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# **symfit Documentation**

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Contents:



# CHAPTER 1

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## Introduction

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Existing fitting modules are not very pythonic in their API and can be difficult for humans to use. This project aims to marry the power of `scipy.optimize` with the readability of `sympy` to create a highly readable and easy to use fitting package which works for projects of any scale.

`symfit` makes it extremely easy to provide guesses for your parameters and to bound them to a certain range:

```
a = Parameter(1.0, min=0.0, max=5.0)
```

To define models to fit to:

```
x = Variable()
A = Parameter()
sig = Parameter(1.0, min=0.0, max=5.0)
x0 = Parameter(1.0, min=0.0)

# Gaussian distrubution
model = A * exp(-(x - x0)**2/(2 * sig**2))
```

And finally, to execute the fit:

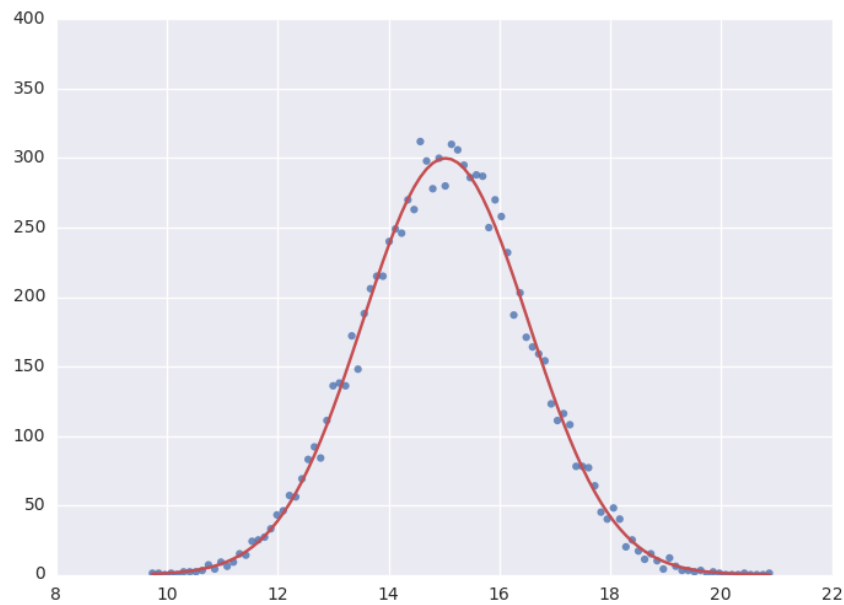
```
fit = Fit(model, xdata, ydata)
fit_result = fit.execute()
```

And to evaluate the model using the best fit parameters:

```
y = model(x=xdata, **fit_result.params)
```

As your models become more complicated, `symfit` really comes into it's own. For example, vector valued functions are both easy to define and beautiful to look at:

```
model = {
    y_1: x**2,
    y_2: 2*x
}
```



And constrained maximization has never been this easy:

```
x, y = parameters('x, y')

model = 2*x*y + 2*x - x**2 - 2*y**2
constraints = [
    Eq(x**3 - y, 0),      # Eq: ==
    Ge(y - 1, 0),         # Ge: >=
]

fit = Fit(- model, constraints=constraints)
fit_result = fit.execute()
```

## 1.1 Technical Reasons

On a more technical note, this symbolic approach turns out to have great technical advantages over using `scipy` directly. In order to fit, the algorithm needs the Jacobian: a matrix containing the derivatives of your model in it's parameters. Because of the symbolic nature of `symfit`, this is determined for you on the fly, saving you the trouble of having to determine the derivatives yourself. Furthermore, having this Jacobian allows good estimation of the errors in your parameters, something `scipy` does not always succeed in.



## CHAPTER 2

---

### Installation

---

If you are using pip, you can simply run

```
pip install symfit
```

from your terminal. If you are using linux and do not use pip, you can download the source from <https://github.com/tBuLi/symfit> and install manually.

Are you not on linux and you do not use pip? That's your own mess.

### 2.1 Contrib module

To also install the dependencies of 3rd party contrib modules such as interactive guesses, install *symfit* using:

```
pip install symfit[contrib]
```

### 2.2 Dependencies

```
pip install sympy
pip install numpy
pip install scipy
```



## 3.1 Simple Example

The example below shows how easy it is to define a model that we could fit to.

```
from symfit import Parameter, Variable

a = Parameter()
b = Parameter()
x = Variable()
model = a * x + b
```

Lets fit this model to some generated data.

```
from symfit import Fit
import numpy as np

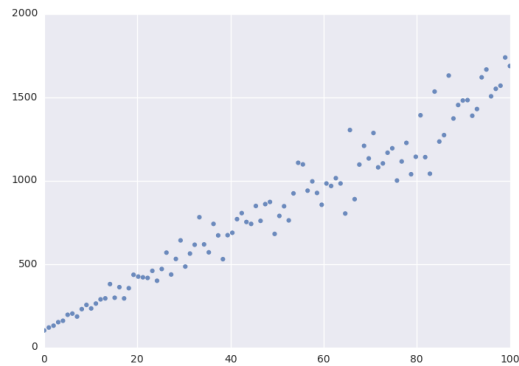
xdata = np.linspace(0, 100, 100) # From 0 to 100 in 100 steps
a_vec = np.random.normal(15.0, scale=2.0, size=(100,))
b_vec = np.random.normal(100.0, scale=2.0, size=(100,))
ydata = a_vec * xdata + b_vec # Point scattered around the line 5 * x + 105

fit = Fit(model, xdata, ydata)
fit_result = fit.execute()
```

Printing `fit_result` will give a full report on the values for every parameter, including the uncertainty, and quality of the fit.

## 3.2 Initial Guess

For fitting to work as desired you should always give a good initial guess for a parameter. The `Parameter` object can therefore be initiated with the following keywords:



- `value` the initial guess value. Defaults to 1.
- `min` Minimal value for the parameter.
- `max` Maximal value for the parameter.
- `fixed` Whether the parameter's value can vary during fitting.

In the example above, we might change our *Parameter*'s to the following after looking at a plot of the data:

```
k = Parameter(value=4, min=3, max=6)

a, b = parameters('a, b')
a.value = 60
a.fixed = True
```

## 3.3 Accessing the Results

A call to *Fit.execute* returns a *FitResults* instance. This object holds all information about the fit. The fitting process does not modify the *Parameter* objects. In the above example, `a.value` will still be 60 and not the value we obtain after fitting. To get the value of fit parameters we can do:

```
>>> print(fit_result.value(a))
>>> 14.66946...
>>> print(fit_result.stdev(a))
>>> 0.3367571...
>>> print(fit_result.value(b))
>>> 104.6558...
>>> print(fit_result.stdev(b))
>>> 19.49172...
>>> print(fit_result.r_squared)
>>> 0.950890866472
```

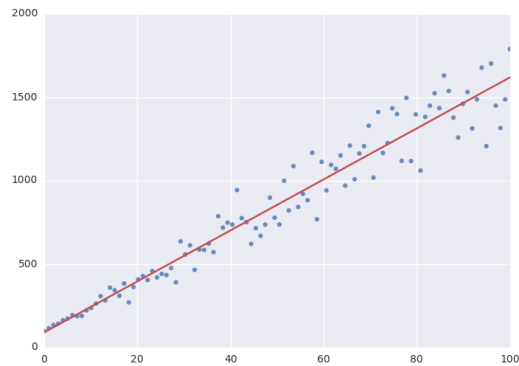
For more *FitResults*, see the *Module Documentation*.

## 3.4 Evaluating the Model

With these parameters, we could now evaluate the model with these parameters so we can make a plot of it. In order to do this, we simply call the model with these values:

```
import matplotlib.pyplot as plt

y = model(x=xdata, a=fit_result.value(a), b=fit_result.value(b))
plt.plot(xdata, y)
plt.show()
```



The model *has* to be called by keyword arguments to prevent any ambiguity. So the following does not work:

```
y = model(xdata, fit_result.value(a), fit_result.value(b))
```

To make life easier, there is a nice shorthand notation to immediately use a fit result:

```
y = model(x=xdata, **fit_result.params)
```

This immediately unpacks an `OrderedDict` containing the optimized fit parameters.

## 3.5 Named Models

More complicated models are also relatively easy to deal with by using named models. Let's try our luck with a bivariate normal distribution:

```
from symfit import parameters, variables, exp, pi, sqrt

x, y, p = variables('x, y, p')
mu_x, mu_y, sig_x, sig_y, rho = parameters('mu_x, mu_y, sig_x, sig_y, rho')

z = (
    (x - mu_x)**2/sig_x**2
    + (y - mu_y)**2/sig_y**2
    - 2 * rho * (x - mu_x) * (y - mu_y)/(sig_x * sig_y)
)

model = {
    p: exp(
        - z / (2 * (1 - rho**2))
        / (2 * pi * sig_x * sig_y * sqrt(1 - rho**2))
    )
}

fit = Fit(model, x=xdata, y=ydata, p=pdata)
```

By using the magic of named models, the flow of information is still relatively clear, even with such a complicated function.

