symfit Documentation

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CHAPTER 1

Introduction

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)
```

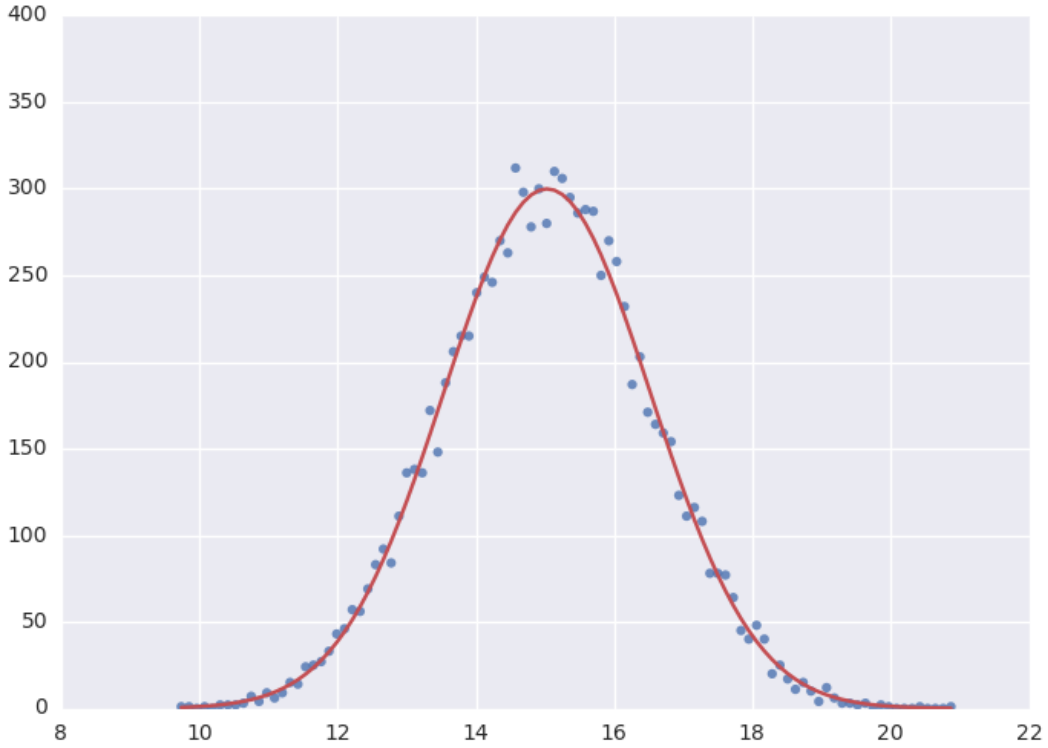
As your models become more complicated, `symfit` really comes into it's own. For example, vector valued functions are both easy to define and beautiful to look at:

```
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: >=
]
```


400
350
300
250
200
150
100
50
0
8
10
12
14
16
18
20
22

```
fit = Maximize(model, constraints=constraints)
```

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 Dependencies

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

CHAPTER 3

Tutorial

3.1 Simple Example

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

```
from symfit.api import Parameter, Variable

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

Lets fit this model to some generated data.

```
from symfit.api 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()
```

