **`model`** (`Model`) – Model to use.
- **`params`** (`Parameters`) – Parameters with initial values for model.
- **`data`** (*`array_like, optional`*) – Data to be modeled.

- **weights** (*array_like, optional*) – Weights to multiply (data-model) for fit residual.
- **method** (*str, optional*) – Name of minimization method to use (default is *'leastsq'*).
- **fcn_args** (*sequence, optional*) – Positional arguments to send to model function.
- **fcn_dict** (*dict, optional*) – Keyword arguments to send to model function.
- **iter_cb** (*callable, optional*) – Function to call on each iteration of fit.
- **scale_covar** (*bool, optional*) – Whether to scale covariance matrix for uncertainty evaluation.
- ****fit_kws** (*optional*) – Keyword arguments to send to minimization routine.

7.3.1 `ModelResult` methods

ModelResult.**eval**(*params=None*, ***kwargs*)

Evaluate model function.

Parameters

- **params** (*Parameters, optional*) – Parameters to use.
- ****kwargs** (*optional*) – Options to send to Model.eval()

Returns **out** – Array for evaluated model.

Return type numpy.ndarray

ModelResult.**eval_components**(*params=None*, ***kwargs*)

Evaluate each component of a composite model function.

Parameters

- **params** (*Parameters, optional*) – Parameters, defaults to ModelResult.params
- ****kwargs** (*optional*) – Leyword arguments to pass to model function.

Returns Keys are prefixes of component models, and values are the estimated model value for each component of the model.

Return type OrderedDict

ModelResult.**fit**(*data=None*, *params=None*, *weights=None*, *method=None*, ***kwargs*)

Re-perform fit for a Model, given data and params.

Parameters

- **data** (*array_like, optional*) – Data to be modeled.
- **params** (*Parameters, optional*) – Parameters with initial values for model.
- **weights** (*array_like, optional*) – Weights to multiply (data-model) for fit residual.
- **method** (*str, optional*) – Name of minimization method to use (default is *'leastsq'*).
- ****kwargs** (*optional*) – Keyword arguments to send to minimization routine.

ModelResult.**fit_report**(*modelpars=None*, *show_correl=True*, *min_correl=0.1*, *sort_pars=False*)

Return a printable fit report.

The report contains fit statistics and best-fit values with uncertainties and correlations.

Parameters

- **modelpars** (`Parameters, optional`) – Known Model Parameters.
- **show_correl** (*bool, optional*) – Whether to show list of sorted correlations (default is True).
- **min_correl** (*float, optional*) – Smallest correlation in absolute value to show (default is 0.1).
- **sort_pars** (*callable, optional*) – Whether to show parameter names sorted in alphanumerical order (default is False). If False, then the parameters will be listed in the order as they were added to the Parameters dictionary. If callable, then this (one argument) function is used to extract a comparison key from each list element.

Returns **text** – Multi-line text of fit report.

Return type str

See also:

fit_report()

`ModelResult.`**`conf_interval`**`(**kwargs)`

Calculate the confidence intervals for the variable parameters.

Confidence intervals are calculated using the `confidence.conf_interval()` function and keyword arguments (***kwargs*) are passed to that function. The result is stored in the *ci_out* attribute so that it can be accessed without recalculating them.

`ModelResult.`**`ci_report`**`(with_offset=True, ndigits=5, **kwargs)`

Return a nicely formatted text report of the confidence intervals.

Parameters

- **with_offset** (*bool, optional*) – Whether to subtract best value from all other values (default is True).
- **ndigits** (*int, optional*) – Number of significant digits to show (default is 5).
- ****kwargs** (*optional*) – Keyword arguments that are passed to the *conf_interval* function.

Returns Text of formatted report on confidence intervals.

Return type str

`ModelResult.`**`eval_uncertainty`**`(params=None, sigma=1, **kwargs)`

Evaluate the uncertainty of the *model function* from the uncertainties for the best-fit parameters. This can be used to give confidence bands for the model.

Parameters

- **params** (`Parameters, optional`) – Parameters, defaults to ModelResult.params.
- **sigma** (*float, optional*) – Confidence level, i.e. how many sigma (default is 1).
- ****kwargs** (*optional*) – Values of options, independent variables, etcetera.

Returns Uncertainty at each value of the model.

Return type numpy.ndarray

Example

```
>>> out = model.fit(data, params, x=x)
>>> dely = out.eval_confidence_band(x=x)
>>> plt.plot(x, data)
>>> plt.plot(x, out.best_fit)
>>> plt.fill_between(x, out.best_fit-dely,
...                  out.best_fit+dely, color='#888888')
```

Notes

1. This is based on the excellent and clear example from https://www.astro.rug.nl/software/kapteyn/kmpfittutorial.html#confidence-and-prediction-intervals, which references the original work of: J. Wolberg,Data Analysis Using the Method of Least Squares, 2006, Springer

2. The value of sigma is number of *sigma* values, and is converted to a probability. Values or 1, 2, or 3 give probalities of 0.6827, 0.9545, and 0.9973, respectively. If the sigma value is < 1, it is interpreted as the probability itself. That is, *sigma=1* and *sigma=0.6827* will give the same results, within precision errors.

`ModelResult.`**`plot`**`(*args, **kws)`

Plot the fit results and residuals using matplotlib, if available.

The method will produce a matplotlib figure with both results of the fit and the residuals plotted. If the fit model included weights, errorbars will also be plotted.

Parameters

- **datafmt** (*str, optional*) – Matplotlib format string for data points.
- **fitfmt** (*str, optional*) – Matplotlib format string for fitted curve.
- **initfmt** (*str, optional*) – Matplotlib format string for initial conditions for the fit.
- **xlabel** (*str, optional*) – Matplotlib format string for labeling the x-axis.
- **ylabel** (*str, optional*) – Matplotlib format string for labeling the y-axis.
- **yerr** (*numpy.ndarray, optional*) – Array of uncertainties for data array.
- **numpoints** (*int, optional*) – If provided, the final and initial fit curves are evaluated not only at data points, but refined to contain *numpoints* points in total.
- **fig** (*matplotlib.figure.Figure, optional*) – The figure to plot on. The default is None, which means use the current pyplot figure or create one if there is none.
- **data_kws** (*dict, optional*) – Keyword arguments passed on to the plot function for data points.
- **fit_kws** (*dict, optional*) – Keyword arguments passed on to the plot function for fitted curve.
- **init_kws** (*dict, optional*) – Keyword arguments passed on to the plot function for the initial conditions of the fit.
- **ax_res_kws** (*dict, optional*) – Keyword arguments for the axes for the residuals plot.
- **ax_fit_kws** (*dict, optional*) – Keyword arguments for the axes for the fit plot.
- **fig_kws** (*dict, optional*) – Keyword arguments for a new figure, if there is one being created.

Returns

Return type A tuple with matplotlib's Figure and GridSpec objects.

Notes

The method combines ModelResult.plot_fit and ModelResult.plot_residuals.

If *yerr* is specified or if the fit model included weights, then matplotlib.axes.Axes.errorbar is used to plot the data. If *yerr* is not specified and the fit includes weights, *yerr* set to 1/self.weights

If *fig* is None then *matplotlib.pyplot.figure(**fig_kws)* is called, otherwise *fig_kws* is ignored.

See also:

`ModelResult.plot_fit()` Plot the fit results using matplotlib.

`ModelResult.plot_residuals()` Plot the fit residuals using matplotlib.

`ModelResult.plot_fit(*args, **kws)`

Plot the fit results using matplotlib, if available.

The plot will include the data points, the initial fit curve, and the best-fit curve. If the fit model included weights or if *yerr* is specified, errorbars will also be plotted.

Parameters

- **ax** (*matplotlib.axes.Axes, optional*) – The axes to plot on. The default in None, which means use the current pyplot axis or create one if there is none.
- **datafmt** (*str, optional*) – Matplotlib format string for data points.
- **fitfmt** (*str, optional*) – Matplotlib format string for fitted curve.
- **initfmt** (*str, optional*) – Matplotlib format string for initial conditions for the fit.
- **xlabel** (*str, optional*) – Matplotlib format string for labeling the x-axis.
- **ylabel** (*str, optional*) – Matplotlib format string for labeling the y-axis.
- **yerr** (*numpy.ndarray, optional*) – Array of uncertainties for data array.
- **numpoints** (*int, optional*) – If provided, the final and initial fit curves are evaluated not only at data points, but refined to contain *numpoints* points in total.
- **data_kws** (*dict, optional*) – Keyword arguments passed on to the plot function for data points.
- **fit_kws** (*dict, optional*) – Keyword arguments passed on to the plot function for fitted curve.
- **init_kws** (*dict, optional*) – Keyword arguments passed on to the plot function for the initial conditions of the fit.
- **ax_kws** (*dict, optional*) – Keyword arguments for a new axis, if there is one being created.

Returns

Return type matplotlib.axes.Axes

Notes

For details about plot format strings and keyword arguments see documentation of matplotlib.axes.Axes.plot.

If *yerr* is specified or if the fit model included weights, then matplotlib.axes.Axes.errorbar is used to plot the data. If *yerr* is not specified and the fit includes weights, *yerr* set to 1/self.weights

If *ax* is None then *matplotlib.pyplot.gca(**ax_kws)* is called.

See also:

`ModelResult.plot_residuals()` Plot the fit residuals using matplotlib.

`ModelResult.plot()` Plot the fit results and residuals using matplotlib.

`ModelResult.`**`plot_residuals`**`(*args, **kws)`

Plot the fit residuals using matplotlib, if available.

If *yerr* is supplied or if the model included weights, errorbars will also be plotted.

Parameters

- **ax** (`matplotlib.axes.Axes, optional`) – The axes to plot on. The default in None, which means use the current pyplot axis or create one if there is none.
- **datafmt** (`str, optional`) – Matplotlib format string for data points.
- **yerr** (`numpy.ndarray, optional`) – Array of uncertainties for data array.
- **data_kws** (`dict, optional`) – Keyword arguments passed on to the plot function for data points.
- **fit_kws** (`dict, optional`) – Keyword arguments passed on to the plot function for fitted curve.
- **ax_kws** (`dict, optional`) – Keyword arguments for a new axis, if there is one being created.

Returns

Return type matplotlib.axes.Axes

Notes

For details about plot format strings and keyword arguments see documentation of matplotlib.axes.Axes.plot.

If *yerr* is specified or if the fit model included weights, then matplotlib.axes.Axes.errorbar is used to plot the data. If *yerr* is not specified and the fit includes weights, *yerr* set to 1/self.weights

If *ax* is None then *matplotlib.pyplot.gca(**ax_kws)* is called.

See also:

`ModelResult.plot_fit()` Plot the fit results using matplotlib.

`ModelResult.plot()` Plot the fit results and residuals using matplotlib.

7.3.2 `ModelResult` attributes

aic
Floating point best-fit Akaike Information Criterion statistic (see *MinimizerResult – the optimization result*).

best_fit
numpy.ndarray result of model function, evaluated at provided independent variables and with best-fit parameters.

best_values
Dictionary with parameter names as keys, and best-fit values as values.

bic
Floating point best-fit Bayesian Information Criterion statistic (see *MinimizerResult – the optimization result*).

chisqr
Floating point best-fit chi-square statistic (see *MinimizerResult – the optimization result*).

ci_out
Confidence interval data (see *Calculation of confidence intervals*) or None if the confidence intervals have not been calculated.

covar
numpy.ndarray (square) covariance matrix returned from fit.

data
numpy.ndarray of data to compare to model.

errorbars
Boolean for whether error bars were estimated by fit.

ier
Integer returned code from scipy.optimize.leastsq.

init_fit
numpy.ndarray result of model function, evaluated at provided independent variables and with initial parameters.

init_params
Initial parameters.

init_values
Dictionary with parameter names as keys, and initial values as values.

iter_cb
Optional callable function, to be called at each fit iteration. This must take take arguments of `(params, iter, resid, *args, **kws)`, where *params* will have the current parameter values, *iter* the iteration, *resid* the current residual array, and **args* and ***kws* as passed to the objective function. See *Using a Iteration Callback Function*.

jacfcn
Optional callable function, to be called to calculate Jacobian array.

lmdif_message
String message returned from scipy.optimize.leastsq.

message
String message returned from `minimize()`.

method
String naming fitting method for `minimize()`.

model
Instance of `Model` used for model.

ndata
Integer number of data points.

nfev
Integer number of function evaluations used for fit.

nfree
Integer number of free parameters in fit.

nvarys
Integer number of independent, freely varying variables in fit.

params
Parameters used in fit. Will have best-fit values.

redchi
Floating point reduced chi-square statistic (see *MinimizerResult – the optimization result*).

residual
numpy.ndarray for residual.

scale_covar
Boolean flag for whether to automatically scale covariance matrix.

success
Boolean value of whether fit succeeded.

weights
numpy.ndarray (or None) of weighting values to be used in fit. If not None, it will be used as a multiplicative factor of the residual array, so that `weights*(data - fit)` is minimized in the least-squares sense.