This syntax also supports vector valued functions:

```
model = {y_1: a * x**2, y_2: 2 * x * b}
```

One thing to note about such models is that now `model(x=xdata)` obviously no longer works as `type(model) == dict`. There is a preferred way to resolve this. If any kind of fitting object has been initiated, it will have a `.model` attribute containing an instance of `Model`. This can again be called:

```
a, b = parameters('a, b')
y_1, y_2, x = variables('y_1, y_2, x')

model = {y_1: a * x**2, y_2: 2 * x * b}
fit = Fit(model, x=xdata, y_1=y_data1, y_2=y_data2)
fit_result = fit.execute()

y_1_result, y_2_result = fit.model(x=xdata, **fit_result.params)
```

This returns a `namedtuple()`, with the components evaluated. So through the magic of tuple unpacking, `y_1` and `y_2` contain the evaluated fit. The dependent variables will be ordered alphabetically in the returned `namedtuple()`. Alternatively, the unpacking can be performed explicitly.

If for some reason no `Fit` is initiated you can make a `Model` object yourself:

```
model = Model(model_dict)
y_1_result, y_2_result = model(x=xdata, a=2.4, b=0.1)
```

or equivalently:

```
outcome = model(x=xdata, a=2.4, b=0.1)
y_1_result = outcome.y_1
y_2_result = outcome.y_2
```

## 3.6 symfit exposes sympy.api

symfit exposes the `sympy` api as well, so mathematical expressions such as `exp`, `sin` and `Pi` are importable from symfit as well. For more, read the [sympy docs](#).

## 4.1 Fit (Least Squares)

The default fitting object does least-squares fitting:

```
from sympfit import parameters, variables, Fit
import numpy as np

# Define a model to fit to.
a, b = parameters('a, b')
x = variables('x')
model = a * x + b

# Generate some data
xdata = np.linspace(0, 100, 100) # From 0 to 100 in 100 steps
a_vec = np.random.normal(15.0, scale=2.0, size=(100,))
b_vec = np.random.normal(100.0, scale=2.0, size=(100,))
# Point scattered around the line 5 * x + 105
ydata = a_vec * xdata + b_vec

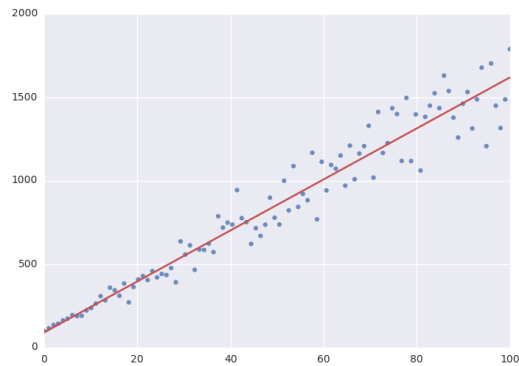
fit = Fit(model, xdata, ydata)
fit_result = fit.execute()
```

The `Fit` object also supports standard deviations. In order to provide these, it's nicer to use a named model:

```
a, b = parameters('a, b')
x, y = variables('x, y')
model = {y: a * x + b}

fit = Fit(model, x=xdata, y=ydata, sigma_y=sigma)
```

**Warning:** `sympfit` assumes these sigma to be from measurement errors by default, and not just as a relative weight. This means the standard deviations on parameters are calculated assuming the absolute size of sigma is



significant. This is the case for measurement errors and therefore for most use cases `symfit` was designed for. If you only want to use the `sigma` for relative weights, then you can use `absolute_sigma=False` as a keyword argument.

Please note that this is the opposite of the convention used by `scipy`'s `curve_fit()`. Looking through their mailing list this seems to have been implemented the opposite way for historical reasons, and was understandably never changed so as not to lose backwards compatibility. Since this is a new project, we don't have that problem.

## 4.2 Constrained Least Squares Fit

The `Fit` takes a `constraints` keyword; a list of relationships between the parameters that has to be respected. As an example of fitting with constraints, we could imagine fitting the angles of a triangle:

```
a, b, c = parameters('a, b, c')
a_i, b_i, c_i = variables('a_i, b_i, c_i')

model = {a_i: a, b_i: b, c_i: c}

data = np.array([
    [10.1, 9., 10.5, 11.2, 9.5, 9.6, 10.],
    [102.1, 101., 100.4, 100.8, 99.2, 100., 100.8],
    [71.6, 73.2, 69.5, 70.2, 70.8, 70.6, 70.1],
])

fit = Fit(
    model=model,
    a_i=data[0],
    b_i=data[1],
    c_i=data[2],
    constraints=[Equality(a + b + c, 180)]
)
fit_result = fit.execute()
```

The line `constraints=[Equality(a + b + c, 180)]` ensures that our basic knowledge of geometry is respected despite my sloppy measurements.

**Note:** Under the hood, a different *Minimizer* is used to perform a constrained fit. `Fit` tries to select the right



*Minimizer* based on the problem you present it with. See *Fit* for more.

## 4.3 (Non)LinearLeastSquares

The *LinearLeastSquares* implements the analytical solution to Least Squares fitting. When your model is linear in it's parameters, consider using this rather than the default *Fit* since this gives the exact solution in one step, no iteration and no guesses needed.

*NonLinearLeastSquares* is the generalization to non-linear models. It works by approximating the model by a linear one around the value of your guesses and repeating that process iteratively. This process is therefore very sensitive to getting good initial guesses.

Notes on these objects:

- Use *NonLinearLeastSquares* instead of *LinearLeastSquares* unless you have a reason not to. *NonLinearLeastSquares* will behave exactly the same as *LinearLeastSquares* when the model is linear.
- Bounds are currently ignored by both. This is because for linear models there can only be one solution. For non-linear models it simply hasn't been considered yet.
- When performance matters, use *Fit* instead of *NonLinearLeastSquares*. These analytical objects are implemented in pure python and are therefore massively outgunned by *Fit* which is ultimately a wrapper to efficient numerical methods such as MINPACK or BFGS implemented in Fortran.

## 4.4 Likelihood

Given a dataset and a model, what values should the model's parameters have to make the observed data most likely? This is the principle of maximum likelihood and the question the Likelihood object can answer for you.

Example:

```
from symfit import Parameter, Variable, exp
from symfit.core.objectives import LogLikelihood
import numpy as np

# Define the model for an exponential distribution (numpy style)
beta = Parameter()
x = Variable()
model = (1 / beta) * exp(-x / beta)

# Draw 100 samples from an exponential distribution with beta=5.5
data = np.random.exponential(5.5, 100)

# Do the fitting!
fit = Fit(model, data, objective=LogLikelihood)
fit_result = fit.execute()
```

`fit_result` is a normal *FitResults* object. As always, bounds on parameters and even constraints are supported.

## 4.5 Minimize/Maximize

Minimize or Maximize a model subject to bounds and/or constraints. As an example I present an example from the [scipy docs](#).

Suppose we want to maximize the following function:

$$f(x, y) = 2xy + 2x - x^2 - 2y^2$$

Subject to the following constraints:

$$x^3 - y = 0$$

$$y - 1 \geq 0$$

In SciPy code the following lines are needed:

```
def func(x, sign=1.0):
    """ Objective function """
    return sign*(2*x[0]*x[1] + 2*x[0] - x[0]**2 - 2*x[1]**2)

def func_deriv(x, sign=1.0):
    """ Derivative of objective function """
    dfdx0 = sign*(-2*x[0] + 2*x[1] + 2)
    dfdx1 = sign*(2*x[0] - 4*x[1])
    return np.array([ dfdx0, dfdx1 ])

cons = ({'type': 'eq',
        'fun' : lambda x: np.array([x[0]**3 - x[1]]),
        'jac' : lambda x: np.array([3.0*(x[0]**2.0), -1.0])},
        {'type': 'ineq',
        'fun' : lambda x: np.array([x[1] - 1]),
        'jac' : lambda x: np.array([0.0, 1.0])})

res = minimize(func, [-1.0, 1.0], args=(-1.0,), jac=func_deriv,
               constraints=cons, method='SLSQP', options={'disp': True})
```

Takes a couple of read-throughs to make sense, doesn't it? Let's do the same problem in symfit:

```
from symfit import parameters, Maximize, Eq, Ge

x, y = parameters('x, y')
model = 2*x*y + 2*x - x**2 - 2*y**2
constraints = [
    Eq(x**3 - y, 0),
    Ge(y - 1, 0),
]

fit = Fit(- model, constraints=constraints)
fit_result = fit.execute()
```

Done! symfit will determine all derivatives automatically, no need for you to think about it. Notice the minus sign in the call to *Fit*. This is because *Fit* will always minimize, so in order to achieve maximization we should minimize *-model*.

**Warning:** You might have noticed that  $x$  and  $y$  are *Parameter*'s in the above problem, which may strike you as weird. However, it makes perfect sense because in this problem they are parameters to be optimised, not independent variables. Furthermore, this way of defining it is consistent with the treatment of *Variable*'s and *Parameter*'s in symfit. Be aware of this when minimizing such problems, as the whole process won't work otherwise.

## 4.6 ODE Fitting

Fitting to a system of ordinary differential equations (ODEs) is also remarkably simple with symfit. Let's do a simple example from reaction kinetics. Suppose we have a reaction  $A + A \rightarrow B$  with rate constant  $k$ . We then need the following system of rate equations:

$$\begin{aligned}\frac{dA}{dt} &= -kA^2 \\ \frac{dB}{dt} &= kA^2\end{aligned}$$

In symfit, this becomes:

```
model_dict = {
    D(a, t): - k * a**2,
    D(b, t): k * a**2,
}
```

We see that the symfit code is already very readable. Let's do a fit to this:

```
tdata = np.array([10, 26, 44, 70, 120])
adata = 10e-4 * np.array([44, 34, 27, 20, 14])
a, b, t = variables('a, b, t')
k = Parameter(0.1)
a0 = 54 * 10e-4

model_dict = {
    D(a, t): - k * a**2,
    D(b, t): k * a**2,
}

ode_model = ODEModel(model_dict, initial={t: 0.0, a: a0, b: 0.0})

fit = Fit(ode_model, t=tdata, a=adata, b=None)
fit_result = fit.execute()
```

That's it! An *ODEModel* behaves just like any other model object, so *Fit* knows how to deal with it! Note that since we don't know the concentration of B, we explicitly set  $b=None$  when calling *Fit* so it will be ignored.