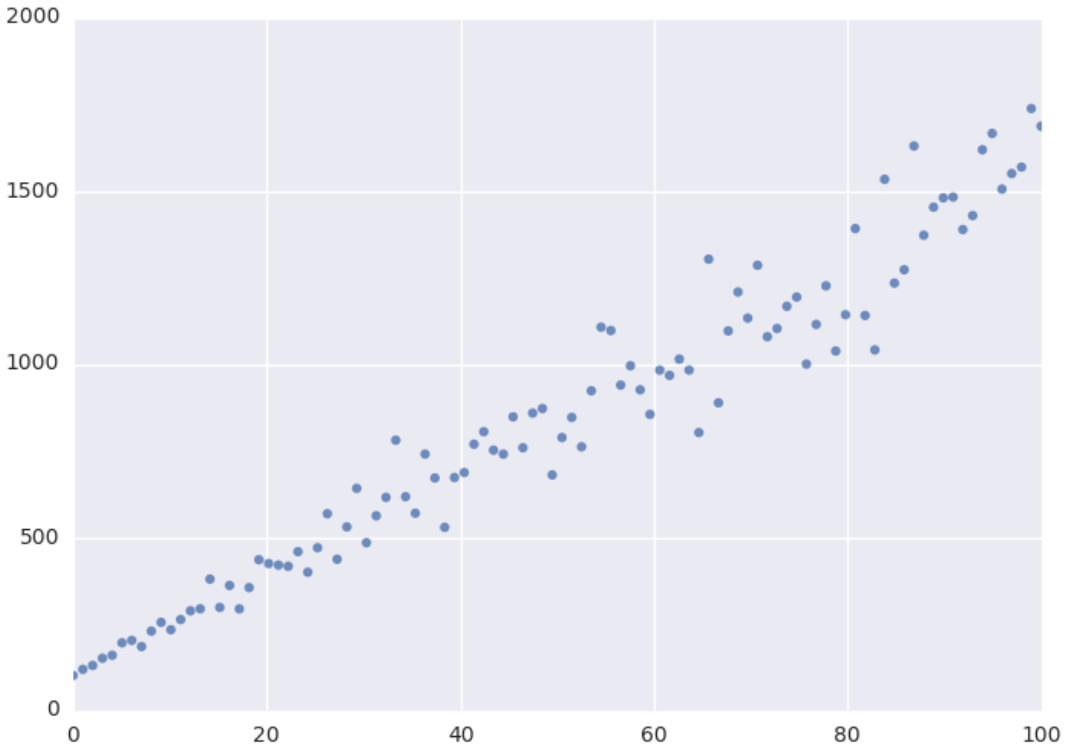
Printing `fit_result` will give a full report on the values for every parameter, including the uncertainty, and quality of the fit.

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.
- `min` Minimal value for the parameter.
- `max` Maximal value for the parameter.
- `fixed` Fix the value of the parameter during the fitting to `value`.

In the example above, we might change our `Parameter`'s to the following after looking at a plot of the data: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```
k = Parameter(value=4, min=3, max=6)

l, m = parameters('b, c')
l.value = 60
l.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, `k.value` will still be `4.0` and not the value we obtain after fitting. To get the value of fit parameters we can do:

```
>>> print(fit_result.params.a)
>>> 14.66946...
>>> print(fit_result.params.a_stdev)
>>> 0.3367571...
>>> print(fit_result.params.b)
>>> 104.6558...
>>> print(fit_result.params.b_stdev)
>>> 19.49172...
>>> print(fit_result.r_squared)
>>> 0.950890866472
```

For more FitResults, see the API docs.