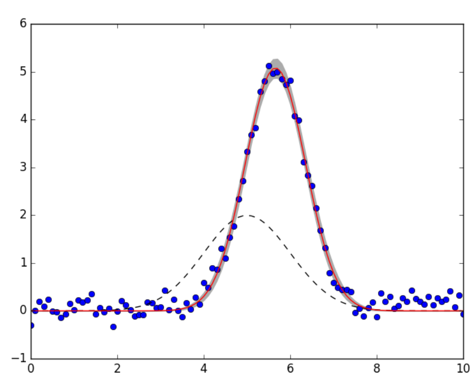
7.3.3 Calculating uncertainties in the model function

We return to the first example above and ask not only for the uncertainties in the fitted parameters but for the range of values that those uncertainties mean for the model function itself. We can use the `ModelResult.eval_uncertainty()` method of the model result object to evaluate the uncertainty in the model with a specified level for $sigma$.

That is, adding:

```
dely = result.eval_uncertainty(sigma=3)
plt.fill_between(x, result.best_fit-dely, result.best_fit+dely, color="#ABABAB")
```

to the example fit to the Gaussian at the beginning of this chapter will give $3-sigma$ bands for the best-fit Gaussian, and produce the figure below.



7.4 Composite Models : adding (or multiplying) Models

One of the more interesting features of the *Model* class is that Models can be added together or combined with basic algebraic operations (add, subtract, multiply, and divide) to give a composite model. The composite model will have parameters from each of the component models, with all parameters being available to influence the whole model. This ability to combine models will become even more useful in the next chapter, when pre-built subclasses of *Model* are discussed. For now, we'll consider a simple example, and build a model of a Gaussian plus a line, as to model a peak with a background. For such a simple problem, we could just build a model that included both components:

```
def gaussian_plus_line(x, amp, cen, wid, slope, intercept):
    "line + 1-d gaussian"

    gauss = (amp/(sqrt(2*pi)*wid)) * exp(-(x-cen)**2 /(2*wid**2))
    line = slope * x + intercept
    return gauss + line
```

and use that with:

```
mod = Model(gaussian_plus_line)
```

But we already had a function for a gaussian function, and maybe we'll discover that a linear background isn't sufficient which would mean the model function would have to be changed.

Instead, lmfit allows models to be combined into a *CompositeModel*. As an alternative to including a linear background in our model function, we could define a linear function:

```
def line(x, slope, intercept):
    "a line"
    return slope * x + intercept
```

and build a composite model with just:

```
mod = Model(gaussian) + Model(line)
```

This model has parameters for both component models, and can be used as:

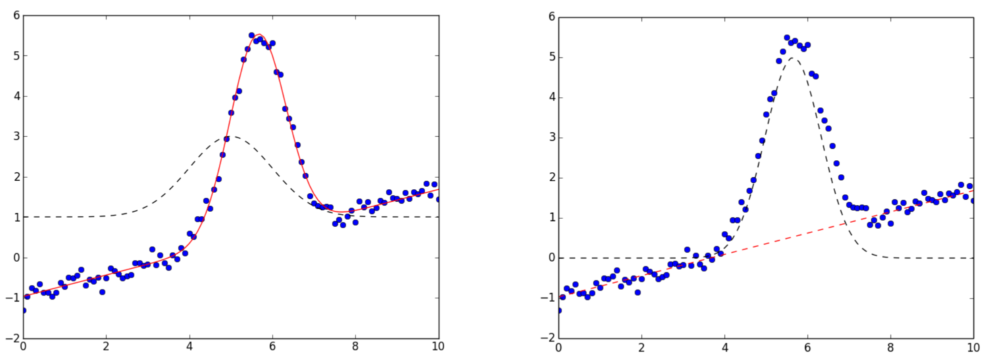
```
#!/usr/bin/env python
#<examples/model_doc2.py>
from numpy import sqrt, pi, exp, loadtxt
from lmfit import Model

import matplotlib.pyplot as plt

data = loadtxt('model1d_gauss.dat')
x = data[:, 0]
y = data[:, 1] + 0.25*x - 1.0

def gaussian(x, amp, cen, wid):
    "1-d gaussian: gaussian(x, amp, cen, wid)"
    return (amp/(sqrt(2*pi)*wid)) * exp(-(x-cen)**2 /(2*wid**2))

def line(x, slope, intercept):
    "line"
    return slope * x + intercept

mod = Model(gaussian) + Model(line)
pars  = mod.make_params( amp=5, cen=5, wid=1, slope=0, intercept=1)
```

```
result = mod.fit(y, pars, x=x)

print(result.fit_report())

plt.plot(x, y,          'bo')
plt.plot(x, result.init_fit, 'k--')
plt.plot(x, result.best_fit, 'r-')
plt.show()
#<end examples/model_doc2.py>
```

which prints out the results:

```
[[Model]]
    (Model(gaussian) + Model(line))
[[Fit Statistics]]
    # function evals   = 44
    # data points      = 101
    # variables        = 5
    chi-square         = 2.579
    reduced chi-square = 0.027
    Akaike info crit   = -360.457
    Bayesian info crit = -347.381
[[Variables]]
    amp:          8.45931061 +/- 0.124145 (1.47%) (init= 5)
    cen:          5.65547872 +/- 0.009176 (0.16%) (init= 5)
    intercept:   -0.96860201 +/- 0.033522 (3.46%) (init= 1)
    slope:        0.26484403 +/- 0.005748 (2.17%) (init= 0)
    wid:          0.67545523 +/- 0.009916 (1.47%) (init= 1)
[[Correlations]] (unreported correlations are <  0.100)
    C(amp, wid)                  =  0.666
    C(cen, intercept)            =  0.129
```

and shows the plot on the left.



On the left, data is shown in blue dots, the total fit is shown in solid red line, and the initial fit is shown as a black dashed line. In the figure on the right, the data is again shown in blue dots, and the Gaussian component shown as a black dashed line, and the linear component shown as a red dashed line. These components were generated after the fit using the Models *ModelResult.eval_components()* method of the *result*:

```
comps = result.eval_components()
```

which returns a dictionary of the components, using keys of the model name (or *prefix* if that is set). This will use the parameter values in *result.params* and the independent variables (*x*) used during the fit. Note that while the `ModelResult` held in *result* does store the best parameters and the best estimate of the model in *result.best_fit*, the original model and parameters in *pars* are left unaltered.

You can apply this composite model to other data sets, or evaluate the model at other values of *x*. You may want to do this to give a finer or coarser spacing of data point, or to extrapolate the model outside the fitting range. This can be done with:

```
xwide = np.linspace(-5, 25, 3001)
predicted = mod.eval(x=xwide)
```

In this example, the argument names for the model functions do not overlap. If they had, the *prefix* argument to `Model` would have allowed us to identify which parameter went with which component model. As we will see in the next chapter, using composite models with the built-in models provides a simple way to build up complex models.

class CompositeModel (*left*, *right*, *op*[, ***kws*])

Combine two models (*left* and *right*) with a binary operator (*op*) into a CompositeModel.

Normally, one does not have to explicitly create a *CompositeModel*, but can use normal Python operators +, '-', *, and / to combine components as in:

```
>>> mod = Model(fcn1) + Model(fcn2) * Model(fcn3)
```

Parameters

- **left** (`Model`) – Left-hand model.
- **right** (`Model`) – Right-hand model.
- **op** (*callable binary operator*) – Operator to combine *left* and *right* models.
- ****kws** (*optional*) – Additional keywords are passed to *Model* when creating this new model.

Notes

1.The two models must use the same independent variable.

Note that when using builtin Python binary operators, a `CompositeModel` will automatically be constructed for you. That is, doing:

```
mod = Model(fcn1) + Model(fcn2) * Model(fcn3)
```

will create a `CompositeModel`. Here, *left* will be *Model(fcn1)*, *op* will be `operator.add()`, and *right* will be another CompositeModel that has a *left* attribute of *Model(fcn2)*, an *op* of `operator.mul()`, and a *right* of *Model(fcn3)*.

To use a binary operator other than '+', '-', '*', or '/' you can explicitly create a `CompositeModel` with the appropriate binary operator. For example, to convolve two models, you could define a simple convolution function, perhaps as:

```
import numpy as np
def convolve(dat, kernel):
    # simple convolution
    npts = min(len(dat), len(kernel))
    pad  = np.ones(npts)
    tmp  = np.concatenate((pad*dat[0], dat, pad*dat[-1]))
```

```
    out  = np.convolve(tmp, kernel, mode='valid')
    noff = int((len(out) - npts)/2)
    return (out[noff:])[:npts]
```

which extends the data in both directions so that the convolving kernel function gives a valid result over the data range. Because this function takes two array arguments and returns an array, it can be used as the binary operator. A full script using this technique is here:

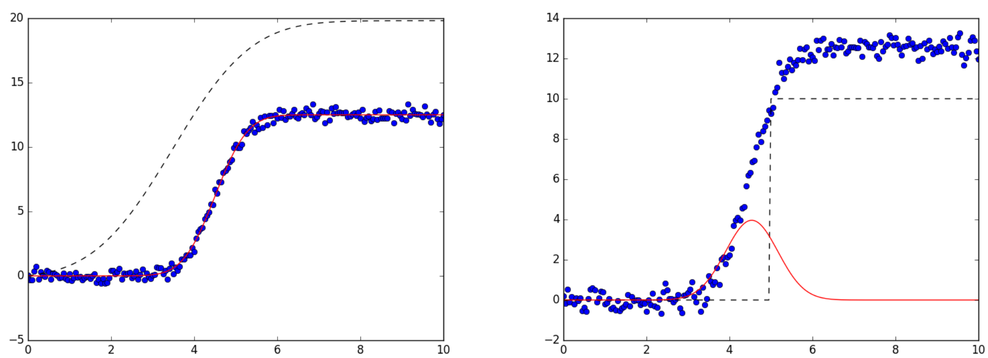
```
#!/usr/bin/env python
#<examples/model_doc3.py>

import numpy as np
from lmfit import Model, CompositeModel
from lmfit.lineshapes import step, gaussian

import matplotlib.pyplot as plt

# create data from broadened step
npts = 201
x = np.linspace(0, 10, npts)
y = step(x, amplitude=12.5, center=4.5, sigma=0.88, form='erf')
y = y + np.random.normal(size=npts, scale=0.35)

def jump(x, mid):
    "heaviside step function"
    o = np.zeros(len(x))
    imid = max(np.where(x<=mid)[0])
    o[imid:] = 1.0
    return o

def convolve(arr, kernel):
    # simple convolution of two arrays
    npts = min(len(arr), len(kernel))
    pad  = np.ones(npts)
    tmp  = np.concatenate((pad*arr[0], arr, pad*arr[-1]))
    out  = np.convolve(tmp, kernel, mode='valid')
    noff = int((len(out) - npts)/2)
    return out[noff:noff+npts]
#
# create Composite Model using the custom convolution operator
mod  = CompositeModel(Model(jump), Model(gaussian), convolve)

pars = mod.make_params(amplitude=1, center=3.5, sigma=1.5, mid=5.0)

# 'mid' and 'center' should be completely correlated, and 'mid' is
# used as an integer index, so a very poor fit variable:
pars['mid'].vary = False

# fit this model to data array y
result =  mod.fit(y, params=pars, x=x)

print(result.fit_report())

plot_components = False

# plot results
plt.plot(x, y,         'bo')
if plot_components:
```

```
    # generate components
    comps = result.eval_components(x=x)
    plt.plot(x, 10*comps['jump'], 'k--')
    plt.plot(x, 10*comps['gaussian'], 'r-')
else:
    plt.plot(x, result.init_fit, 'k--')
    plt.plot(x, result.best_fit, 'r-')
plt.show()
# #<end examples/model_doc3.py>
```

which prints out the results:

```
[[Model]]
    (Model(jump) <function convolve at 0x109ee4488> Model(gaussian))
[[Fit Statistics]]
    # function evals   = 27
    # data points      = 201
    # variables        = 3
    chi-square         = 22.091
    reduced chi-square = 0.112
    Akaike info crit   = -437.837
    Bayesian info crit = -427.927
[[Variables]]
    mid:          5 (fixed)
    sigma:        0.64118585 +/- 0.013233 (2.06%) (init= 1.5)
    center:       4.51633608 +/- 0.009567 (0.21%) (init= 3.5)
    amplitude:    0.62654849 +/- 0.001813 (0.29%) (init= 1)
[[Correlations]] (unreported correlations are <  0.100)
    C(center, amplitude)          =  0.344
    C(sigma, amplitude)           =  0.280
```

and shows the plots:



Using composite models with built-in or custom operators allows you to build complex models from testable sub-components.