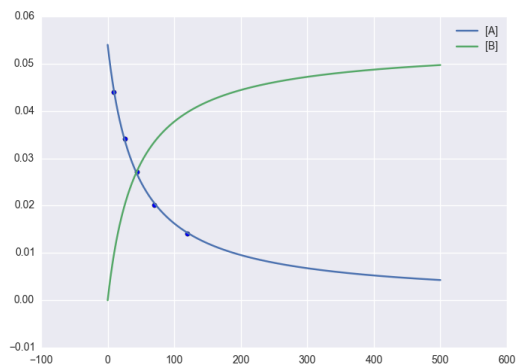
**Warning:** Fitting to ODEs is extremely difficult from an algorithmic point of view, since these systems are usually very sensitive to the parameters. Using (very) good initial guesses for the parameters and initial values is critical.

Upon every iteration of performing the fit the *ODEModel* is integrated again from the initial point using the new guesses for the parameters.

We can plot it just like always:

```
# Generate some data
tvec = np.linspace(0, 500, 1000)

A, B = ode_model(t=tvec, **fit_result.params)
plt.plot(tvec, A, label='[A]')
plt.plot(tvec, B, label='[B]')
plt.scatter(tdata, adata)
plt.legend()
plt.show()
```



As an example of the power of symfit's ODE syntax, let's have a look at a system with 2 equilibria: compound AA + B  $\leftrightarrow$  AAB and AAB + B  $\leftrightarrow$  BAAB.

In symfit these can be implemented as:

```
AA, B, AAB, BAAB, t = variables('AA, B, AAB, BAAB, t')
k, p, l, m = parameters('k, p, l, m')

AA_0 = 10 # Some made up initial amount of [AA]
B = AA_0 - BAAB + AA # [B] is not independent.

model_dict = {
    D(BAAB, t): l * AAB * B - m * BAAB,
    D(AAB, t): k * A * B - p * AAB - l * AAB * B + m * BAAB,
    D(A, t): -k * A * B + p * AAB,
}
```

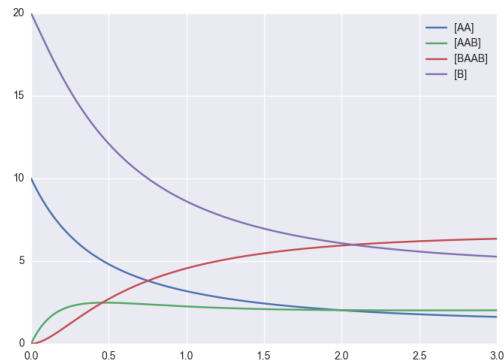
The result is as readable as one can reasonably expect from a multicomponent system (and while using chemical notation). Let's plot the model for some kinetics constants:

```
model = ODEModel(model_dict, initial={t: 0.0, AA: AA_0, AAB: 0.0, BAAB: 0.0})

# Generate some data
tdata = np.linspace(0, 3, 1000)
# Eval the normal way.
AA, AAB, BAAB = model(t=tdata, k=0.1, l=0.2, m=0.3, p=0.3)

plt.plot(tdata, AA, color='red', label='[AA]')
plt.plot(tdata, AAB, color='blue', label='[AAB]')
plt.plot(tdata, BAAB, color='green', label='[BAAB]')
plt.plot(tdata, B(BAAB=BAAB, AA=AA), color='pink', label='[B]')
# plt.plot(tdata, AA + AAB + BAAB, color='black', label='total')
```

```
plt.legend()
plt.show()
```



More common examples, such as dampened harmonic oscillators also work as expected:

```
# Oscillator strength
k = Parameter()
# Mass, just there for the physics
m = 1
# Dampening factor
gamma = Parameter()

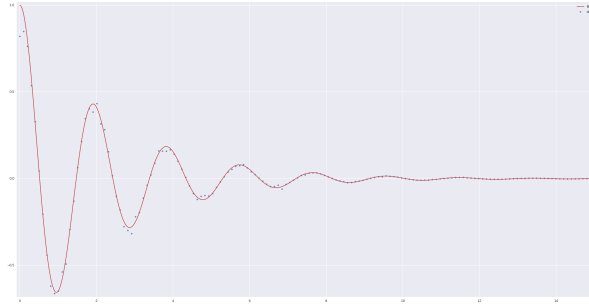
x, v, t = symfit.variables('x, v, t')

# Define the force based on Hooke's law, and dampening
a = (-k * x - gamma * v)/m
model_dict = {
    D(x, t): v,
    D(v, t): a,
}
ode_model = ODEModel(model_dict, initial={t: 0, v: 0, x: 1})

# Let's create some data...
times = np.linspace(0, 15, 150)
data = ode_model(times, k=11, gamma=0.9, m=m.value).x
# ... and add some noise to it.
noise = np.random.normal(1, 0.1, data.shape) # 10% error
data *= noise

fit = Fit(ode_model, t=times, x=data)
fit_result = fit.execute()
```

**Note:** Evaluating the model above will produce a named tuple with values for both  $x$  and  $v$ . Since we are only interested in the values for  $x$ , we immediately select it with `.x`.



## 4.7 Global Fitting

In a global fitting problem, we fit to multiple datasets where one or more parameters might be shared. The same syntax used for ODE fitting makes this problem very easy to solve in `symfit`.

As a simple example, suppose we have two datasets measuring exponential decay, with the same background, but different amplitude and decay rate.

$$f(x) = y_0 + a * e^{-b*x}$$

In order to fit to this, we define the following model:

```
x_1, x_2, y_1, y_2 = variables('x_1, x_2, y_1, y_2')
y0, a_1, a_2, b_1, b_2 = parameters('y0, a_1, a_2, b_1, b_2')

model = Model({
    y_1: y0 + a_1 * exp(- b_1 * x_1),
    y_2: y0 + a_2 * exp(- b_2 * x_2),
})
```

Note that `y0` is shared between the components. Fitting is then done in the normal way:

```
fit = Fit(model, x_1=xdata1, x_2=xdata2, y_1=ydata1, y_2=ydata2)
fit_result = fit.execute()
```

**Warning:** The regression coefficient is not properly defined for vector-valued models, but it is still listed! Until this is fixed, please recalculate it on your own for every component using the bestfit parameters.

Do not cite the overall  $R^2$  given by `symfit`.

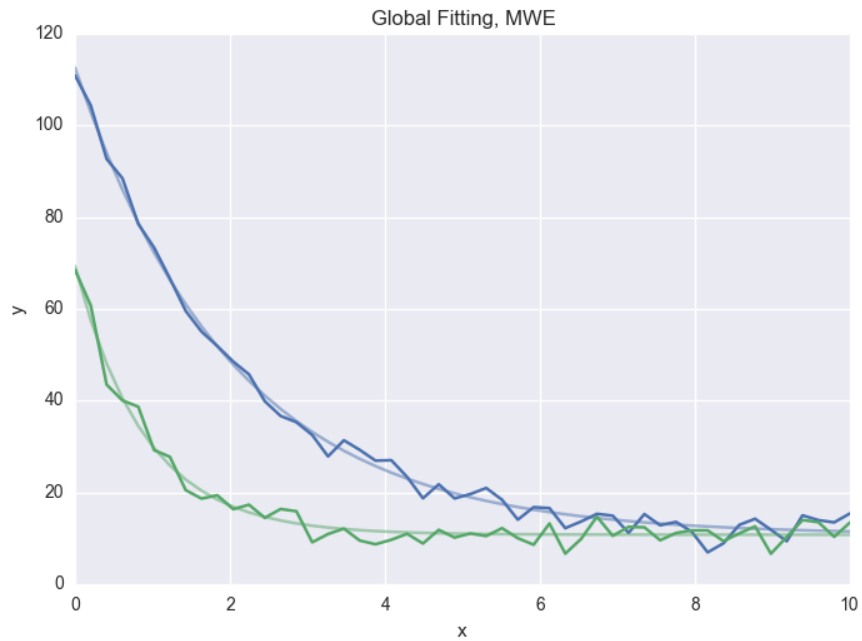
### 4.7.1 Advanced usage

In general, the separate components of the model can be whatever you need them to be. You can mix and match which variables and parameters should be coupled and decoupled ad lib. Some examples are given below.

Same parameters and same function, different (in)dependent variables:

```
datasets = [data_1, data_2, data_3, data_4, data_5, data_6]

xs = variables('x_1, x_2, x_3, x_4, x_5, x_6')
ys = variables('y_1, y_2, y_3, y_4, y_5, y_6')
zs = variables('z_{}'.format(i) for i in range(1, 7))
```



```
a, b = parameters('a, b')

model_dict = {
    z: a/(y * b) * exp(- a * x)
    for x, y, z in zip(xs, ys, zs)
}
```

## 4.8 What if the model is unnamed?

Then you'll have to use the ordering. Variables throughout `symfit`'s objects are internally ordered in the following way: first independent variables, then dependent variables, then sigma variables, and lastly parameters when applicable. Within each group alphabetical ordering applies.