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.params.a, b=fit_result.params.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.params.a, fit_result.params.b)
```

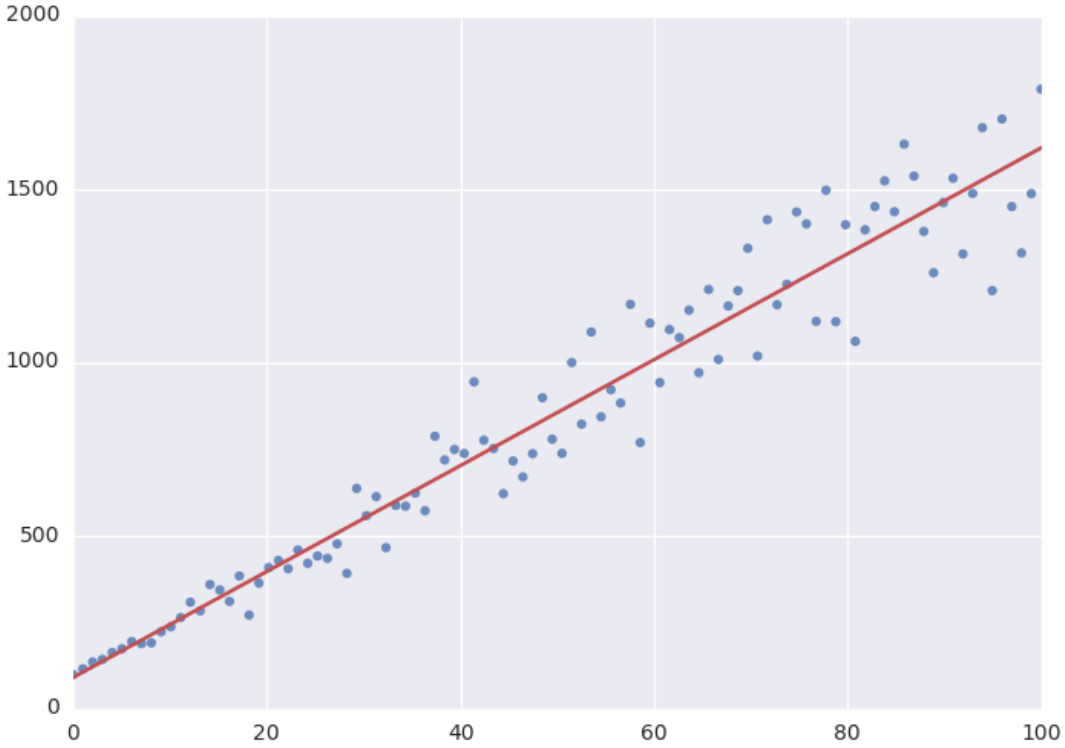
To make life easier, there is a nice shorthand notation to immediately use a fit result:

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

This unpacks the .params object as a dict. For more info view ParameterDict.

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: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```
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_
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 very 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` atribute containing an instance of `Model`. This can again be called:

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

y_1, y_2 = fit.model(x=xdata, **fit_result.params)
```

This returns a tuple with the components evaluated so through the magic of tuple unpacking‘‘y_1‘‘ and `y_2` contain the evaluated fit. Nice!

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

```
from symfit import Model

model_dict = {y_1: a * x**2, y_2: 2 * x * b}
model = Model.from_dict(model_dict)

y_1, y_2 = fit.model(x=xdata, a=2.4, b=0.1)
```

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.

CHAPTER 4

Fitting Types

4.1 Fit (LeastSquares)

The default fitting object does least-squares fitting:

```
from symfit 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,))
ydata = a_vec * xdata + b_vec # Point scattered around the line 5 * x + 105

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:

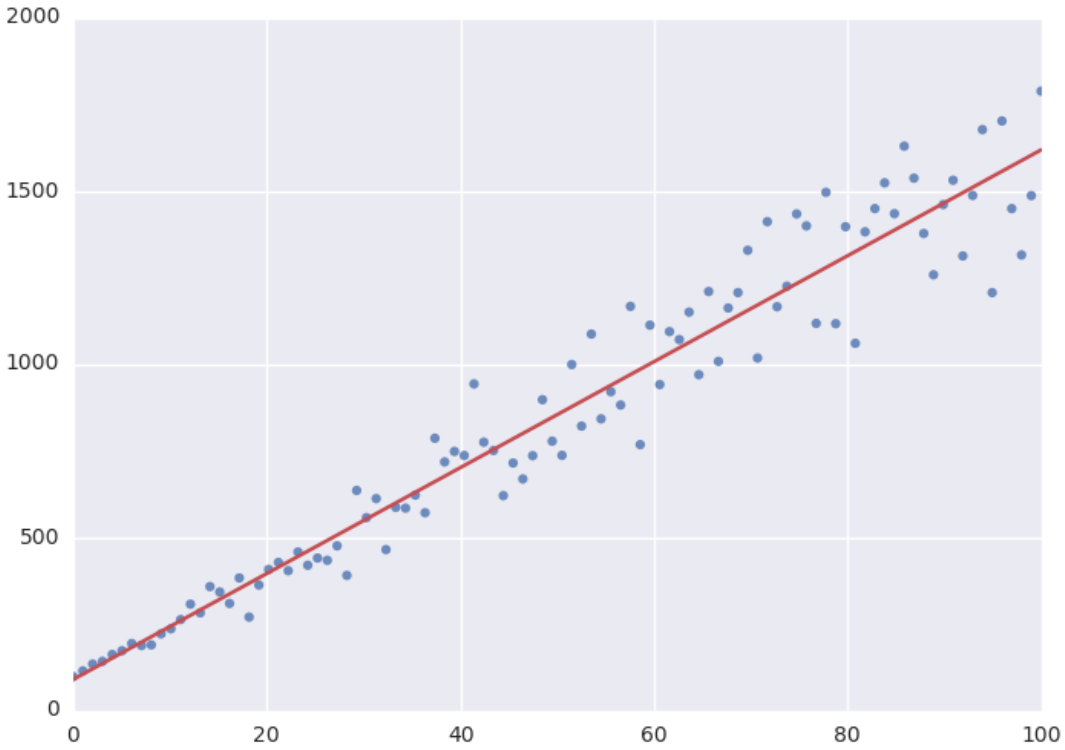
```
a, b = parameters('a, b')
x, y = variables('x, y')
model = {y: a * x + b}