CHAPTER

EIGHT

BUILT-IN FITTING MODELS IN THE MODELS MODULE

Lmfit provides several builtin fitting models in the `models` module. These pre-defined models each subclass from the `model.Model` class of the previous chapter and wrap relatively well-known functional forms, such as Gaussians, Lorentzian, and Exponentials that are used in a wide range of scientific domains. In fact, all the models are all based on simple, plain Python functions defined in the `lineshapes` module. In addition to wrapping a function into a `model.Model`, these models also provide a `guess()` method that is intended to give a reasonable set of starting values from a data array that closely approximates the data to be fit.

As shown in the previous chapter, a key feature of the `mode.Model` class is that models can easily be combined to give a composite `model.CompositeModel`. Thus, while some of the models listed here may seem pretty trivial (notably, *ConstantModel* and *LinearModel*), the main point of having these is to be able to use them in composite models. For example, a Lorentzian plus a linear background might be represented as:

```
>>> from lmfit.models import LinearModel, LorentzianModel
>>> peak = LorentzianModel()
>>> background  = LinearModel()
>>> model = peak + background
```

All the models listed below are one dimensional, with an independent variable named `x`. Many of these models represent a function with a distinct peak, and so share common features. To maintain uniformity, common parameter names are used whenever possible. Thus, most models have a parameter called `amplitude` that represents the overall height (or area of) a peak or function, a `center` parameter that represents a peak centroid position, and a `sigma` parameter that gives a characteristic width. Many peak shapes also have a parameter `fwhm` (constrained by `sigma`) giving the full width at half maximum and a parameter `height` (constrained by `sigma` and `amplitude`) to give the maximum peak height.

After a list of builtin models, a few examples of their use is given.

8.1 Peak-like models

There are many peak-like models available. These include *GaussianModel*, *LorentzianModel*, *VoigtModel* and some less commonly used variations. The `guess()` methods for all of these make a fairly crude guess for the value of `amplitude`, but also set a lower bound of 0 on the value of `sigma`.

8.1.1 GaussianModel

class GaussianModel (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Gaussian or normal distribution lineshape. (see http://en.wikipedia.org/wiki/Normal_distribution), with three Parameters: `amplitude`, `center`, and `sigma`. In addition, parameters `fwhm` and

height are included as constraints to report full width at half maximum and maximum peak height, respectively.

$$f(x; A, \mu, \sigma) = \frac{A}{\sigma\sqrt{2\pi}} e^{[-(x-\mu)^2/2\sigma^2]}$$

where the parameter amplitude corresponds to A, center to μ, and sigma to σ. The full width at half maximum is $2\sigma\sqrt{2\ln 2}$, approximately 2.3548σ.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to Model.

8.1.2 LorentzianModel

class LorentzianModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Lorentzian or Cauchy-Lorentz distribution function (see http://en.wikipedia.org/wiki/Cauchy_distribution), with three Parameters: amplitude, center, and sigma. In addition, parameters fwhm and height are included as constraints to report full width at half maximum and maximum peak height, respectively.

$$f(x; A, \mu, \sigma) = \frac{A}{\pi} \big[\frac{\sigma}{(x-\mu)^2 + \sigma^2}\big]$$

where the parameter amplitude corresponds to A, center to μ, and sigma to σ. The full width at half maximum is 2σ.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to Model.

8.1.3 VoigtModel

class VoigtModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Voigt distribution function (see http://en.wikipedia.org/wiki/Voigt_profile>), with four Parameters: `amplitude`, `center`, `sigma`, and `gamma`. By default, `gamma` is constrained to have value equal to `sigma`, though it can be varied independently. In addition, parameters `fwhm` and `height` are included as constraints to report full width at half maximum and maximum peak height, respectively. The definition for the Voigt function used here is

$$f(x; A, \mu, \sigma, \gamma) = \frac{A \textrm{Re}[w(z)]}{\sigma\sqrt{2 \pi}}$$

where

$$\begin{aligned} z &= \frac{x-\mu +i\gamma}{\sigma\sqrt{2}} \\ w(z) &= e^{-z^2}{\operatorname{erfc}}(-iz) \end{aligned}$$

and `erfc()` is the complimentary error function. As above, `amplitude` corresponds to A, `center` to μ, and `sigma` to σ. The parameter `gamma` corresponds to γ. If `gamma` is kept at the default value (constrained to `sigma`), the full width at half maximum is approximately 3.6013σ.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.4 PseudoVoigtModel

class PseudoVoigtModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a pseudo-Voigt distribution function (see http://en.wikipedia.org/wiki/Voigt_profile#Pseudo-Voigt_Approximation), which is a weighted sum of a Gaussian and Lorentzian distribution functions with that share values for `amplitude` (A), `center` (μ) and full width at half maximum (and so have constrained values of `sigma` (σ). A parameter `fraction` (α) controls the relative weight of the Gaussian and Lorentzian components, giving the full definition of

$$f(x; A, \mu, \sigma, \alpha) = \frac{(1-\alpha)A}{\sigma_g\sqrt{2\pi}} e^{[{-{(x-\mu)^2}/{{2\sigma_g}^2}}]} + \frac{\alpha A}{\pi} \big[\frac{\sigma}{(x - \mu)^2 + \sigma^2}\big]$$

where $\sigma_g = {\sigma}/{\sqrt{2\ln{2}}}$ so that the full width at half maximum of each component and of the sum is 2σ. The `guess()` function always sets the starting value for `fraction` at 0.5.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.

- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.5 MoffatModel

class MoffatModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on the Moffat distribution function (see https://en.wikipedia.org/wiki/Moffat_distribution), with four Parameters: `amplitude` (A), `center` (μ), a width parameter `sigma` (σ) and an exponent `beta` (β).

$$f(x; A, \mu, \sigma, \beta) = A\big[(\frac{x-\mu}{\sigma})^2 + 1\big]^{-\beta}$$

the full width have maximum is $2\sigma\sqrt{2^{1/\beta}-1}$. The `guess()` function always sets the starting value for `beta` to 1.

Note that for ($\beta = 1$) the Moffat has a Lorentzian shape.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.6 Pearson7Model

class Pearson7Model(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Pearson VII distribution (see http://en.wikipedia.org/wiki/Pearson_distribution#The_Pearson_type_VII_distribution), with four parameers: `amplitude` (A), `center` (μ), `sigma` (σ), and `exponent` (m) in

$$f(x; A, \mu, \sigma, m) = \frac{A}{\sigma\beta(m-\frac{1}{2}, \frac{1}{2})}\big[1 + \frac{(x-\mu)^2}{\sigma^2}\big]^{-m}$$

where β is the beta function (see scipy.special.beta in `scipy.special`). The `guess()` function always gives a starting value for `exponent` of 1.5.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.7 StudentsTModel

class StudentsTModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Student's t distribution function (see http://en.wikipedia.org/wiki/Student%27s_t-distribution), with three Parameters: `amplitude` (A), `center` (μ) and `sigma` (σ) in

$$f(x; A, \mu, \sigma) = \frac{A \Gamma(\frac{\sigma+1}{2})}{\sqrt{\sigma\pi}\,\Gamma(\frac{\sigma}{2})} \Bigg[1 + \frac{(x-\mu)^2}{\sigma}\Bigg]^{-\frac{\sigma+1}{2}}$$

where $\Gamma(x)$ is the gamma function.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.8 BreitWignerModel

class BreitWignerModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Breit-Wigner-Fano function (see http://en.wikipedia.org/wiki/Fano_resonance>), with four Parameters: `amplitude` (A), `center` (μ), `sigma` (σ), and `q` (q) in

$$f(x; A, \mu, \sigma, q) = \frac{A (q\sigma/2 + x - \mu)^2}{(\sigma/2)^2 + (x - \mu)^2}$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.

- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.9 `LognormalModel`

class LognormalModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on the Log-normal distribution function (see http://en.wikipedia.org/wiki/Lognormal), with three Parameters `amplitude` (A), `center` (μ) and `sigma` (σ) in

$$f(x; A, \mu, \sigma) = \frac{A e^{-(\ln(x)-\mu)/2\sigma^2}}{x}$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.10 `DampedOcsillatorModel`

class DampedOscillatorModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on the Damped Harmonic Oscillator Amplitude (see http://en.wikipedia.org/wiki/Harmonic_oscillator#Amplitude_part), with three Parameters: `amplitude` (A), `center` (μ) and `sigma` (σ) in

$$f(x; A, \mu, \sigma) = \frac{A}{\sqrt{[1 - (x/\mu)^2]^2 + (2\sigma x/\mu)^2}}$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.

- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.11 `DampedHarmonicOcsillatorModel`

class DampedHarmonicOscillatorModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a variation of the Damped Harmonic Oscillator (see http://en.wikipedia.org/wiki/Harmonic_oscillator), following the definition given in DAVE/PAN (see https://www.ncnr.nist.gov/dave/) with four Parameters: `amplitude` (A), `center` (μ), `sigma` (σ), and `gamma` (γ) in

$$f(x; A, \mu, \sigma, \gamma) = \frac{A\sigma}{\pi[1 - \exp(-x/\gamma)]}\Big[\frac{1}{(x-\mu)^2 + \sigma^2} - \frac{1}{(x+\mu)^2 + \sigma^2}\Big]$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.12 `ExponentialGaussianModel`

class ExponentialGaussianModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model of an Exponentially modified Gaussian distribution (see http://en.wikipedia.org/wiki/Exponentially_modified_Gaussian_distribution) with four Parameters `amplitude` (A), `center` (μ), `sigma` (σ), and `gamma` (γ) in

$$f(x; A, \mu, \sigma, \gamma) = \frac{A\gamma}{2} \exp\big[\gamma({\mu - x + \gamma\sigma^2/2})\big] {\operatorname{erfc}}\Big(\frac{\mu + \gamma\sigma^2 - x}{\sqrt{2}\sigma}\Big)$$

where `erfc()` is the complimentary error function.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.

- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.13 SkewedGaussianModel

class SkewedGaussianModel (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A variation of the Exponential Gaussian, this uses a skewed normal distribution (see http://en.wikipedia.org/wiki/Skew_normal_distribution), with Parameters `amplitude` (A), `center` (μ), `sigma` (σ), and `gamma` (γ) in

$$f(x; A, \mu, \sigma, \gamma) = \frac{A}{\sigma\sqrt{2\pi}} e^{[-(x-\mu)^2/2\sigma^2]} \Big\{ 1 + \mathrm{erf}\big[\frac{\gamma(x-\mu)}{\sigma\sqrt{2}}\big] \Big\}$$

where `erf()` is the error function.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.1.14 DonaichModel

class DonaichModel (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model of an Doniach Sunjic asymmetric lineshape (see http://www.casaxps.com/help_manual/line_shapes.htm), used in photo-emission, with four Parameters `amplitude` (A), `center` (μ), `sigma` (σ), and `gamma` (γ) in

$$f(x; A, \mu, \sigma, \gamma) = A \frac{\cos\big[\pi\gamma/2 + (1-\gamma)\arctan{(x-\mu)/\sigma}\big]}{\big[1 + (x-\mu)/\sigma\big]^{(1-\gamma)/2}}$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.

- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.2 Linear and Polynomial Models

These models correspond to polynomials of some degree. Of course, lmfit is a very inefficient way to do linear regression (see numpy.polyfit or scipy.stats.linregress), but these models may be useful as one of many components of composite model.

8.2.1 ConstantModel

class ConstantModel(*independent_vars=['x'], prefix='', missing=None, **kwargs*)

Constant model, with a single Parameter: `c`.

Note that this is 'constant' in the sense of having no dependence on the independent variable `x`, not in the sense of being non- varying. To be clear, `c` will be a Parameter that will be varied in the fit (by default, of course).

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.2.2 LinearModel

class LinearModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

Linear model, with two Parameters `intercept` and `slope`.

Defined as:

$$f(x; m, b) = mx + b$$

with `slope` for m and `intercept` for b.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.

- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.2.3 `QuadraticModel`

class QuadraticModel(*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A quadratic model, with three Parameters `a`, `b`, and `c`.

Defined as:

$$f(x; a, b, c) = ax^2 + bx + c$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.2.4 `PolynomialModel`

class PolynomialModel(*degree, independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A polynomial model with up to 7 Parameters, specfied by `degree`.

$$f(x; c_0, c_1, \ldots, c_7) = \sum_{i=0,7} c_i x^i$$

with parameters `c0`, `c1`, ..., `c7`. The supplied `degree` will specify how many of these are actual variable parameters. This uses numpy.polyval for its calculation of the polynomial.

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.

- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.3 Step-like models

Two models represent step-like functions, and share many characteristics.

8.3.1 StepModel

class StepModel (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Step function, with three Parameters: `amplitude` (A), `center` (μ) and `sigma` (σ) and four choices for functional form:

- `linear` (the default)
- `atan` or `arctan` for an arc-tangent function
- `erf` for an error function
- `logistic` for a logistic function (see http://en.wikipedia.org/wiki/Logistic_function).

The step function starts with a value 0, and ends with a value of A rising to $A/2$ at μ, with σ setting the characteristic width. The forms are

$$\begin{aligned} f(x;A,\mu,\sigma,\mathrm{form}='\mathrm{linear}') &= A\min\left[1,\max\left(0,\alpha\right)\right] \\ f(x;A,\mu,\sigma,\mathrm{form}='\mathrm{arctan}') &= A[1/2+\arctan\left(\alpha\right)/\pi] \\ f(x;A,\mu,\sigma,\mathrm{form}='\mathrm{erf}') &= A[1+\mathrm{erf}(\alpha)]/2 \\ f(x;A,\mu,\sigma,\mathrm{form}='\mathrm{logistic}') &= A[1-\frac{1}{1+e^{\alpha}}] \end{aligned}$$

where $\alpha = (x-\mu)/\sigma$.

Parameters

- **independent_vars** (`['x']`) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.3.2 `RectangleModel`

class **`RectangleModel`** (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Step-up and Step-down function, with five Parameters: `amplitude` (A), `center1` (μ_1), `center2` (μ_2), *sigma1'* (σ_1) and `sigma2` (σ_2) and four choices for functional form (which is used for both the Step up and the Step down:

- `linear` (the default)
- `atan` or `arctan` for an arc-tangent function
- `erf` for an error function
- `logistic` for a logistic function (see http://en.wikipedia.org/wiki/Logistic_function).

The function starts with a value 0, transitions to a value of A, taking the value $A/2$ at μ_1, with σ_1 setting the characteristic width. The function then transitions again to the value $A/2$ at μ_2, with σ_2 setting the characteristic width. The forms are

$$
\begin{aligned}
f(x; A, \mu, \sigma, \mathrm{form} = '\mathrm{linear}') &= A\{\min[1, \max(0, \alpha_1)] + \min[-1, \max(0, \alpha_2)]\} \\
f(x; A, \mu, \sigma, \mathrm{form} = '\mathrm{arctan}') &= A[\arctan(\alpha_1) + \arctan(\alpha_2)]/\pi \\
f(x; A, \mu, \sigma, \mathrm{form} = '\mathrm{erf}') &= A[\mathrm{erf}(\alpha_1) + \mathrm{erf}(\alpha_2)]/2 \\
f(x; A, \mu, \sigma, \mathrm{form} = '\mathrm{logistic}') &= A[1 - \frac{1}{1 + e^{\alpha_1}} - \frac{1}{1 + e^{\alpha_2}}]
\end{aligned}
$$

where $\alpha_1 = (x - \mu_1)/\sigma_1$ and $\alpha_2 = -(x - \mu_2)/\sigma_2$.

Parameters

- **`independent_vars`** (*['x']*) – Arguments to func that are independent variables.
- **`prefix`** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **`missing`** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- **`**kwargs`** (*optional*) – Keyword arguments to pass to `Model`.

8.4 Exponential and Power law models

8.4.1 `ExponentialModel`

class **`ExponentialModel`** (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on an exponential decay function (see http://en.wikipedia.org/wiki/Exponential_decay) with two Parameters: `amplitude` (A), and `decay` (τ), in:

$$f(x; A, \tau) = Ae^{-x/\tau}$$

Parameters

- **`independent_vars`** (*['x']*) – Arguments to func that are independent variables.

- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.4.2 PowerLawModel

class PowerLawModel (*independent_vars=['x'], prefix='', missing=None, name=None, **kwargs*)

A model based on a Power Law (see http://en.wikipedia.org/wiki/Power_law>), with two Parameters: `amplitude` (A), and `exponent` (k), in:

$$f(x; A, k) = Ax^k$$

Parameters

- **independent_vars** (*['x']*) – Arguments to func that are independent variables.
- **prefix** (*string, optional*) – String to prepend to parameter names, needed to add two Models that have parameter names in common.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kwargs** (*optional*) – Keyword arguments to pass to `Model`.

8.5 User-defined Models

As shown in the previous chapter (*Modeling Data and Curve Fitting*), it is fairly straightforward to build fitting models from parametrized Python functions. The number of model classes listed so far in the present chapter should make it clear that this process is not too difficult. Still, it is sometimes desirable to build models from a user-supplied function. This may be especially true if model-building is built-in to some larger library or application for fitting in which the user may not be able to easily build and use a new model from Python code.

The *ExpressionModel* allows a model to be built from a user-supplied expression. This uses the asteval module also used for mathematical constraints as discussed in *Using Mathematical Constraints*.

8.5.1 ExpressionModel

class ExpressionModel (*expr, independent_vars=None, init_script=None, missing=None, **kws*)

Model from User-supplied expression.

Parameters

- **expr** (*str*) – Mathematical expression for model.
- **independent_vars** (*list of strings or None, optional*) – Variable names to use as independent variables.
- **init_script** (*string or None, optional*) – Initial script to run in asteval interpreter.
- **missing** (*str or None, optional*) – How to handle NaN and missing values in data. One of:
  - 'none' or None: Do not check for null or missing values (default).
  - 'drop': Drop null or missing observations in data. if pandas is installed, *pandas.isnull* is used, otherwise *numpy.isnan* is used.
  - 'raise': Raise a (more helpful) exception when data contains null or missing values.
- ****kws** (*optional*) – Keyword arguments to pass to `Model`.

Notes

1.each instance of ExpressionModel will create and using its own version of an asteval interpreter.

2.prefix is **not supported** for ExpressionModel

Since the point of this model is that an arbitrary expression will be supplied, the determination of what are the parameter names for the model happens when the model is created. To do this, the expression is parsed, and all symbol names are found. Names that are already known (there are over 500 function and value names in the asteval namespace, including most Python builtins, more than 200 functions inherited from NumPy, and more than 20 common lineshapes defined in the `lineshapes` module) are not converted to parameters. Unrecognized name are expected to be names either of parameters or independent variables. If *independent_vars* is the default value of None, and if the expression contains a variable named *x*, that will be used as the independent variable. Otherwise, *independent_vars* must be given.

For example, if one creates an `ExpressionModel` as:

```
>>> mod = ExpressionModel('off + amp * exp(-x/x0) * sin(x*phase)')
```

The name *exp* will be recognized as the exponent function, so the model will be interpreted to have parameters named *off*, *amp*, *x0* and *phase*. In addition, *x* will be assumed to be the sole independent variable. In general, there is no obvious way to set default parameter values or parameter hints for bounds, so this will have to be handled explicitly.

To evaluate this model, you might do the following:

```
>>> x = numpy.linspace(0, 10, 501)
>>> params = mod.make_params(off=0.25, amp=1.0, x0=2.0, phase=0.04)
>>> y = mod.eval(params, x=x)
```

While many custom models can be built with a single line expression (especially since the names of the lineshapes like *gaussian*, *lorentzian* and so on, as well as many NumPy functions, are available), more complex models will inevitably require multiple line functions. You can include such Python code with the *init_script* argument. The text of this script is evaluated when the model is initialized (and before the actual expression is parsed), so that you can define functions to be used in your expression.

As a probably unphysical example, to make a model that is the derivative of a Gaussian function times the logarithm of a Lorentzian function you may could to define this in a script:

```
>>> script = """
def mycurve(x, amp, cen, sig):
    loren = lorentzian(x, amplitude=amp, center=cen, sigma=sig)
    gauss = gaussian(x, amplitude=amp, center=cen, sigma=sig)
    return log(loren)*gradient(gauss)/gradient(x)
"""
```

and then use this with `ExpressionModel` as:

```
>>> mod = ExpressionModel('mycurve(x, height, mid, wid)',
                          init_script=script,
                          independent_vars=['x'])
```

As above, this will interpret the parameter names to be *height*, *mid*, and *wid*, and build a model that can be used to fit data.

8.6 Example 1: Fit Peaked data to Gaussian, Lorentzian, and Voigt profiles

Here, we will fit data to three similar line shapes, in order to decide which might be the better model. We will start with a Gaussian profile, as in the previous chapter, but use the built-in `GaussianModel` instead of writing one ourselves. This is a slightly different version from the one in previous example in that the parameter names are different, and have built-in default values. We will simply use:

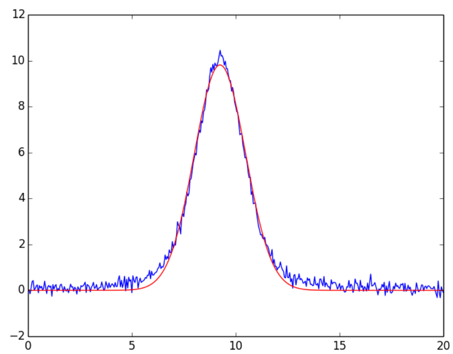
```
from numpy import loadtxt
from lmfit.models import GaussianModel

data = loadtxt('test_peak.dat')
x = data[:, 0]
y = data[:, 1]

mod = GaussianModel()

pars = mod.guess(y, x=x)
out  = mod.fit(y, pars, x=x)
print(out.fit_report(min_correl=0.25))
```

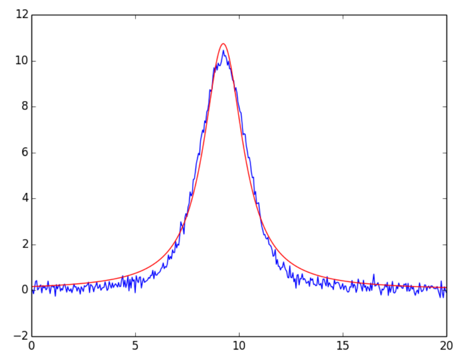
which prints out the results:

```
[[Model]]
    Model(gaussian)
[[Fit Statistics]]
    # function evals   = 23
    # data points      = 401
    # variables        = 3
    chi-square         = 29.994
    reduced chi-square = 0.075
    Akaike info crit   = -1033.774
    Bayesian info crit = -1021.792
[[Variables]]
    sigma:       1.23218319 +/- 0.007374 (0.60%) (init= 1.35)
    center:      9.24277049 +/- 0.007374 (0.08%) (init= 9.25)
    amplitude:   30.3135571 +/- 0.157126 (0.52%) (init= 29.08159)
    fwhm:        2.90156963 +/- 0.017366 (0.60%)  == '2.3548200*sigma'
    height:      9.81457973 +/- 0.050872 (0.52%)  == '0.3989423*amplitude/max(1.e-15,
↪sigma)'
```

```
[[Correlations]] (unreported correlations are <  0.250)
    C(sigma, amplitude)          =  0.577
```

We see a few interesting differences from the results of the previous chapter. First, the parameter names are longer. Second, there are `fwhm` and `height` parameters, to give the full width at half maximum and maximum peak height. And third, the automated initial guesses are pretty good. A plot of the fit:





Fit to peak with Gaussian (left) and Lorentzian (right) models.

shows a decent match to the data – the fit worked with no explicit setting of initial parameter values. Looking more closing, the fit is not perfect, especially in the tails of the peak, suggesting that a different peak shape, with longer tails, should be used. Perhaps a Lorentzian would be better? To do this, we simply replace `GaussianModel` with `LorentzianModel` to get a *LorentzianModel*:

```
from lmfit.models import LorentzianModel
mod = LorentzianModel()
```

with the rest of the script as above. Perhaps predictably, the first thing we try gives results that are worse:

```
[[Model]]
    Model(lorentzian)
[[Fit Statistics]]
    # function evals   = 27
    # data points      = 401
    # variables        = 3
    chi-square         = 53.754
    reduced chi-square = 0.135
    Akaike info crit   = -799.830
    Bayesian info crit = -787.848
[[Variables]]
    sigma:       1.15484517 +/- 0.013156 (1.14%) (init= 1.35)
    center:      9.24438944 +/- 0.009275 (0.10%) (init= 9.25)
    amplitude:   38.9728645 +/- 0.313857 (0.81%) (init= 36.35199)
    fwhm:        2.30969034 +/- 0.026312 (1.14%)  == '2.0000000*sigma'
    height:      10.7420881 +/- 0.086336 (0.80%)  == '0.3183099*amplitude/max(1.e-15,␣
↪sigma)'
[[Correlations]] (unreported correlations are <  0.250)
    C(sigma, amplitude)          =  0.709
```