It is therefore always possible to assign data to variables in an unambiguous way using this ordering. For example:

```
fit = Fit(model, x_data, y_data, sigma_y_data)
```





---

## Style Guide & Best Practices

---

### 5.1 Style Guide

Anything Raymond Hettinger says wins the argument until I have time to write a proper style guide.

### 5.2 Best Practices

- It is recommended to always use named models. So not:

```
model = a * x**2
fit = Fit(model, xdata, ydata)
```

but:

```
model = {y: a * x**2}
fit = Fit(model, x=xdata, y=ydata)
```

In this simple example the two are equivalent but for multidimensional data using ordered arguments can become ambiguous and difficult to read. To increase readability, it is therefore recommended to always use named models.

- Evaluating a (vector valued) model returns a `namedtuple()`. You can access the elements by either tuple unpacking, or by using the variable names. Note that if you use tuple unpacking, the results will be ordered alphabetically. The following:

```
model = Model({y_1: x**2, y_2: x**3})
sol_1, sol_2 = model(x=xdata)
```

is therefore equivalent to:

```
model = Model({y_1: x**2, y_2: x**3})
solutions = model(x=xdata)
```

```
sol_1 = solutions.y_1  
sol_2 = solutions.y_2
```

Using numerical indexing (or something similar) is not recommended as it is less readable than the options given above:

```
sol_1 = model(x=xdata)[0]
```

Essays on mathematical and implementation details.

## 6.1 On Likelihood Fitting

The `LogLikelihood` objective function should be used to perform log-likelihood maximization. The `__call__()` and `eval_jacobian()` definitions have been changed to facilitate what one would expect from Likelihood fitting:

`__call__` gives the value of log-likelihood at the given values of  $\vec{p}$  and  $\vec{x}_i$ , where  $\vec{p}$  is a shorthand notation for all parameter, and  $\vec{x}_i$  the same shorthand for all independent variables.

$$\log L(\vec{p}|\vec{x}_i) = \sum_{i=1}^N \log f(\vec{p}|\vec{x}_i)$$

`eval_jacobian()` gives the derivative with respect to every parameter of the log-likelihood:

$$\nabla_{\vec{p}} \log L(\vec{p}|\vec{x}_i) = \sum_{i=1}^N \frac{1}{f(\vec{p}|\vec{x}_i)} \nabla_{\vec{p}} f(\vec{p}|\vec{x}_i)$$

Where  $\nabla_{\vec{p}}$  is the derivative with respect to all parameters  $\vec{p}$ . The function therefore returns a vector of length `len(p)` containing the Jacobian evaluated at the given values of  $\vec{p}$  and  $\vec{x}$ .

## 6.2 On Standard Deviations

This essay is meant as a reflection on the implementation of Standard Deviations and/or measurement errors in `symfit`. Although reading this essay in it's entirety will only be interesting to a select few, I urge anyone who uses `symfit` to read the following summarizing bullet points, as `symfit` is **not** backward-compatible with `scipy`.

- standard deviations are assumed to be measurement errors by default, not relative weights. This is the opposite of the `scipy` definition. Set `absolute_sigma=False` when calling `Fit` to get the `scipy` behavior.

### 6.2.1 Analytical Example

The implementation of standard deviations should be in agreement with cases to which the analytical solution is known. `symfit` was build such that this is true. Let's follow the example outlined by [\[taldcroft\]](#). We'll be sampling from a normal distribution with  $\mu = 0.0$  and varying  $\sigma$ . It can be shown that given a sample from such a distribution:

$$\mu = 0.0$$
$$\sigma_{\mu} = \frac{\sigma}{\sqrt{N}}$$

where  $N$  is the size of the sample. We see that the error in the sample mean scales with the  $\sigma$  of the distribution.

In order to reproduce this with `symfit`, we recognize that determining the avarage of a set of numbers is the same as fitting to a constant. Therefore we will fit to samples generated from distributions with  $\sigma = 1.0$  and  $\sigma = 10.0$  and check if this matches the analytical values. Let's set  $N = 10000$ .

```
N = 10000
sigma = 10.0
np.random.seed(10)
yn = np.random.normal(size=N, scale=sigma)

a = Parameter('a')
y = Variable('y')
model = {y: a}

fit = Fit(model, y=yn, sigma_y=sigma)
fit_result = fit.execute()

fit_no_sigma = Fit(model, y=yn)
fit_result_no_sigma = fit_no_sigma.execute()
```

This gives the following results:

- $a = 5.102056e-02 \pm 1.000000e-01$  when `sigma_y` is provided. This matches the analytical prediction.
- $a = 5.102056e-02 \pm 9.897135e-02$  without `sigma_y` provided. This is incorrect.

If we run the above code example with `sigma = 1.0`, we get the following results:

- $a = 5.102056e-03 \pm 9.897135e-03$  when `sigma_y` is provided. This matches the analytical prediction.
- $a = 5.102056e-03 \pm 9.897135e-03$  without `sigma_y` provided. This is also correct, since providing no weights is the same as setting the weights to 1.

To conclude, if `symfit` is provided with the standard deviations, it will give the expected result by default. As shown in [\[taldcroft\]](#) and `symfit`'s tests, `scipy.optimize.curve_fit()` has to be provided with the `absolute_sigma=True` setting to do the same.

---

**Important:** We see that even if the weight provided to every data point is the same, the *scale* of the weight still effects the result. `scipy` was build such that the opposite is true: if all datapoints have the same weight, the error in the parameters does not depend on the scale of the weight.

This difference is due to the fact that `symfit` is build for areas of science where one is dealing with measurement errors. And with measurement errors, the size of the errors obviously matters for the certainty of the fit parameters, even if the errors are the same for every measurement.

If you want the `scipy` behavior, initiate `Fit` with `absolute_sigma=False`.

---

## 6.3 Comparison to Mathematica

In Mathematica, the default setting is also to use relative weights, which we just argued is not correct when dealing with measurement errors. In [\[Mathematica\]](#) this problem is discussed very nicely, and it is shown how to solve this in Mathematica.

Since `symfit` is a fitting tool for the practical man, measurement errors are assumed by default.

## 6.4 Internal API Structure

Here we describe how the code is organized internally. This is only really relevant for advanced users and developers.

### 6.4.1 Fitting 101

Fitting a model to data is, at it's most basic, a parameter optimisation, and depending on whether you do a least-squares fit or a loglikelihood fit your objective function changes. This means we can split the process of fitting in three distinct, isolated parts:: the *Model*, the Objective and the Minimizer.

In practice, *Fit* will choose an appropriate objective and minimizer, but you can also give it specific instances and classes; just in case you know better.

For both the minimizers and objectives there are abstract base classes, which describe the minimal API required. There are corresponding abstract classes for e.g. *ConstrainedMinimizer*.

### 6.4.2 Objectives

Objectives wrap both the Model and the data supplied, and when called must return a scalar. This scalar will be *minimized*, so when you need something maximized, be sure to add a negation in the right place(s). They must be called with the parameter values as keyword arguments. Be sure to inherit from the abstract base class(es) so you're sure you define all the methods that are expected.

### 6.4.3 Minimizers

Minimizers minimize. They are provided with a function to minimize (the objective) and the *Parameter*s as a function of which the objective should be minimized. Note that once again there are different base classes for minimizers that take e.g. bounds or support gradients. Their *execute()* method takes the metaparameters for the minimization. Again, be sure to inherit from the appropriate base class(es) if you're implementing your own minimizer to make sure all the expected methods are there. And if you're wrapping Scipy style minimizers, have a look at *ScipyMinimize* to avoid a duplication of efforts.

### 6.4.4 Example

Let's say we have some data:

```
xdata = np.linspace(0, 100, 25)
a_vec = np.random.normal(15, scale=2, size=xdata.shape)
b_vec = np.random.normal(100, scale=2, size=xdata.shape)
ydata = a_vec * xdata + b_vec
```

And we want to fit it to some model:

```
a = Parameter(value=0, min=0, max=1000)
b = Parameter(value=0, min=0, max=1000)
x = Variable()
model = a * x + b
```

If we want to fit this normally (but with a specified minimizer), we'd write the following:

```
fit = Fit(model, xdata, ydata, minimizer=BFGS)
fit_result = fit.execute()
```

Now instead, we want to call the minimizer directly. We first define a custom objective function (actually just a chi squared):

```
def f(x, a, b):
    return a * x + b

def chi_squared(a, b):
    return np.sum((ydata - f(xdata, a, b))**2)

custom_minimize = BFGS(chi_squared, [a, b])
custom_minimize.execute()
```

You'll see that the result of both will be the same!

---

### Dependencies and Credits

---

Always pay credit where credit's due. `symfit` uses the following projects to make it's sexy interface possible:

- `leastsqbound-scipy` is used to bound parameters to a given domain.
- `seaborn` was used to make the beautifully styled plots in the example code. All you have to do to sexify your matplotlib plot's is import seaborn, even if you don't use it's special plotting facilities, so I highly recommend it.
- `numpy` and `scipy` are of course used to do efficient data processing.
- `sympy` is used for the manipulation of the symbolic expressions that give this project it's high readability.





This page contains documentation to everything `symfit` has to offer.