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

`symfit` 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 'wrong' way for historical reasons, and was understandably never changed so as not to loose backwards compatibility. Since this is a new project, we don't have that problem.

`Fit` currently simply wraps `NumericalLeastSquares`, but might become more intelligent in the future.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4.2 (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 `NumericalLeastSquares` 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.

Note's 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 `NumericalLeastSquares` instead of `NonLinearLeastSquares`. These analytical objects are implemented in pure python and are therefore massively outgunned by `NumericalLeastSquares` which is ultimately a wrapper to MINPACK.

4.3 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, Likelihood, exp
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 = Likelihood(model, data)
fit_result = fit.execute()
```

Off-course `fit_result` is a normal `FitResults` object. Because `scipy.optimize.minimize` is used to do the actual work, bounds on parameters, and even constraints are supported. For more information on this subject, check out `symfit`'s `Minimize`.

4.4 Minimize/Maximize

Minimize or Maximize a model subject to bounds and/or constraints. It is a wrapper to `scipy.optimize.minimize`. 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:

$$x^3 - y = 0$$

$$y - 1 >= 0$$

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 = Maximize(model, constraints=constraints)
fit_result = fit.execute()
```

Done! `symfit` will determine all derivatives automatically, no need for you to think about it.

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 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 using `Minimize`, as the whole process won't work otherwise.

4.5 ODE Fitting

Fitting to a system of ODEs is also remarkedly simple with `symfit`. Let's do a simple example from reaction kinetics. Suppose we have a reaction A + A -> B with rate constant k. We then need the following system of rate equations:

$$\frac{dA}{dt} = -kA^2$$
$$\frac{dB}{dt} = kA^2$$

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.