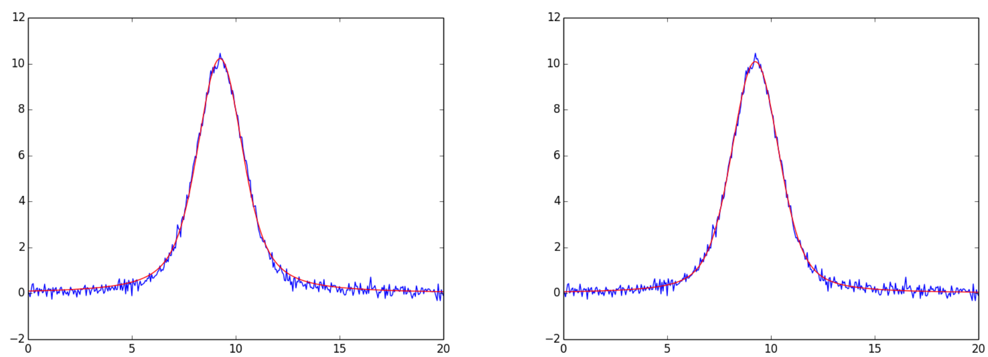
with the plot shown on the right in the figure above. The tails are now too big, and the value for χ^2 almost doubled. A Voigt model does a better job. Using *VoigtModel*, this is as simple as using:

```
from lmfit.models import VoigtModel
mod = VoigtModel()
```

with all the rest of the script as above. This gives:

```
[[Model]]
    Model(voigt)
[[Fit Statistics]]
    # function evals   = 19
    # data points      = 401
    # variables        = 3
    chi-square         = 14.545
    reduced chi-square = 0.037
    Akaike info crit   = -1324.006
    Bayesian info crit = -1312.024
[[Variables]]
    amplitude:   35.7554017 +/- 0.138614 (0.39%) (init= 43.62238)
    sigma:       0.73015574 +/- 0.003684 (0.50%) (init= 0.8775)
    center:      9.24411142 +/- 0.005054 (0.05%) (init= 9.25)
    gamma:       0.73015574 +/- 0.003684 (0.50%)  == 'sigma'
    fwhm:        2.62951718 +/- 0.013269 (0.50%)  == '3.6013100*sigma'
    height:      19.5360268 +/- 0.075691 (0.39%)  == '0.3989423*amplitude/max(1.e-15,
↪sigma)'
[[Correlations]] (unreported correlations are <  0.250)
    C(sigma, amplitude)          =  0.651
```

which has a much better value for χ^2 and an obviously better match to the data as seen in the figure below (left).



Fit to peak with Voigt model (left) and Voigt model with `gamma` varying independently of `sigma` (right).

Can we do better? The Voigt function has a γ parameter (`gamma`) that can be distinct from `sigma`. The default behavior used above constrains `gamma` to have exactly the same value as `sigma`. If we allow these to vary separately, does the fit improve? To do this, we have to change the `gamma` parameter from a constrained expression and give it a starting value using something like:

```
mod = VoigtModel()
pars = mod.guess(y, x=x)
pars['gamma'].set(value=0.7, vary=True, expr='')
```

which gives:

```
[[Model]]
    Model(voigt)
[[Fit Statistics]]
    # function evals   = 23
    # data points      = 401
    # variables        = 4
    chi-square         = 10.930
```

```
    reduced chi-square = 0.028
    Akaike info crit   = -1436.576
    Bayesian info crit = -1420.600
[[Variables]]
    amplitude:   34.1914716 +/- 0.179468 (0.52%) (init= 43.62238)
    sigma:       0.89518950 +/- 0.014154 (1.58%) (init= 0.8775)
    center:      9.24374845 +/- 0.004419 (0.05%) (init= 9.25)
    gamma:       0.52540156 +/- 0.018579 (3.54%) (init= 0.7)
    fwhm:        3.22385492 +/- 0.050974 (1.58%)  == '3.6013100*sigma'
    height:      15.2374711 +/- 0.299235 (1.96%)  == '0.3989423*amplitude/max(1.e-15,␣
↪sigma)'
[[Correlations]] (unreported correlations are <  0.250)
    C(sigma, gamma)              = -0.928
    C(gamma, amplitude)          =  0.821
    C(sigma, amplitude)          = -0.651
```

and the fit shown on the right above.

Comparing the two fits with the Voigt function, we see that χ^2 is definitely improved with a separately varying `gamma` parameter. In addition, the two values for `gamma` and `sigma` differ significantly – well outside the estimated uncertainties. More compelling, reduced χ^2 is improved even though a fourth variable has been added to the fit. In the simplest statistical sense, this suggests that `gamma` is a significant variable in the model. In addition, we can use both the Akaike or Bayesian Information Criteria (see *Akaike and Bayesian Information Criteria*) to assess how likely the model with variable `gamma` is to explain the data than the model with `gamma` fixed to the value of `sigma`. According to theory, $\exp(-(\mathrm{AIC1}-\mathrm{AIC0})/2)$ gives the probability that a model with AIC1 is more likely than a model with AIC0. For the two models here, with AIC values of -1432 and -1321 (Note: if we had more carefully set the value for `weights` based on the noise in the data, these values might be positive, but there difference would be roughly the same), this says that the model with `gamma` fixed to `sigma` has a probability less than 1.e-25 of being the better model.

8.7 Example 2: Fit data to a Composite Model with pre-defined models

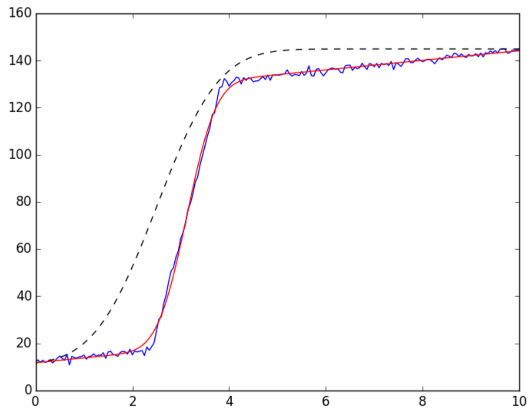
Here, we repeat the point made at the end of the last chapter that instances of `model.Model` class can be added together to make a *composite model*. By using the large number of built-in models available, it is therefore very simple to build models that contain multiple peaks and various backgrounds. An example of a simple fit to a noisy step function plus a constant:

```
#!/usr/bin/env python
#<examples/doc_stepmodel.py>
import numpy as np
from lmfit.models import StepModel, LinearModel

import matplotlib.pyplot as plt

x = np.linspace(0, 10, 201)
y = np.ones_like(x)
y[:48] = 0.0
y[48:77] = np.arange(77-48)/(77.0-48)
y = 110.2 * (y + 9e-3*np.random.randn(len(x))) + 12.0 + 2.22*x

step_mod = StepModel(form='erf', prefix='step_')
line_mod = LinearModel(prefix='line_')
```

```
pars =  line_mod.make_params(intercept=y.min(), slope=0)
pars += step_mod.guess(y, x=x, center=2.5)

mod = step_mod + line_mod
out = mod.fit(y, pars, x=x)

print(out.fit_report())

plt.plot(x, y)
plt.plot(x, out.init_fit, 'k--')
plt.plot(x, out.best_fit, 'r-')
plt.show()
#<end examples/doc_stepmodel.py>
```

After constructing step-like data, we first create a *StepModel* telling it to use the `erf` form (see details above), and a *ConstantModel*. We set initial values, in one case using the data and `guess()` method for the initial step function paramaters, and `make_params()` arguments for the linear component. After making a composite model, we run `fit()` and report the results, which gives:

```
[[Model]]
    (Model(step, prefix='step_', form='erf') + Model(linear, prefix='line_'))
[[Fit Statistics]]
    # function evals   = 51
    # data points      = 201
    # variables        = 5
    chi-square         = 584.829
    reduced chi-square = 2.984
    Akaike info crit   = 224.671
    Bayesian info crit = 241.187
[[Variables]]
    line_slope:       2.03039786 +/- 0.092221 (4.54%) (init= 0)
    line_intercept:   11.7234542 +/- 0.274094 (2.34%) (init= 10.7816)
    step_amplitude:   112.071629 +/- 0.647316 (0.58%) (init= 134.0885)
    step_sigma:       0.67132341 +/- 0.010873 (1.62%) (init= 1.428571)
    step_center:      3.12697699 +/- 0.005151 (0.16%) (init= 2.5)
[[Correlations]] (unreported correlations are <  0.100)
    C(line_slope, step_amplitude)   = -0.878
    C(step_amplitude, step_sigma)   =  0.563
    C(line_slope, step_sigma)      = -0.455
    C(line_intercept, step_center)   =  0.427
    C(line_slope, line_intercept)   = -0.308
    C(line_slope, step_center)     = -0.234
    C(line_intercept, step_sigma)   = -0.139
    C(line_intercept, step_amplitude)   = -0.121
    C(step_amplitude, step_center)   =  0.109
```



with a plot of

8.8 Example 3: Fitting Multiple Peaks – and using Prefixes

As shown above, many of the models have similar parameter names. For composite models, this could lead to a problem of having parameters for different parts of the model having the same name. To overcome this, each `model.Model` can have a `prefix` attribute (normally set to a blank string) that will be put at the beginning of each parameter name. To illustrate, we fit one of the classic datasets from the NIST StRD suite involving a decaying exponential and two gaussians.

```
#!/usr/bin/env python
#<examples/doc_nistgauss.py>
import numpy as np
from lmfit.models import GaussianModel, ExponentialModel
import sys
import matplotlib.pyplot as plt

dat = np.loadtxt('NIST_Gauss2.dat')
x = dat[:, 1]
y = dat[:, 0]

exp_mod = ExponentialModel(prefix='exp_')
pars = exp_mod.guess(y, x=x)

gauss1  = GaussianModel(prefix='g1_')
pars.update( gauss1.make_params())

pars['g1_center'].set(105, min=75, max=125)
pars['g1_sigma'].set(15, min=3)
pars['g1_amplitude'].set(2000, min=10)

gauss2  = GaussianModel(prefix='g2_')

pars.update(gauss2.make_params())

pars['g2_center'].set(155, min=125, max=175)
pars['g2_sigma'].set(15, min=3)
pars['g2_amplitude'].set(2000, min=10)

mod = gauss1 + gauss2 + exp_mod
```

```
init = mod.eval(pars, x=x)
plt.plot(x, y)
plt.plot(x, init, 'k--')

out = mod.fit(y, pars, x=x)

comps = out.eval_components(x=x)

print(out.fit_report(min_correl=0.5))

plt.plot(x, out.best_fit, 'r-')
plt.plot(x, comps['g1_'], 'b--')
plt.plot(x, comps['g2_'], 'b--')
plt.plot(x, comps['exp_'], 'k--')

plt.show()
#<end examples/doc_nistgauss.py>
```

where we give a separate prefix to each model (they all have an `amplitude` parameter). The `prefix` values are attached transparently to the models.

Note that the calls to `make_param()` used the bare name, without the prefix. We could have used the prefixes, but because we used the individual model `gauss1` and `gauss2`, there was no need.

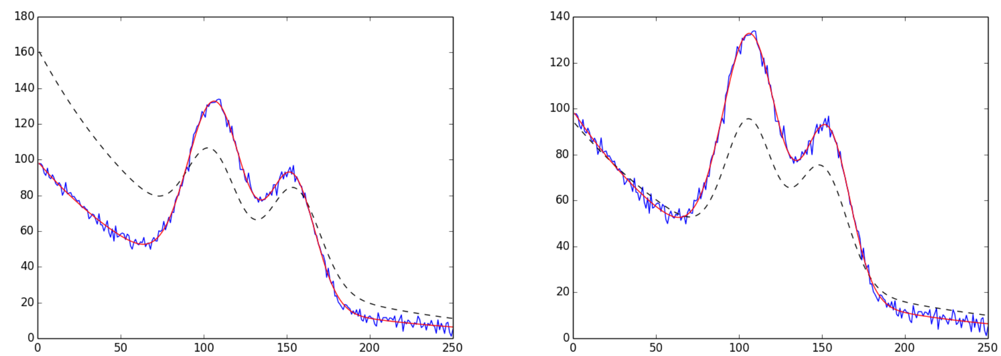
Note also in the example here that we explicitly set bounds on many of the parameter values.