## 8.1 Fit

**class** `symfit.core.fit.BaseFit` (*model*, *\*ordered\_data*, *absolute\_sigma=None*, *\*\*named\_data*)

Bases: `symfit.core.fit.TakesData`

Abstract base class for all fitting objects.

**error\_func** (*\*args*, *\*\*kwargs*)

Every fit object has to define an `error_func` method, giving the function to be minimized.

**eval\_jacobian** (*\*args*, *\*\*kwargs*)

Every fit object has to define an `eval_jacobian` method, giving the jacobian of the function to be minimized.

**execute** (*\*args*, *\*\*kwargs*)

Every fit object has to define an `execute` method. Any `*` and `**` arguments will be passed to the fitting module that is being wrapped, e.g. `leastsq`.

**Args** *kwargs*

**Returns** Instance of `FitResults`

**class** `symfit.core.fit.BaseModel` (*model*)

Bases: `collections.abc.Mapping`

ABC for `Model`'s. Makes sure models are iterable. Models can be initiated from Mappings or Iterables of Expressions, or from an expression directly. Expressions are not enforced for ducktyping purposes.

**\_\_eq\_\_** (*other*)

`Model`'s are considered equal when they have the same dependent variables, and the same expressions for those dependent variables. The same is defined here as passing `sympy ==` for the vars themselves, and as `expr1 - expr2 == 0` for the expressions. For more info check the [sympy docs](#).

**Parameters** *other* – Instance of `Model`.

**Returns** bool

`__getitem__` (*dependent\_var*)

Returns the expression belonging to a given dependent variable.

**Parameters** `dependent_var` (`Variable`) – Instance of `Variable`

**Returns** The expression belonging to `dependent_var`

`__init__` (*model*)

Initiate a Model from a dict:

```
a = Model({y: x**2})
```

Preferred way of initiating `Model`, since now you know what the dependent variable is called.

**Parameters** `model` – dict of `Expr`, where dependent variables are the keys.

`__iter__` ()

**Returns** iterable over `self.model_dict`

`__len__` ()

**Returns** the number of dependent variables for this model.

`__neg__` ()

**Returns** new model with opposite sign. Does not change the model in-place, but returns a new copy.

**bounds**

**Returns** List of tuples of all bounds on parameters.

**shared\_parameters**

**Returns** bool, indicating if parameters are shared between the vector components of this model.

**vars**

**Returns** Returns a list of dependent, independent and sigma variables, in that order.

**class** `symfit.core.fit.CallableModel` (*model*)

Bases: `symfit.core.fit.BaseModel`

Defines a callable model. The usual rules apply to the ordering of the arguments:

- first independent variables, then dependent variables, then parameters.
- within each of these groups they are ordered alphabetically.

`__call__` (*\*args, \*\*kwargs*)

Evaluate the model for a certain value of the independent vars and parameters. Signature for this function contains independent vars and parameters, NOT dependent and sigma vars.

Can be called with both ordered and named parameters. Order is independent vars first, then parameters. Alphabetical order within each group.

**Parameters**

- **args** –
- **kwargs** –

**Returns** A namedtuple of all the dependent vars evaluated at the desired point. Will always return a tuple, even for scalar valued functions. This is done for consistency.

**eval\_components** (\*args, \*\*kwargs)

Evaluate the components of the model with the given data. Used for numerical evaluation.

**eval\_jacobian** (\*args, \*\*kwargs)

**Returns** The jacobian matrix of the function.

**finite\_difference** (\*args, dx=1e-08, \*\*kwargs)

Calculates a numerical approximation of the Jacobian of the model using the sixth order central finite difference method. Accepts a *dx* keyword to tune the relative stepsize used. Makes 6\*n\_params calls to the model.

**Returns** A numerical approximation of the Jacobian of the model as a list with length n\_components containing numpy arrays of shape (n\_params, n\_datapoints)

**numerical\_components**

**Returns** lambda functions of each of the components in model\_dict, to be used in numerical calculation.

**class** symfit.core.fit.Constraint (constraint, model)

Bases: *symfit.core.fit.Model*

Constraints are a special type of model in that they have a type: >=, == etc. They are made to have lhs - rhs == 0 of the original expression.

For example, Eq(y + x, 4) -> Eq(y + x - 4, 0)

Since a constraint belongs to a certain model, it has to be initiated with knowledge of it's parent model. This is important because all numerical\_ methods are done w.r.t. the parameters and variables of the parent model, not the constraint! This is because the constraint might not have all the parameter or variables that the model has, but in order to compute for example the Jacobian we still want to derive w.r.t. all the parameters, not just those present in the constraint.

**\_\_init\_\_** (constraint, model)

**Parameters**

- **constraint** – constraint that model should be subjected to.
- **model** – A constraint is always tied to a model.

**\_\_neg\_\_** ()

**Returns** new model with opposite sign. Does not change the model in-place, but returns a new copy.

**jacobian**

**Returns** Jacobian 'Matrix' filled with the symbolic expressions for all the partial derivatives. Partial derivatives are of the components of the function with respect to the Parameter's, not the independent Variable's.

**numerical\_components**

**Returns** lambda functions of each of the components in model\_dict, to be used in numerical calculation.

**numerical\_jacobian**

**Returns** lambda functions of the jacobian matrix of the function, which can be used in numerical optimization.

**class** symfit.core.fit.Fit (model, \*ordered\_data, constraints=None, objective=None, minimizer=None, \*\*named\_data)

Bases: *symfit.core.fit.TakesData*, *symfit.core.fit.HasCovarianceMatrix*

Your one stop fitting solution! Based on the nature of the input, this object will attempt to select the right fitting type for your problem.

If you need very specific control over how the problem is solved, you can pass it the minimizer or objective function you would like to use.

Example usage:

```
a, b = parameters('a, b')
x, y = variables('x, y')

model = {y: a * x + b}

# Fit will use its default settings
fit = Fit(model, x=xdata, y=ydata)
fit_result = fit.execute()

# Use Nelder-Mead instead
fit = Fit(model, x=xdata, y=ydata, minimizer=NelderMead)
fit_result = fit.execute()
```

```
__init__(model, *ordered_data, constraints=None, objective=None, minimizer=None,
**named_data)
```

#### Parameters

- **model** – (dict of) sympy expression(s) or Model object.
- **constraints** – iterable of Relation objects to be used as constraints.
- **absolute\_sigma** (*bool*) – True by default. If the sigma is only used for relative weights in your problem, you could consider setting it to False, but if your sigma are measurement errors, keep it at True. Note that curve\_fit has this set to False by default, which is wrong in experimental science.
- **objective** – Have Fit use your specified objective. Can be one of the predefined *symfit* objectives or any callable which accepts fit parameters and returns a scalar.
- **minimizer** – Have Fit use your specified *symfit.core.minimizers.BaseMinimizer*.
- **ordered\_data** – data for dependent, independent and sigma variables. Assigned in the following order: independent vars are assigned first, then dependent vars, then sigma's in dependent vars. Within each group they are assigned in alphabetical order.
- **named\_data** – assign dependent, independent and sigma variables data by name.

```
execute (**minimize_options)
```

Execute the fit.

**Parameters minimize\_options** – keyword arguments to be passed to the specified minimizer.

**Returns** FitResults instance

```
class symfit.core.fit.HasCovarianceMatrix
```

Bases: *object*

Mixin class for calculating the covariance matrix for any model that has a well-defined Jacobian  $J$ . The covariance is then approximated as  $J^T W J$ , where W contains the weights of each data point.

Supports vector valued models, but is unable to estimate covariances for those, just variances. Therefore, take the result with a grain of salt for vector models.

**covariance\_matrix** (*best\_fit\_params*)

Given best fit parameters, this function finds the covariance matrix. This matrix gives the (co)variance in the parameters.

**Parameters** *best\_fit\_params* – dict of best fit parameters as given by .best\_fit\_params()

**Returns** covariance matrix.

**class** symfit.core.fit.LinearLeastSquares (\*args, \*\*kwargs)

Bases: *symfit.core.fit.BaseFit*

Experimental. Solves the linear least squares problem analytically. Involves no iterations or approximations, and therefore gives the best possible fit to the data.

The `Model` provided has to be linear.

Currently, since this object still has to mature, it suffers from the following limitations:

- It does not check if the model can be linearized by a simple substitution. For example,  $\exp(a * x) \rightarrow b * \exp(x)$ . You will have to do this manually.
- Does not use bounds or guesses on the `Parameter`'s. Then again, it doesn't have to, since you have an exact solution. No guesses required.
- It only works with scalar functions. This is strictly enforced.

**\_\_init\_\_** (\*args, \*\*kwargs)

**Raises** `ModelError` in case of a non-linear model or when a vector valued function is provided.

**best\_fit\_params** ()

Fits to the data and returns the best fit parameters.

**Returns** dict containing parameters and their best-fit values.

**covariance\_matrix** (*best\_fit\_params*)

Given best fit parameters, this function finds the covariance matrix. This matrix gives the (co)variance in the parameters.

**Parameters** *best\_fit\_params* – dict of best fit parameters as given by .best\_fit\_params()

**Returns** covariance matrix.

**execute** ()

Execute an analytical (Linear) Least Squares Fit. This object works by symbolically solving when  $\nabla \chi^2 = 0$ .

To perform this task the expression of  $\nabla \chi^2$  is determined, ignoring that  $\chi^2$  involves summing over all terms. Then the sum is performed by substituting the variables by their respective data and summing all terms, while leaving the parameters symbolic.