The fit results printed out are:

```
[[Model]]
    ((Model(gaussian, prefix='g1_') + Model(gaussian, prefix='g2_')) +
↪Model(exponential, prefix='exp_'))
[[Fit Statistics]]
    # function evals   = 66
    # data points      = 250
    # variables        = 8
    chi-square         = 1247.528
    reduced chi-square = 5.155
    Akaike info crit   = 417.865
    Bayesian info crit = 446.036
[[Variables]]
    exp_amplitude:   99.0183282 +/- 0.537487 (0.54%) (init= 162.2102)
    exp_decay:       90.9508859 +/- 1.103105 (1.21%) (init= 93.24905)
    g1_sigma:        16.6725753 +/- 0.160481 (0.96%) (init= 15)
    g1_center:       107.030954 +/- 0.150067 (0.14%) (init= 105)
    g1_amplitude:    4257.77319 +/- 42.38336 (1.00%) (init= 2000)
    g1_fwhm:         39.2609139 +/- 0.377905 (0.96%)  == '2.3548200*g1_sigma'
    g1_height:       101.880231 +/- 0.592170 (0.58%)  == '0.3989423*g1_amplitude/
↪max(1.e-15, g1_sigma)'
    g2_sigma:        13.8069484 +/- 0.186794 (1.35%) (init= 15)
    g2_center:       153.270100 +/- 0.194667 (0.13%) (init= 155)
    g2_amplitude:    2493.41770 +/- 36.16947 (1.45%) (init= 2000)
    g2_fwhm:         32.5128782 +/- 0.439866 (1.35%)  == '2.3548200*g2_sigma'
    g2_height:       72.0455934 +/- 0.617220 (0.86%)  == '0.3989423*g2_amplitude/
↪max(1.e-15, g2_sigma)'
[[Correlations]] (unreported correlations are <  0.500)
    C(g1_sigma, g1_amplitude)     =  0.824
    C(g2_sigma, g2_amplitude)     =  0.815
    C(exp_amplitude, exp_decay)   = -0.695
```

```
    C(g1_sigma, g2_center)         =  0.684
    C(g1_center, g2_amplitude)     = -0.669
    C(g1_center, g2_sigma)         = -0.652
    C(g1_amplitude, g2_center)     =  0.648
    C(g1_center, g2_center)        =  0.621
    C(g1_sigma, g1_center)         =  0.507
    C(exp_decay, g1_amplitude)     = -0.507
```

We get a very good fit to this problem (described at the NIST site as of average difficulty, but the tests there are generally deliberately challenging) by applying reasonable initial guesses and putting modest but explicit bounds on the parameter values. This fit is shown on the left:



One final point on setting initial values. From looking at the data itself, we can see the two Gaussian peaks are reasonably well separated but do overlap. Furthermore, we can tell that the initial guess for the decaying exponential component was poorly estimated because we used the full data range. We can simplify the initial parameter values by using this, and by defining an `index_of()` function to limit the data range. That is, with:

```
def index_of(arrval, value):
    "return index of array *at or below* value "
    if value < min(arrval):  return 0
    return max(np.where(arrval<=value)[0])

ix1 = index_of(x,  75)
ix2 = index_of(x, 135)
ix3 = index_of(x, 175)

exp_mod.guess(y[:ix1], x=x[:ix1])
gauss1.guess(y[ix1:ix2], x=x[ix1:ix2])
gauss2.guess(y[ix2:ix3], x=x[ix2:ix3])
```

we can get a better initial estimate. The fit converges to the same answer, giving to identical values (to the precision printed out in the report), but in few steps, and without any bounds on parameters at all:

```
[[Model]]
    ((Model(gaussian, prefix='g1_') + Model(gaussian, prefix='g2_')) + 
↪Model(exponential,  prefix='exp_'))
[[Fit Statistics]]
    # function evals   = 48
    # data points      = 250
    # variables        = 8
    chi-square         = 1247.528
    reduced chi-square = 5.155
    Akaike info crit   = 417.865
```

```
    Bayesian info crit = 446.036
[[Variables]]
    exp_amplitude:   99.0183281 +/- 0.537487 (0.54%) (init= 94.53724)
    exp_decay:       90.9508862 +/- 1.103105 (1.21%) (init= 111.1985)
    g1_sigma:        16.6725754 +/- 0.160481 (0.96%) (init= 14.5)
    g1_center:       107.030954 +/- 0.150067 (0.14%) (init= 106.5)
    g1_amplitude:    4257.77322 +/- 42.38338 (1.00%) (init= 2126.432)
    g1_fwhm:         39.2609141 +/- 0.377905 (0.96%)  == '2.3548200*g1_sigma'
    g1_height:       101.880231 +/- 0.592171 (0.58%)  == '0.3989423*g1_amplitude/
↪max(1.e-15, g1_sigma)'
    g2_sigma:        13.8069481 +/- 0.186794 (1.35%) (init= 15)
    g2_center:       153.270100 +/- 0.194667 (0.13%) (init= 150)
    g2_amplitude:    2493.41766 +/- 36.16948 (1.45%) (init= 1878.892)
    g2_fwhm:         32.5128777 +/- 0.439866 (1.35%)  == '2.3548200*g2_sigma'
    g2_height:       72.0455935 +/- 0.617221 (0.86%)  == '0.3989423*g2_amplitude/
↪max(1.e-15, g2_sigma)'
[[Correlations]] (unreported correlations are <  0.500)
    C(g1_sigma, g1_amplitude)     =  0.824
    C(g2_sigma, g2_amplitude)     =  0.815
    C(exp_amplitude, exp_decay)   = -0.695
    C(g1_sigma, g2_center)        =  0.684
    C(g1_center, g2_amplitude)    = -0.669
    C(g1_center, g2_sigma)        = -0.652
    C(g1_amplitude, g2_center)    =  0.648
    C(g1_center, g2_center)       =  0.621
    C(g1_sigma, g1_center)        =  0.507
    C(exp_decay, g1_amplitude)    = -0.507
```

This script is in the file `doc_nistgauss2.py` in the examples folder, and the fit result shown on the right above shows an improved initial estimate of the data.

CHAPTER

NINE

CALCULATION OF CONFIDENCE INTERVALS

The lmfit `confidence` module allows you to explicitly calculate confidence intervals for variable parameters. For most models, it is not necessary since the estimation of the standard error from the estimated covariance matrix is normally quite good.

But for some models, the sum of two exponentials for example, the approximation begins to fail. For this case, lmfit has the function `conf_interval()` to calculate confidence intervals directly. This is substantially slower than using the errors estimated from the covariance matrix, but the results are more robust.

9.1 Method used for calculating confidence intervals

The F-test is used to compare our null model, which is the best fit we have found, with an alternate model, where one of the parameters is fixed to a specific value. The value is changed until the difference between χ_0^2 and χ_f^2 can't be explained by the loss of a degree of freedom within a certain confidence.

$$F(P_{fix}, N-P) = \left(\frac{\chi_f^2}{\chi_0^2} - 1\right) \frac{N-P}{P_{fix}}$$

N is the number of data points, *P* the number of parameters of the null model. P_{fix} is the number of fixed parameters (or to be more clear, the difference of number of parameters between our null model and the alternate model).

Adding a log-likelihood method is under consideration.

9.2 A basic example

First we create an example problem:

```
>>> import lmfit
>>> import numpy as np
>>> x = np.linspace(0.3,10,100)
>>> y = 1/(0.1*x)+2+0.1*np.random.randn(x.size)
>>> pars = lmfit.Parameters()
>>> pars.add_many(('a', 0.1), ('b', 1))
>>> def residual(p):
...     a = p['a'].value
...     b = p['b'].value
...     return 1/(a*x)+b-y
```

before we can generate the confidence intervals, we have to run a fit, so that the automated estimate of the standard errors can be used as a starting point:

```
>>> mini = lmfit.Minimizer(residual, pars)
>>> result = mini.minimize()
>>> print(lmfit.fit_report(result.params))
[Variables]]
    a:   0.09943895 +/- 0.000193 (0.19%) (init= 0.1)
    b:   1.98476945 +/- 0.012226 (0.62%) (init= 1)
[[Correlations]] (unreported correlations are <  0.100)
    C(a, b)                      =  0.601
```

Now it is just a simple function call to calculate the confidence intervals:

```
>>> ci = lmfit.conf_interval(mini, result)
>>> lmfit.printfuncs.report_ci(ci)
     99.70%    95.00%    67.40%     0.00%    67.40%    95.00%    99.70%
a    0.09886   0.09905   0.09925   0.09944   0.09963   0.09982   0.10003
b    1.94751   1.96049   1.97274   1.97741   1.99680   2.00905   2.02203
```

This shows the best-fit values for the parameters in the *0.00%* column, and parameter values that are at the varying confidence levels given by steps in σ. As we can see, the estimated error is almost the same, and the uncertainties are well behaved: Going from 1 σ (68% confidence) to 3 σ (99.7% confidence) uncertainties is fairly linear. It can also be seen that the errors are fairy symmetric around the best fit value. For this problem, it is not necessary to calculate confidence intervals, and the estimates of the uncertainties from the covariance matrix are sufficient.

9.3 An advanced example

Now we look at a problem where calculating the error from approximated covariance can lead to misleading result – two decaying exponentials. In fact such a problem is particularly hard for the Levenberg-Marquardt method, so we first estimate the results using the slower but robust Nelder-Mead method, and *then* use Levenberg-Marquardt to estimate the uncertainties and correlations

```
import lmfit
import numpy as np
import matplotlib
# matplotlib.use('WXAgg')

import matplotlib.pyplot as plt

x = np.linspace(1, 10, 250)
np.random.seed(0)
y = 3.0*np.exp(-x/2) -5.0*np.exp(-(x-0.1)/10.) + 0.1*np.random.randn(len(x))

p = lmfit.Parameters()
p.add_many(('a1', 4.), ('a2', 4.), ('t1', 3.), ('t2', 3.))

def residual(p):
   return p['a1']*np.exp(-x/p['t1']) + p['a2']*np.exp(-(x-0.1)/p['t2'])-y

# create Minimizer
mini = lmfit.Minimizer(residual, p)

# first solve with Nelder-Mead
out1 = mini.minimize(method='Nelder')

# then solve with Levenberg-Marquardt using the
# Nelder-Mead solution as a starting point
```

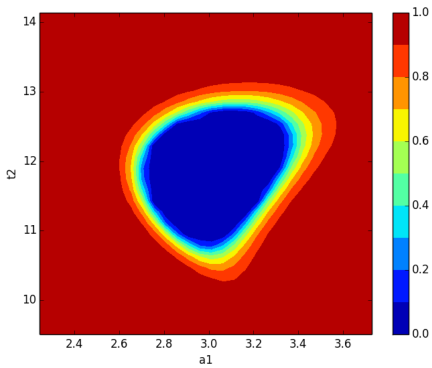
```
out2 = mini.minimize(method='leastsq', params=out1.params)

lmfit.report_fit(out2.params, min_correl=0.5)

ci, trace = lmfit.conf_interval(mini, out2, sigmas=[1, 2],
                                trace=True, verbose=False)
lmfit.printfuncs.report_ci(ci)

plot_type = 2
if plot_type == 0:
    plt.plot(x, y)
    plt.plot(x, residual(out2.params)+y )

elif plot_type == 1:
    cx, cy, grid = lmfit.conf_interval2d(mini, out2, 'a2','t2',30,30)
    plt.contourf(cx, cy, grid, np.linspace(0,1,11))
    plt.xlabel('a2')
    plt.colorbar()
    plt.ylabel('t2')

elif plot_type == 2:
    cx, cy, grid = lmfit.conf_interval2d(mini, out2, 'a1','t2',30,30)
    plt.contourf(cx, cy, grid, np.linspace(0,1,11))
    plt.xlabel('a1')
    plt.colorbar()
    plt.ylabel('t2')


elif plot_type == 3:
    cx1, cy1, prob = trace['a1']['a1'], trace['a1']['t2'],trace['a1']['prob']
    cx2, cy2, prob2 = trace['t2']['t2'], trace['t2']['a1'],trace['t2']['prob']
    plt.scatter(cx1, cy1, c=prob, s=30)
    plt.scatter(cx2, cy2, c=prob2, s=30)
    plt.gca().set_xlim((2.5, 3.5))
    plt.gca().set_ylim((11, 13))
    plt.xlabel('a1')
    plt.ylabel('t2')

if plot_type > 0:
    plt.show()
```

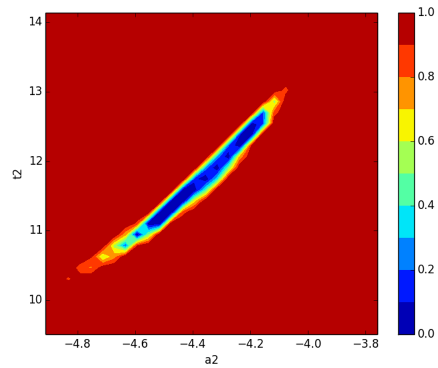
which will report:

```
[[Variables]]
    a1:   2.98622120 +/- 0.148671 (4.98%) (init= 2.986237)
    a2:  -4.33526327 +/- 0.115275 (2.66%) (init=-4.335256)
    t1:   1.30994233 +/- 0.131211 (10.02%) (init= 1.309932)
    t2:   11.8240350 +/- 0.463164 (3.92%) (init= 11.82408)
[[Correlations]] (unreported correlations are <  0.500)
    C(a2, t2)                    =  0.987
    C(a2, t1)                    = -0.925
    C(t1, t2)                    = -0.881
    C(a1, t1)                    = -0.599
      95.00%     68.00%      0.00%     68.00%     95.00%
a1   2.71850    2.84525    2.98622    3.14874    3.34076
a2  -4.63180   -4.46663   -4.33526   -4.22883   -4.14178
t2  10.82699   11.33865   11.82404   12.28195   12.71094
t1   1.08014    1.18566    1.30994    1.45566    1.62579
```

Again we called `conf_interval()`, this time with tracing and only for 1- and 2-σ. Comparing these two different estimates, we see that the estimate for *a1* is reasonably well approximated from the covariance matrix, but the estimates for *a2* and especially for *t1*, and *t2* are very asymmetric and that going from 1 σ (68% confidence) to 2 σ (95% confidence) is not very predictable.