The resulting system of equations is then easily solved with `sympy.solve`.

**Returns** `FitResult`

**static is\_linear** (*model*)

Test whether model is of linear form in it's parameters.

Currently this function does not recognize if a model can be considered linear by a simple substitution, such as  $\exp(k x) = k' \exp(x)$ .

**Parameters** *model* – `Model` instance

**Returns** True or False

**class** `symfit.core.fit.Model(model)`

Bases: `symfit.core.fit.CallableModel`

Model represents a symbolic function and all it's derived properties such as sum of squares, jacobian etc. Models can be initiated from several objects:

```
a = Model({y: x**2})
b = Model(y=x**2)
```

Models are callable. The usual rules apply to the ordering of the arguments:

- first independent variables, then dependent variables, then parameters.
- within each of these groups they are ordered alphabetically.

Models are also iterable, behaving as their internal `model_dict`. In the example above, `a[y]` returns `x**2`, `len(a) == 1`, `y in a == True`, etc.

**\_\_str\_\_()**

Printable representation of this model.

**Returns** `str`

**chi**

**Returns** Symbolic Square root of  $\chi^2$ . Required for MINPACK optimization only. Denoted as  $\sqrt{\chi^2}$

**chi\_jacobian**

Return a symbolic jacobian of the  $\sqrt{\chi^2}$  function. Vector of derivatives w.r.t. each parameter. Not a Matrix but a vector! This is because that's what leastsq needs.

**chi\_squared**

**Returns** Symbolic  $\chi^2$

**chi\_squared\_jacobian**

Return a symbolic jacobian of the  $\chi^2$  function. Vector of derivatives w.r.t. each parameter. Not a Matrix but a vector!

**eval\_components** (*\*args*, *\*\*kwargs*)

**Returns** lambda functions of each of the components in `model_dict`, to be used in numerical calculation.

**eval\_jacobian** (*\*args*, *\*\*kwargs*)

**Returns** Jacobian evaluated at the specified point.

**jacobian**

**Returns** Jacobian 'Matrix' filled with the symbolic expressions for all the partial derivatives. Partial derivatives are of the components of the function with respect to the Parameter's, not the independent Variable's.

**numerical\_chi**

**Returns** lambda function of the `.chi` method, to be used in MINPACK optimisation.

**numerical\_chi\_jacobian**

**Returns** lambda functions of the jacobian of the `.chi` method, which can be used in numerical optimization.

**numerical\_chi\_squared**

**Returns** lambda function of the `.chi_squared` method, to be used in numerical optimisation.

**numerical\_chi\_squared\_jacobian**

**Returns** lambda functions of the jacobian of the `.chi_squared` method.

**numerical\_jacobian**

**Returns** lambda functions of the jacobian matrix of the function, which can be used in numerical optimization.

**exception** `symfit.core.fit.ModelError`

Bases: `Exception`

Raised when a problem occurs with a model.

**class** `symfit.core.fit.NonLinearLeastSquares(*args, **kwargs)`

Bases: `symfit.core.fit.BaseFit`

Experimental. Implements non-linear least squares [\[wiki\\_nllsq\]](#). Works by a two step process: First the model is linearised by doing a first order taylor expansion around the guesses for the parameters. Then a LinearLeastSquares fit is performed. This is iterated until a fit of sufficient quality is obtained.

Sensitive to good initial guesses. Providing good initial guesses is a must.

**execute** (*relative\_error=1e-08, max\_iter=500*)

Perform a non-linear least squares fit.

**Parameters**

- **relative\_error** – Relative error between the sum of squares of subsequent iterations. Once smaller than the value specified, the fit is considered complete.
- **max\_iter** – Maximum number of iterations before giving up.

**Returns** Instance of `FitResults`.

**class** `symfit.core.fit.ODEModel(model_dict, initial, *lsoda_args, **lsoda_kwargs)`

Bases: `symfit.core.fit.CallableModel`

Model build from a system of ODEs. When the model is called, the ODE is integrated using the LSODA package.

Currently the initial conditions are assumed to specify the first point to begin the integration from. This is enforced. In future versions one should be allowed to specify the initial value as a parameter.

**\_\_call\_\_** (*\*args, \*\*kwargs*)

Evaluate the model for a certain value of the independent vars and parameters. Signature for this function contains independent vars and parameters, NOT dependent and sigma vars.

Can be called with both ordered and named parameters. Order is independent vars first, then parameters. Alphabetical order within each group.

**Parameters**

- **args** – Ordered arguments for the parameters and independent variables
- **kwargs** – Keyword arguments for the parameters and independent variables

**Returns** A namedtuple of all the dependent vars evaluated at the desired point. Will always return a tuple, even for scalar valued functions. This is done for consistency.

**\_\_getitem\_\_** (*dependent\_var*)

Gives the function defined for the derivative of `dependent_var`. e.g.  $y' = f(y, t)$ , `model[y] -> f(y, t)`

**Parameters** `dependent_var` –

### Returns

`__init__` (*model\_dict*, *initial*, *\*lsoda\_args*, *\*\*lsoda\_kwargs*)

### Parameters

- **model\_dict** – Dictionary specifying ODEs. e.g. `model_dict = {D(y, x): a * x**2}`
- **initial** – dict of initial conditions for the ODE. Must be provided! e.g. `initial = {y: 1.0, x: 0.0}`
- **lsoda\_args** – args to pass to the lsoda solver. See [scipy's odeint](#) for more info.
- **lsoda\_kwargs** – kwargs to pass to the lsoda solver.

`__iter__` ()

**Returns** iterable over `self.model_dict`

`__neg__` ()

**Returns** new model with opposite sign. Does not change the model in-place, but returns a new copy.

**eval\_components** (*\*args*, *\*\*kwargs*)

Numerically integrate the system of ODEs.

### Parameters

- **args** – Ordered arguments for the parameters and independent variables
- **kwargs** – Keyword arguments for the parameters and independent variables

### Returns

**class** `symfit.core.fit.TakesData` (*model*, *\*ordered\_data*, *absolute\_sigma=None*, *\*\*named\_data*)

Bases: `object`

An base class for everything that takes data. Most importantly, it takes care of linking the provided data to variables. The allowed variables are extracted from the model.

`__init__` (*model*, *\*ordered\_data*, *absolute\_sigma=None*, *\*\*named\_data*)

### Parameters

- **model** – (dict of) sympy expression or `Model` object.
- **absolute\_sigma** (*bool*) – True by default. If the sigma is only used for relative weights in your problem, you could consider setting it to False, but if your sigma are measurement errors, keep it at True. Note that `curve_fit` has this set to False by default, which is wrong in experimental science.
- **ordered\_data** – data for dependent, independent and sigma variables. Assigned in the following order: independent vars are assigned first, then dependent vars, then sigma's in dependent vars. Within each group they are assigned in alphabetical order.
- **named\_data** – assign dependent, independent and sigma variables data by name.

Standard deviation can be provided to any variable. They have to be prefixed with `sigma_`. For example, let `x` be a `Variable`. Then `sigma_x` will give the stdev in `x`.

### data\_shapes

Returns the shape of the data. In most cases this will be the same for all variables of the same type, if not this raises an `Exception`.



Ignores variables which are set to None by design so we know that those None variables can be assumed to have the same shape as the other in calculations where this is needed, such as the covariance matrix.

**Returns** Tuple of all independent var shapes, dependent var shapes.

#### **dependent\_data**

Read-only Property

**Returns** Data belonging to each dependent variable as a dict with variable names as key, data as value.

**Return type** `collections.OrderedDict`

#### **independent\_data**

Read-only Property

**Returns** Data belonging to each independent variable as a dict with variable names as key, data as value.

**Return type** `collections.OrderedDict`

#### **initial\_guesses**

**Returns** Initial guesses for every parameter.

#### **sigma\_data**

Read-only Property

**Returns** Data belonging to each sigma variable as a dict with variable names as key, data as value.

**Return type** `collections.OrderedDict`

**class** `symfit.core.fit.TaylorModel` (*model*)

Bases: `symfit.core.fit.Model`

A first-order Taylor expansion of a model around given parameter values ( $p_0$ ). Is used by NonLinearLeast-Squares. Currently only a first order expansion is implemented.

**\_\_init\_\_** (*model*)

Make a first order Taylor expansion of *model*.

**Parameters** *model* – Instance of `Model`

**\_\_str\_\_** ()

When printing a `TaylorModel`, the point around which the expansion took place is included.

For example, a Taylor expansion of  $\{y: \sin(w * x)\}$  at  $w = 0$  would be printed as:

```
@{w: 0.0} -> y(x; w) = w*x
```

#### **p0**

Property of the  $p_0$  around which to expand. Should be set by the names of the parameters themselves.

Example:

```
a = Parameter()
x, y = variables('x, y')
model = TaylorModel({y: sin(a * x)})

model.p0 = {a: 0.0}
```

#### **params**

`params` returns only the *free* parameters. Strictly speaking, the expression for a `TaylorModel` contains

both the parameters  $\vec{p}$  and  $p_0$  around which to expand, but params should only give  $\vec{p}$ . To get a mapping to the  $\vec{p}_0$ , use `.params_0`.

`symfit.core.fit.r_squared(model, fit_result, data)`  
 Calculates the coefficient of determination,  $R^2$ , for the fit.

(Is not defined properly for vector valued functions.)

#### Parameters

- **model** – Model instance
- **fit\_result** – FitResults instance
- **data** – data with which the fit was performed.

## 8.2 Argument

**class** `symfit.core.argument.Argument` (*name=None, \*\*assumptions*)

Bases: `sympy.core.symbol.Symbol`

Base class for symfit symbols. This helps make symfit symbols distinguishable from sympy symbols.

The `Argument` class also makes DRY possible in defining `Argument`'s: it uses `inspect` to read the lhs of the assignment and uses that as the name for the `Argument` is none is explicitly set.

For example:

```
x = Variable()
print(x.name)
>> 'x'
```

**class** `symfit.core.argument.Parameter` (*value=1.0, min=None, max=None, fixed=False, name=None, \*\*assumptions*)

Bases: `symfit.core.argument.Argument`

Parameter objects are used to facilitate bounds on function parameters.

**\_\_call\_\_** (*\*values, \*\*named\_values*)

Call an expression to evaluate it at the given point.

Future improvements: I would like if func and signature could be buffered after the first call so they don't have to be recalculated for every call. However, nothing can be stored on self as sympy uses `__slots__` for efficiency. This means there is no instance dict to put stuff in! And I'm pretty sure it's ill advised to hack into the `__slots__` of `Expr`.

However, for the moment I don't really notice a performance penalty in running tests.

p.s. In the current setup signature is not even needed since no introspection is possible on the `Expr` before calling it anyway, which makes calculating the signature absolutely useless. However, I hope that someday some monkey patching expert in shining armour comes by and finds a way to store it in `__signature__` upon `__init__` of any `symfit` expr such that calling `inspect_sig.signature` on a symbolic expression will tell you which arguments to provide.

#### Parameters

- **self** – Any subclass of `sympy.Expr`
- **values** – Values for the Parameters and Variables of the `Expr`.

- **named\_values** – Values for the vars and params by name. `named_values` is allowed to contain too many values, as this sometimes happens when using `**fit_result.params` on a submodel. The irrelevant params are simply ignored.

**Returns** The function evaluated at `values`. The type depends entirely on the input. Typically an array or a float but nothing is enforced.

`__init__` (*value=1.0, min=None, max=None, fixed=False, name=None, \*\*assumptions*)

#### Parameters

- **value** – Initial guess value.
- **min** – Lower bound on the parameter value.
- **max** – Upper bound on the parameter value.
- **fixed** (*bool*) – Fix the parameter to `value` during fitting.
- **name** – Name of the Parameter.
- **assumptions** – assumptions to pass to `sympy`.

`class` `symfit.core.argument.Variable` (*name=None, \*\*assumptions*)

Bases: `symfit.core.argument.Argument`

Variable type.

## 8.3 Operators

Monkey Patching module.

This module makes `sympy` Expressions callable, which makes the whole project feel more consistent.

`symfit.core.operators.call` (*self, \*values, \*\*named\_values*)

Call an expression to evaluate it at the given point.

Future improvements: I would like if `func` and `signature` could be buffered after the first call so they don't have to be recalculated for every call. However, nothing can be stored on `self` as `sympy` uses `__slots__` for efficiency. This means there is no instance dict to put stuff in! And I'm pretty sure it's ill advised to hack into the `__slots__` of `Expr`.

However, for the moment I don't really notice a performance penalty in running tests.

p.s. In the current setup `signature` is not even needed since no introspection is possible on the `Expr` before calling it anyway, which makes calculating the signature absolutely useless. However, I hope that someday some monkey patching expert in shining armour comes by and finds a way to store it in `__signature__` upon `__init__` of any `symfit` `expr` such that calling `inspect_sig.signature` on a symbolic expression will tell you which arguments to provide.

#### Parameters

- **self** – Any subclass of `sympy.Expr`
- **values** – Values for the Parameters and Variables of the `Expr`.
- **named\_values** – Values for the vars and params by name. `named_values` is allowed to contain too many values, as this sometimes happens when using `**fit_result.params` on a submodel. The irrelevant params are simply ignored.

**Returns** The function evaluated at `values`. The type depends entirely on the input. Typically an array or a float but nothing is enforced.

## 8.4 Fit Results

**class** `symfit.core.fit_results.FitResults` (*model*, *popt*, *covariance\_matrix*, *infodic*, *mesg*, *ier*, *\*\*gof\_qualifiers*)

Bases: `object`

Class to display the results of a fit in a nice and unambiguous way. All things related to the fit are available on this class, e.g. - parameter values + stdev - R squared (Regression coefficient.) or other fit quality qualifiers. - fitting status message - covariance matrix

Contains the attribute *params*, which is an `OrderedDict` containing all the parameter names and their optimized values. Can be `**` unpacked when evaluating *Model*'s.

`__getattr__` (*item*)

Return the requested *item* if it can be found in the *gof\_qualifiers* dict.

**Parameters** *item* – Name of Goodness of Fit qualifier.

**Returns** Goodness of Fit qualifier if present.

`__init__` (*model*, *popt*, *covariance\_matrix*, *infodic*, *mesg*, *ier*, *\*\*gof\_qualifiers*)

Excuse the ugly names of most of these variables, they are inherited from *scipy*. Will be changed.

**Parameters**

- **model** – *Model* that was fit to.
- **popt** – best fit parameters, same ordering as in *model.params*.
- **pcov** – covariance matrix.
- **infodic** – dict with fitting info.
- **mesg** – Status message.
- **ier** – Number of iterations.
- **gof\_qualifiers** – Any remaining keyword arguments should be Goodness of fit (g.o.f.) qualifiers.

`__str__` ()

Pretty print the results as a table.

**covariance** (*param\_1*, *param\_2*)

Return the covariance between *param\_1* and *param\_2*.

**Parameters**

- **param\_1** – *Parameter* Instance.
- **param\_2** – *Parameter* Instance.

**Returns** Covariance of the two params.

**stdev** (*param*)

Return the standard deviation in a given parameter as found by the fit.

**Parameters** *param* – *Parameter* Instance.

**Returns** Standard deviation of *param*.

**value** (*param*)

Return the value in a given parameter as found by the fit.

**Parameters** *param* – *Parameter* Instance.

**Returns** Value of `param`.

**variance** (*param*)

Return the variance in a given parameter as found by the fit.

**Parameters** `param` – Parameter Instance.

**Returns** Variance of `param`.

## 8.5 Minimizers

**class** `symfit.core.minimizers.BaseMinimizer` (*objective, parameters*)

Bases: `object`

ABC for all Minimizers.

**\_\_init\_\_** (*objective, parameters*)

**Parameters**

- **objective** – Objective function to be used.
- **parameters** – List of *Parameter* instances

**execute** (*\*\*options*)

The execute method should implement the actual minimization procedure, and should return a *FitResults* instance. :param options: options to be used by the minimization procedure. :return: an instance of *FitResults*.

**class** `symfit.core.minimizers.BoundedMinimizer` (*objective, parameters*)

Bases: `symfit.core.minimizers.BaseMinimizer`

ABC for Minimizers that support bounds.

**class** `symfit.core.minimizers.ConstrainedMinimizer` (*\*args, constraints=None, \*\*kwargs*)

Bases: `symfit.core.minimizers.BaseMinimizer`

ABC for Minimizers that support constraints

**class** `symfit.core.minimizers.DummyModel` (*params*)

Bases: `tuple`

**\_\_getnewargs\_\_** ()

Return self as a plain tuple. Used by copy and pickle.

**static** **\_\_new\_\_** (*\_cls, params*)

Create new instance of DummyModel(params,)

**\_\_repr\_\_** ()

Return a nicely formatted representation string

**params**

Alias for field number 0

**class** `symfit.core.minimizers.GradientMinimizer` (*\*args, jacobian=None, \*\*kwargs*)

Bases: `symfit.core.minimizers.BaseMinimizer`

ABC for Minizers that support the use of a jacobian

**class** `symfit.core.minimizers.MINPACK` (*\*args, \*\*kwargs*)

Bases: `symfit.core.minimizers.ScipyMinimize`, `symfit.core.minimizers.GradientMinimizer`, `symfit.core.minimizers.BoundedMinimizer`

Wrapper to scipy's implementation of MINPACK, since it is the industry standard.

**execute** (*\*\*minpack\_options*)

**Parameters** *minpack\_options* – Any named arguments to be passed to leastsqbound

**class** `symfit.core.minimizers.ScipyMinimize` (*\*args, \*\*kwargs*)

Bases: `object`

Mix-in class that handles the execute calls to `scipy.optimize.minimize`.

**static** `scipy_constraints` (*constraints, data*)

Returns all constraints in a scipy compatible format.

**Returns** dict of scipy compatible statements.

**wrap\_func** (*func*)

Given an objective function *func*, make sure it is always called via keyword arguments with the relevant parameter names.

**Parameters** *func* – Function to be wrapped to keyword only calls.

**Returns** wrapped function

## 8.6 Objectives

**class** `symfit.core.objectives.BaseObjective` (*model, data*)

Bases: `object`

ABC for objective functions. Implements basic data handling.

**\_\_call\_\_** (*\*\*parameters*)

Evaluate the objective function for given parameter values.

**Parameters** *parameters* –

**Returns** float

**\_\_init\_\_** (*model, data*)

**Parameters**

- **model** – *symfit* style model.
- **data** – data for all the variables of the model.