Let plots mad of the confidence region are shown the figure on the left below for *a1* and *t2*, and for *a2* and *t2* on the right:



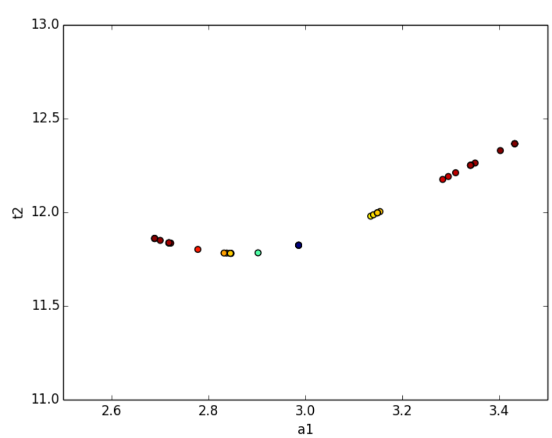


Neither of these plots is very much like an ellipse, which is implicitly assumed by the approach using the covariance matrix.

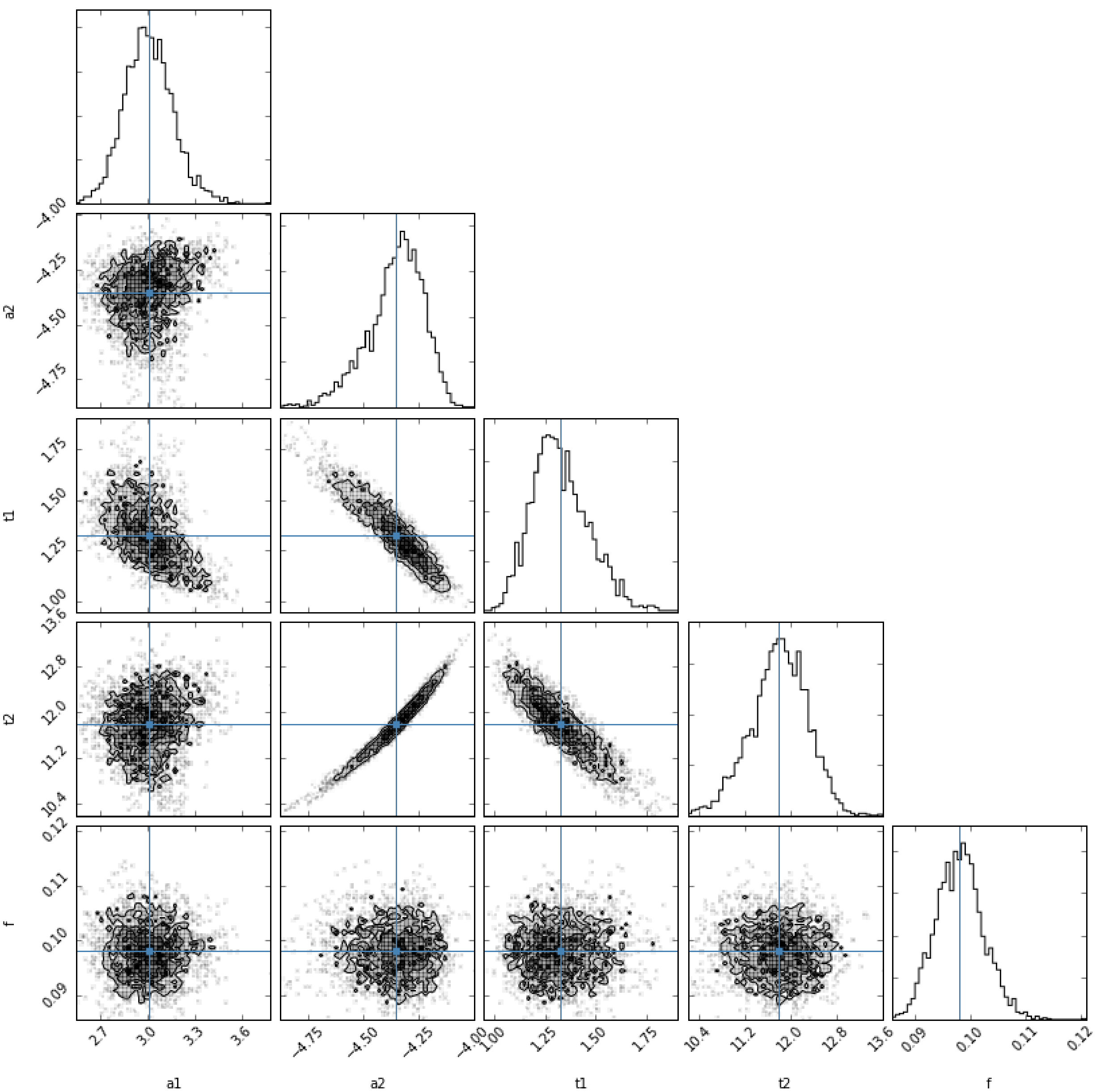
The trace returned as the optional second argument from `conf_interval()` contains a dictionary for each variable parameter. The values are dictionaries with arrays of values for each variable, and an array of corresponding probabilities for the corresponding cumulative variables. This can be used to show the dependence between two parameters:

```
>>> x, y, prob = trace['a1']['a1'], trace['a1']['t2'],trace['a1']['prob']
>>> x2, y2, prob2 = trace['t2']['t2'], trace['t2']['a1'],trace['t2']['prob']
>>> plt.scatter(x, y, c=prob ,s=30)
>>> plt.scatter(x2, y2, c=prob2, s=30)
>>> plt.gca().set_xlim((1, 5))
>>> plt.gca().set_ylim((5, 15))
>>> plt.xlabel('a1')
>>> plt.ylabel('t2')
>>> plt.show()
```

which shows the trace of values:



The `Minimizer.emcee()` method uses Markov Chain Monte Carlo to sample the posterior probability distribution. These distributions demonstrate the range of solutions that the data supports. The following image was obtained by using `Minimizer.emcee()` on the same problem.



Credible intervals (the Bayesian equivalent of the frequentist confidence interval) can be obtained with this method. MCMC can be used for model selection, to determine outliers, to marginalise over nuisance parameters, etcetera. For example, you may have fractionally underestimated the uncertainties on a dataset. MCMC can be used to estimate the true level of uncertainty on each datapoint. A tutorial on the possibilities offered by MCMC can be found at[1].

9.4 Confidence Interval Functions

conf_interval(*minimizer*, *result*, *p_names=None*, *sigmas=(1, 2, 3)*, *trace=False*, *maxiter=200*, *verbose=False*, *prob_func=None*)

Calculate the confidence interval for parameters.

The parameter for which the ci is calculated will be varied, while the remaining parameters are re-optimized for

[1] http://jakevdp.github.io/blog/2014/03/11/frequentism-and-bayesianism-a-practical-intro/

minimizing chi-square. The resulting chi-square is used to calculate the probability with a given statistic (e.g., F-test). This function uses a 1d-rootfinder from SciPy to find the values resulting in the searched confidence region.

Parameters

- **minimizer** (Minimizer) – The minimizer to use, holding objective function.
- **result** (MinimizerResult) – The result of running minimize().
- **p_names** (*list, optional*) – Names of the parameters for which the ci is calculated. If None, the ci is calculated for every parameter.
- **sigmas** (*list, optional*) – The sigma-levels to find. Default is [1, 2, 3]. See Note below.
- **trace** (*bool, optional*) – Defaults to False, if True, each result of a probability calculation is saved along with the parameter. This can be used to plot so-called "profile traces".
- **maxiter** (*int, optional*) – Maximum of iteration to find an upper limit. Default is 200.
- **verbose** (*bool, optional*) – Print extra debuging information. Default is False.
- **prob_func** (*None or callable, optional*) – Function to calculate the probability from the optimized chi-square. Default is None and uses built-in f_compare (F-test).

Returns

- **output** (*dict*) – A dictionary that contains a list of (sigma, vals)-tuples for each name.
- **trace_dict** (*dict, optional*) – Only if trace is True. Is a dict, the key is the parameter which was fixed. The values are again a dict with the names as keys, but with an additional key 'prob'. Each contains an array of the corresponding values.

Note: The values for *sigma* are taken as the number of standard deviations for a normal distribution and converted to probabilities. That is, the default `sigma=(1, 2, 3)` will use probabilities of 0.6827, 0.9545, and 0.9973. If any of the sigma values is less than 1, that will be interpreted as a probability. That is, a value of 1 and 0.6827 will give the same results, within precision.

See also:

`conf_interval2d()`

Examples

```
>>> from lmfit.printfuncs import *
>>> mini = minimize(some_func, params)
>>> mini.leastsq()
True
>>> report_errors(params)
... #report
>>> ci = conf_interval(mini)
>>> report_ci(ci)
... #report
```

Now with quantiles for the sigmas and using the trace.

```
>>> ci, trace = conf_interval(mini, sigmas=(0.5, 1, 2, 3), trace=True)
>>> fixed = trace['para1']['para1']
>>> free = trace['para1']['not_para1']
>>> prob = trace['para1']['prob']
```

This makes it possible to plot the dependence between free and fixed parameters.

conf_interval2d (*minimizer*, *result*, *x_name*, *y_name*, *nx=10*, *ny=10*, *limits=None*, *prob_func=None*)
Calculate confidence regions for two fixed parameters.

The method itself is explained in *conf_interval*: here we are fixing two parameters.

Parameters

- **minimizer** (Minimizer) – The minimizer to use, holding objective function.
- **result** (MinimizerResult) – The result of running minimize().
- **x_name** (*str*) – The name of the parameter which will be the x direction.
- **y_name** (*str*) – The name of the parameter which will be the y direction.
- **nx** (*int, optional*) – Number of points in the x direction.
- **ny** (*int, optional*) – Number of points in the y direction.
- **limits** (*tuple, optional*) – Should have the form ((x_upper, x_lower),(y_upper, y_lower)). If not given, the default is 5 std-errs in each direction.
- **prob_func** (*None or callable, optional*) – Function to calculate the probability from the optimized chi-square. Default is None and uses built-in f_compare (F-test).

Returns

- **x** (*numpy.ndarray*) – X-coordinates (same shape as nx).
- **y** (*numpy.ndarray*) – Y-coordinates (same shape as ny).
- **grid** (*numpy.ndarray*) – Grid containing the calculated probabilities (with shape (nx, ny)).

Examples

```
>>> mini = Minimizer(some_func, params)
>>> result = mini.leastsq()
>>> x, y, gr = conf_interval2d(mini, result, 'para1','para2')
>>> plt.contour(x,y,gr)
```

ci_report (*ci*, *with_offset=True*, *ndigits=5*)
Return text of a report for confidence intervals.

Parameters

- **with_offset** (*bool, optional*) – Whether to subtract best value from all other values (default is True).
- **ndigits** (*int, optional*) – Number of significant digits to show (default is 5).

Returns Text of formatted report on confidence intervals.

Return type str

CHAPTER

TEN

BOUNDS IMPLEMENTATION

This section describes the implementation of `Parameter` bounds. The MINPACK-1 implementation used in scipy.optimize.leastsq for the Levenberg-Marquardt algorithm does not explicitly support bounds on parameters, and expects to be able to fully explore the available range of values for any Parameter. Simply placing hard constraints (that is, resetting the value when it exceeds the desired bounds) prevents the algorithm from determining the partial derivatives, and leads to unstable results.

Instead of placing such hard constraints, bounded parameters are mathematically transformed using the formulation devised (and documented) for MINUIT. This is implemented following (and borrowing heavily from) the leastsqbound from J. J. Helmus. Parameter values are mapped from internally used, freely variable values $P_{\rm internal}$ to bounded parameters $P_{\rm bounded}$. When both `min` and `max` bounds are specified, the mapping is:

$$\begin{aligned} P_{\rm internal} &= \arcsin\big(\frac{2(P_{\rm bounded} - {\rm min})}{({\rm max} - {\rm min})} - 1\big) \\ P_{\rm bounded} &= {\rm min} + \big(\sin(P_{\rm internal}) + 1\big) \frac{({\rm max} - {\rm min})}{2} \end{aligned}$$

With only an upper limit `max` supplied, but `min` left unbounded, the mapping is:

$$\begin{aligned} P_{\rm internal} &= \sqrt{({\rm max} - P_{\rm bounded} + 1)^2 - 1} \\ P_{\rm bounded} &= {\rm max} + 1 - \sqrt{P_{\rm internal}^2 + 1} \end{aligned}$$

With only a lower limit `min` supplied, but `max` left unbounded, the mapping is:

$$\begin{aligned} P_{\rm internal} &= \sqrt{(P_{\rm bounded} - {\rm min} + 1)^2 - 1} \\ P_{\rm bounded} &= {\rm min} - 1 + \sqrt{P_{\rm internal}^2 + 1} \end{aligned}$$

With these mappings, the value for the bounded Parameter cannot exceed the specified bounds, though the internally varied value can be freely varied.

It bears repeating that code from leastsqbound was adopted to implement the transformation described above. The challenging part (thanks again to Jonathan J. Helmus!) here is to re-transform the covariance matrix so that the uncertainties can be estimated for bounded Parameters. This is included by using the derivate $dP_{\rm internal}/dP_{\rm bounded}$ from the equations above to re-scale the Jacobin matrix before constructing the covariance matrix from it. Tests show that this re-scaling of the covariance matrix works quite well, and that uncertainties estimated for bounded are quite reasonable. Of course, if the best fit value is very close to a boundary, the derivative estimated uncertainty and correlations for that parameter may not be reliable.

The MINUIT documentation recommends caution in using bounds. Setting bounds can certainly increase the number of function evaluations (and so computation time), and in some cases may cause some instabilities, as the range of acceptable parameter values is not fully explored. On the other hand, preliminary tests suggest that using `max` and `min` to set clearly outlandish bounds does not greatly affect performance or results.

CHAPTER

ELEVEN

USING MATHEMATICAL CONSTRAINTS

Being able to fix variables to a constant value or place upper and lower bounds on their values can greatly simplify modeling real data. These capabilities are key to lmfit's Parameters. In addition, it is sometimes highly desirable to place mathematical constraints on parameter values. For example, one might want to require that two Gaussian peaks have the same width, or have amplitudes that are constrained to add to some value. Of course, one could rewrite the objective or model function to place such requirements, but this is somewhat error prone, and limits the flexibility so that exploring constraints becomes laborious.

To simplify the setting of constraints, Parameters can be assigned a mathematical expression of other Parameters, builtin constants, and builtin mathematical functions that will be used to determine its value. The expressions used for constraints are evaluated using the asteval module, which uses Python syntax, and evaluates the constraint expressions in a safe and isolated namespace.

This approach to mathematical constraints allows one to not have to write a separate model function for two Gaussians where the two `sigma` values are forced to be equal, or where amplitudes are related. Instead, one can write a more general two Gaussian model (perhaps using `GaussianModel`) and impose such constraints on the Parameters for a particular fit.

11.1 Overview

Just as one can place bounds on a Parameter, or keep it fixed during the fit, so too can one place mathematical constraints on parameters. The way this is done with lmfit is to write a Parameter as a mathematical expression of the other parameters and a set of pre-defined operators and functions. The constraint expressions are simple Python statements, allowing one to place constraints like:

```
pars = Parameters()
pars.add('frac_curve1', value=0.5, min=0, max=1)
pars.add('frac_curve2', expr='1-frac_curve1')
```

as the value of the *frac_curve1* parameter is updated at each step in the fit, the value of *frac_curve2* will be updated so that the two values are constrained to add to 1.0. Of course, such a constraint could be placed in the fitting function, but the use of such constraints allows the end-user to modify the model of a more general-purpose fitting function.

Nearly any valid mathematical expression can be used, and a variety of built-in functions are available for flexible modeling.

11.2 Supported Operators, Functions, and Constants

The mathematical expressions used to define constrained Parameters need to be valid python expressions. As you'd expect, the operators '+', '-', '*', '/', '**', are supported. In fact, a much more complete set can be used, including Python's bit- and logical operators:

```
+, -, *, /, **, &, |, ^, <<, >>, %, and, or,
==, >, >=, <, <=, !=, ~, not, is, is not, in, not in
```

The values for *e* (2.7182818...) and *pi* (3.1415926...) are available, as are several supported mathematical and trigonometric function:

```
abs, acos, acosh, asin, asinh, atan, atan2, atanh, ceil,
copysign, cos, cosh, degrees, exp, fabs, factorial,
floor, fmod, frexp, fsum, hypot, isinf, isnan, ldexp,
log, log10, log1p, max, min, modf, pow, radians, sin,
sinh, sqrt, tan, tanh, trunc
```

In addition, all Parameter names will be available in the mathematical expressions. Thus, with parameters for a few peak-like functions:

```
pars = Parameters()
pars.add('amp_1', value=0.5, min=0, max=1)
pars.add('cen_1', value=2.2)
pars.add('wid_1', value=0.2)
```

The following expression are all valid:

```
pars.add('amp_2', expr='(2.0 - amp_1**2)')
pars.add('cen_2', expr='cen_1 * wid_2 / max(wid_1, 0.001)')
pars.add('wid_2', expr='sqrt(pi)*wid_1')
```

In fact, almost any valid Python expression is allowed. A notable example is that Python's 1-line *if expression* is supported:

```
pars.add('bounded', expr='param_a if test_val/2. > 100 else param_b')
```

which is equivalent to the more familiar:

```
if test_val/2. > 100:
    bounded = param_a
else:
    bounded = param_b
```

11.3 Using Inequality Constraints

A rather common question about how to set up constraints that use an inequality, say, $x + y \leq 10$. This can be done with algebraic constraints by recasting the problem, as $x + y = \delta$ and $\delta \leq 10$. That is, first, allow x to be held by the freely varying parameter *x*. Next, define a parameter *delta* to be variable with a maximum value of 10, and define parameter *y* as *delta* - *x*:

```
pars = Parameters()
pars.add('x',     value = 5, vary=True)
pars.add('delta', value = 5, max=10, vary=True)
pars.add('y',     expr='delta-x')
```

The essential point is that an inequality still implies that a variable (here, *delta*) is needed to describe the constraint. The secondary point is that upper and lower bounds can be used as part of the inequality to make the definitions more convenient.

11.4 Advanced usage of Expressions in lmfit

The expression used in a constraint is converted to a Python Abstract Syntax Tree, which is an intermediate version of the expression – a syntax-checked, partially compiled expression. Among other things, this means that Python's own parser is used to parse and convert the expression into something that can easily be evaluated within Python. It also means that the symbols in the expressions can point to any Python object.

In fact, the use of Python's AST allows a nearly full version of Python to be supported, without using Python's built-in `eval()` function. The asteval module actually supports most Python syntax, including for- and while-loops, conditional expressions, and user-defined functions. There are several unsupported Python constructs, most notably the class statement, so that new classes cannot be created, and the import statement, which helps make the asteval module safe from malicious use.

One important feature of the asteval module is that you can add domain-specific functions into the it, for later use in constraint expressions. To do this, you would use the `asteval` attribute of the `Minimizer` class, which contains a complete AST interpreter. The asteval interpreter uses a flat namespace, implemented as a single dictionary. That means you can preload any Python symbol into the namespace for the constraints:

```
def mylorentzian(x, amp, cen, wid):
    "lorentzian function: wid = half-width at half-max"
    return (amp  / (1 + ((x-cen)/wid)**2))

fitter = Minimizer()
fitter.asteval.symtable['lorentzian'] = mylorentzian
```

and this `lorentzian()` function can now be used in constraint expressions.

CHAPTER TWELVE

RELEASE NOTES

This section discusses changes between versions, especially changes significant to the use and behavior of the library. This is not meant to be a comprehensive list of changes. For such a complete record, consult the lmfit github repository.

12.1 Version 0.9.6 Release Notes

Support for SciPy 0.14 has been dropped: SciPy 0.15 is now required. This is especially important for lmfit maintenance, as it means we can now rely on SciPy having code for differential evolution and do not need to keep a local copy.

A brute force method was added, which can be used either with `Minimizer.brute()` or using the *method='brute'* option to `Minimizer.minimize()`. This method requires finite bounds on all varying parameters, or that parameters have a finite *brute_step* attribute set to specify the step size.

Custom cost functions can now be used for the scalar minimizers using the *reduce_fcn* option.

Many improvements to documentation and docstrings in the code were made. As part of that effort, all API documentation in this main Sphinx documentation now derives from the docstrings.

Uncertainties in the resulting best-fit for a model can now be calculated from the uncertainties in the model parameters.

Parameters have two new attributes: *brute_step*, to specify the step size when using the *brute* method, and *user_data*, which is unused but can be used to hold additional information the user may desire. This will be preserved on copy and pickling.

Several bug fixes and cleanups.

Versioneer was updated to 0.18.

Tests can now be run either with nose or pytest.

12.2 Version 0.9.5 Release Notes

Support for Python 2.6 and SciPy 0.13 has been dropped.

12.3 Version 0.9.4 Release Notes

Some support for the new *least_squares* routine from SciPy 0.17 has been added.

Parameters can now be used directly in floating point or array expressions, so that the Parameter value does not need *sigma = params['sigma'].value*. The older, explicit usage still works, but the docs, samples, and tests have been updated to use the simpler usage.

Support for Python 2.6 and SciPy 0.13 is now explicitly deprecated and wil be dropped in version 0.9.5.

12.4 Version 0.9.3 Release Notes

Models involving complex numbers have been improved.

The *emcee* module can now be used for uncertainty estimation.

Many bug fixes, and an important fix for performance slowdown on getting parameter values.

ASV benchmarking code added.

12.5 Version 0.9.0 Release Notes

This upgrade makes an important, non-backward-compatible change to the way many fitting scripts and programs will work. Scripts that work with version 0.8.3 will not work with version 0.9.0 and vice versa. The change was not made lightly or without ample discussion, and is really an improvement. Modifying scripts that did work with 0.8.3 to work with 0.9.0 is easy, but needs to be done.

12.5.1 Summary

The upgrade from 0.8.3 to 0.9.0 introduced the `MinimizerResult` class (see *MinimizerResult – the optimization result*) which is now used to hold the return value from `minimize()` and `Minimizer.minimize()`. This returned object contains many goodness of fit statistics, and holds the optimized parameters from the fit. Importantly, the parameters passed into `minimize()` and `Minimizer.minimize()` are no longer modified by the fit. Instead, a copy of the passed-in parameters is made which is changed and returns as the `params` attribute of the returned `MinimizerResult`.

12.5.2 Impact

This upgrade means that a script that does:

```
my_pars = Parameters()
my_pars.add('amp',     value=300.0, min=0)
my_pars.add('center', value=  5.0, min=0, max=10)
my_pars.add('decay',  value=  1.0, vary=False)

result = minimize(objfunc, my_pars)
```

will still work, but that `my_pars` will **NOT** be changed by the fit. Instead, `my_pars` is copied to an internal set of parameters that is changed in the fit, and this copy is then put in `result.params`. To look at fit results, use `result.params`, not `my_pars`.

This has the effect that `my_pars` will still hold the starting parameter values, while all of the results from the fit are held in the `result` object returned by `minimize()`.

If you want to do an initial fit, then refine that fit to, for example, do a pre-fit, then refine that result different fitting method, such as:

```
result1 = minimize(objfunc, my_pars, method='nelder')
result1.params['decay'].vary = True
result2 = minimize(objfunc, result1.params, method='leastsq')
```

and have access to all of the starting parameters `my_pars`, the result of the first fit `result1`, and the result of the final fit `result2`.

12.5.3 Discussion

The main goal for making this change were to

1. give a better return value to `minimize()` and `Minimizer.minimize()` that can hold all of the information about a fit. By having the return value be an instance of the `MinimizerResult` class, it can hold an arbitrary amount of information that is easily accessed by attribute name, and even be given methods. Using objects is good!
2. To limit or even eliminate the amount of "state information" a `Minimizer` holds. By state information, we mean how much of the previous fit is remembered after a fit is done. Keeping (and especially using) such information about a previous fit means that a `Minimizer` might give different results even for the same problem if run a second time. While it's desirable to be able to adjust a set of `Parameters` re-run a fit to get an improved result, doing this by changing an internal attribute (`Minimizer.params`) has the undesirable side-effect of not being able to "go back", and makes it somewhat cumbersome to keep track of changes made while adjusting parameters and re-running fits.

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