**dependent\_data**

Read-only Property

**Returns** Data belonging to each dependent variable as a dict with variable names as key, data as value.

**Return type** `collections.OrderedDict`

**independent\_data**

Read-only Property

**Returns** Data belonging to each independent variable as a dict with variable names as key, data as value.

**Return type** `collections.OrderedDict`

**sigma\_data**

Read-only Property

**Returns** Data belonging to each sigma variable as a dict with variable names as key, data as value.

**Return type** `collections.OrderedDict`

**class** `symfit.core.objectives.GradientObjective` (*model, data*)

Bases: `symfit.core.objectives.BaseObjective`

ABC for objectives that support gradient methods.

**eval\_jacobian** (*\*\*parameters*)

Evaluate the jacobian for given parameter values.

**Parameters** *parameters* –

**Returns** float

**class** `symfit.core.objectives.LeastSquares` (*model, data*)

Bases: `symfit.core.objectives.GradientObjective`

Objective representing the  $\chi^2$  of a model.

**\_\_call\_\_** (*\*, flatten\_components=True, \*\*parameters*)

**Parameters**

- **parameters** – values of the *Parameter*’s to evaluate  $\chi^2$  at.
- **flatten\_components** – if *True*, return the total  $\chi^2$ . If *False*, return the  $\chi^2$  per component of the *BaseModel*.

**Returns** scalar or list of scalars depending on the value of *flatten\_components*.

**eval\_jacobian** (*\*\*parameters*)

Jacobian of  $\chi^2$  in the *Parameter*’s ( $\nabla_{\vec{p}}\chi^2$ ).

**Parameters** *parameters* – values of the *Parameter*’s to evaluate  $\nabla_{\vec{p}}\chi^2$  at.

**Returns** *np.array* of length equal to the number of parameters..

**class** `symfit.core.objectives.LogLikelihood` (*model, data*)

Bases: `symfit.core.objectives.GradientObjective`

Error function to be minimized by a minimizer in order to *maximize* the log-likelihood.

**\_\_call\_\_** (*\*\*parameters*)

**Parameters** *parameters* – values for the fit parameters.

**Returns** scalar value of log-likelihood

**eval\_jacobian** (*\*, apply\_func=<function nansum>, \*\*parameters*)

Jacobian for log-likelihood is defined as  $\nabla_{\vec{p}}(\log(L(\vec{p}|\vec{x})))$ .

**Parameters**

- **parameters** – values for the fit parameters.
- **apply\_func** – Function to apply to each component before returning it. The default is to sum away along the datapoint dimension using *np.nansum*.

**Returns** array of length number of *Parameter*’s in the model, with all partial derivatives evaluated at *p*, data.

**class** `symfit.core.objectives.MinimizeModel` (*model, \*args, \*\*kwargs*)

Bases: `symfit.core.objectives.BaseObjective`

Objective to use when the model itself is the quantity that should be minimized. This is only supported for scalar models.

**class** `symfit.core.objectives.VectorLeastSquares` (*model, data*)

Bases: `symfit.core.objectives.GradientObjective`

Implemented for MINPACK only. Returns the residuals/sigma before squaring and summing, rather than chi2 itself.

**\_\_call\_\_** (\*, *flatten\_components=True*, \*\**parameters*)

Returns the value of the square root of  $\chi^2$ , summing over the components.

This function now supports setting variables to None.

#### Parameters

- **p** – array of parameter values.
- **flatten\_components** – If True, summing is performed over the data indices (default).

**Returns**  $\sqrt{\chi^2}$

## 8.7 Support

This module contains support functions and convenience methods used throughout symfit. Some are used predominantly internally, others are designed for users.

**class** `symfit.core.support.D`

Bases: `sympy.core.function.Derivative`

Convenience wrapper for `sympy.Derivative`. Used most notably in defining `ODEModel`'s.

**class** `symfit.core.support.RequiredKeyword`

Bases: `object`

Flag variable to indicate that this is a required keyword.

**exception** `symfit.core.support.RequiredKeywordError`

Bases: `Exception`

Error raised in case a keyword-only argument is not treated as such.

`symfit.core.support.cache` (*func*)

Decorator function that gets a method as its input and either buffers the input, or returns the buffered output. Used in conjunction with properties to take away the standard buffering logic.

**Parameters** **func** –

**Returns**

**class** `symfit.core.support.deprecated` (*replacement=None*)

Bases: `object`

Decorator to raise a DeprecationWarning.

**\_\_init\_\_** (*replacement=None*)

**Parameters** **replacement** – The function which should now be used instead.

`symfit.core.support.jacobian` (*expr, symbols*)

Derive a symbolic expr w.r.t. each symbol in symbols. This returns a symbolic jacobian vector.

**Parameters**



- **expr** – A sympy Expr.
- **symbols** – The symbols w.r.t. which to derive.

`symfit.core.support.key2str(target)`

In `symfit` there are many dicts with symbol: value pairs. These can not be used immediately as `**kwargs`, even though this would make a lot of sense from the context. This function wraps such dict to make them usable as `**kwargs` immediately.

**Parameters** `target` – dict to be made save

**Returns** dict of `str(symbol): value pairs`.

**class** `symfit.core.support.keywordonly(**kwonly_arguments)`

Bases: `object`

Decorator class which wraps a python 2 function into one with keyword-only arguments.

Example:

```
@keywordonly(floor=True)
def f(x, **kwargs):
    floor = kwargs.pop('floor')
    return np.floor(x**2) if floor else x**2
```

This decorator is not much more than:

```
floor = kwargs.pop('floor') if 'floor' in kwargs else True
```

However, I prefer it's usage because:

- it's clear from reading the function declaration there is an option to provide this argument. The information on possible keywords is where you'd expect it to be.
- you're guaranteed that the pop works.
- It is fully inspect compatible such that sphynx is able to index these properly as keyword only arguments just like it would for native py3 keyword only arguments.

Please note that this decorator needs a `**` argument on the wrapped function in order to work.

**\_\_call\_\_** (*func*)

Returns a decorated version of *func*, who's signature now includes the keyword-only arguments.

**Parameters** `func` – the function to be decorated

**Returns** the decorated function

`symfit.core.support.parameters(names)`

Convenience function for the creation of multiple parameters.

**Parameters** `names` – string of parameter names. Should be comma seperated. Example: `a, b = parameters('a, b')`

`symfit.core.support.seperate_symbols(func)`

Seperate the symbols in symbolic function *func*. Return them in alphabetical order.

**Parameters** `func` – scipy symbolic function.

**Returns** (`vars, params`), a tuple of all variables and parameters, each sorted in alphabetical order.

**Raises** `TypeError` – only `symfit` Variable and Parameter are allowed, not sympy Symbols.

`symfit.core.support.sympy_to_py(func, vars, params)`

Turn a symbolic expression into a Python lambda function, which has the names of the variables and parameters as it's argument names.

**Parameters**

- **func** – sympy expression
- **vars** – variables in this model
- **params** – parameters in this model

**Returns** lambda function to be used for numerical evaluation of the model. Ordering of the arguments will be vars first, then params.

`symfit.core.support.sympy_to_scipy(func, vars, params)`

Convert a symbolic expression to one scipy digs. Not used by symfit any more.

**Parameters**

- **func** – sympy expression
- **vars** – variables
- **params** – parameters

**Returns** Scipy-style function to be used for numerical evaluation of the model.

`symfit.core.support.variables(names)`

Convenience function for the creation of multiple variables.

**Parameters** **names** – string of variable names. Should be comma seperated. Example: x, y = variables('x, y')

## 8.8 Distributions

Some common distributions are defined in this module. That way, users can easily build more complicated expressions without making them look hard.

I have deliberately chosen to start these function with a capital, e.g. Gaussian instead of gaussian, because this makes the resulting expressions more readable.

`symfit.distributions.Exp(x, l)`

Exponential Distribution pdf. :param x: free variable. :param l: rate parameter. :return: sympy.Expr for an Exponential Distribution pdf.

`symfit.distributions.Gaussian(x, mu, sig)`

Gaussian pdf. :param x: free variable. :param mu: mean of the distribution. :param sig: standard deviation of the distribution. :return: sympy.Expr for a Gaussian pdf.

## 8.9 Contrib

Contrib modules are modules and extensions to symfit provided by other people. This usually means the code is of slightly less quality, and may not survive future versions.

```
class symfit.contrib.interactive_guess.interactive_guess.InteractiveGuess2D(*args,
                                                                              n_points=100,
                                                                              **kwargs)
    Bases: symfit.core.fit.TakesData
```

A class that provides an graphical, interactive way of guessing initial fitting parameters.

**\_\_init\_\_** (\*args, n\_points=100, \*\*kwargs)

Create a matplotlib window with sliders for all parameters in this model, so that you may graphically guess initial fitting parameters. n\_points is the number of points drawn for the plot. Data points are plotted as blue points, the proposed model as a red line.

Slider extremes are taken from the parameters where possible. If these are not provided, the minimum is 0; and the maximum is value\*2. If no initial value is provided, it defaults to 1.

This will modify the values of the parameters present in model.

**Parameters** n\_points (*int*) – The number of points used for drawing the fitted function.

**\_\_str\_\_** ()

Represent the guesses in a human readable way.

**Returns** string with the guessed values.

**execute** (\*, block=True, show=True, \*\*kwargs)

Execute the interactive guessing procedure.

**Parameters**

- **show** (*bool*) – Whether or not to show the figure. Useful for testing.
- **block** – Blocking call to matplotlib



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