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

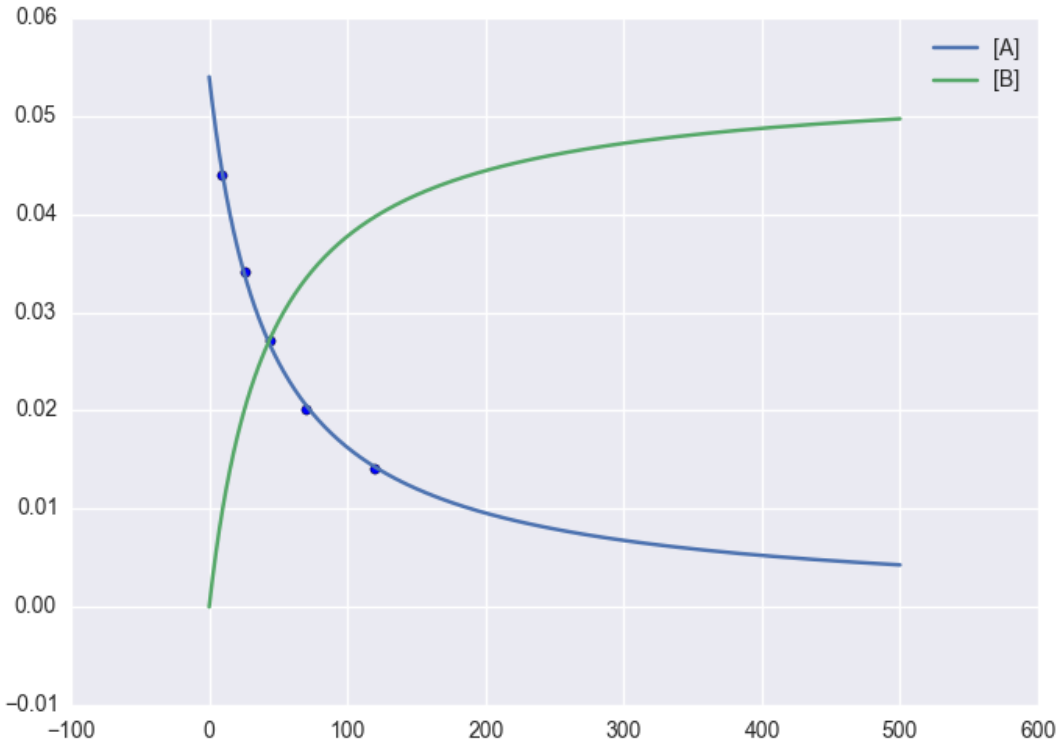
We can plot it just like always:

```
# 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 <-> AAB and AAB + B <-> d.

In `symfit` these can be implemented as:

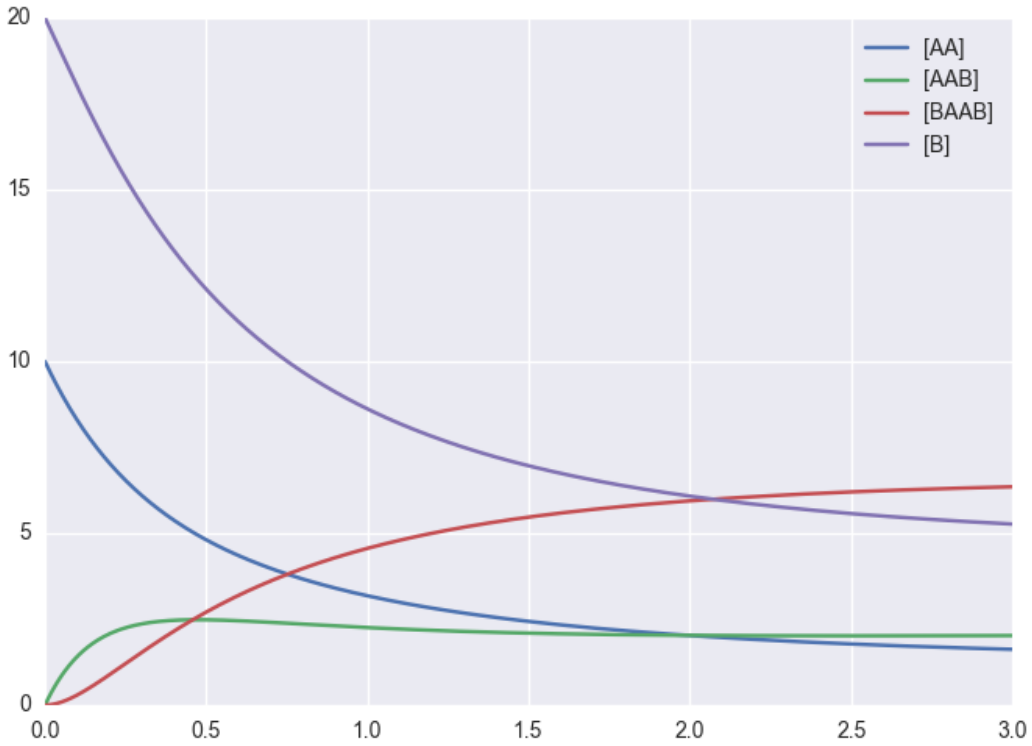
```
AA, B, AAB, BAAB, t = variables('AA, B, AAB, BAAB, t')
k, p, l, m = parameters('k, p, l, m')
```




```
AA_0 = 10 # Some made up initial amound 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()
```



4.6 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.

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

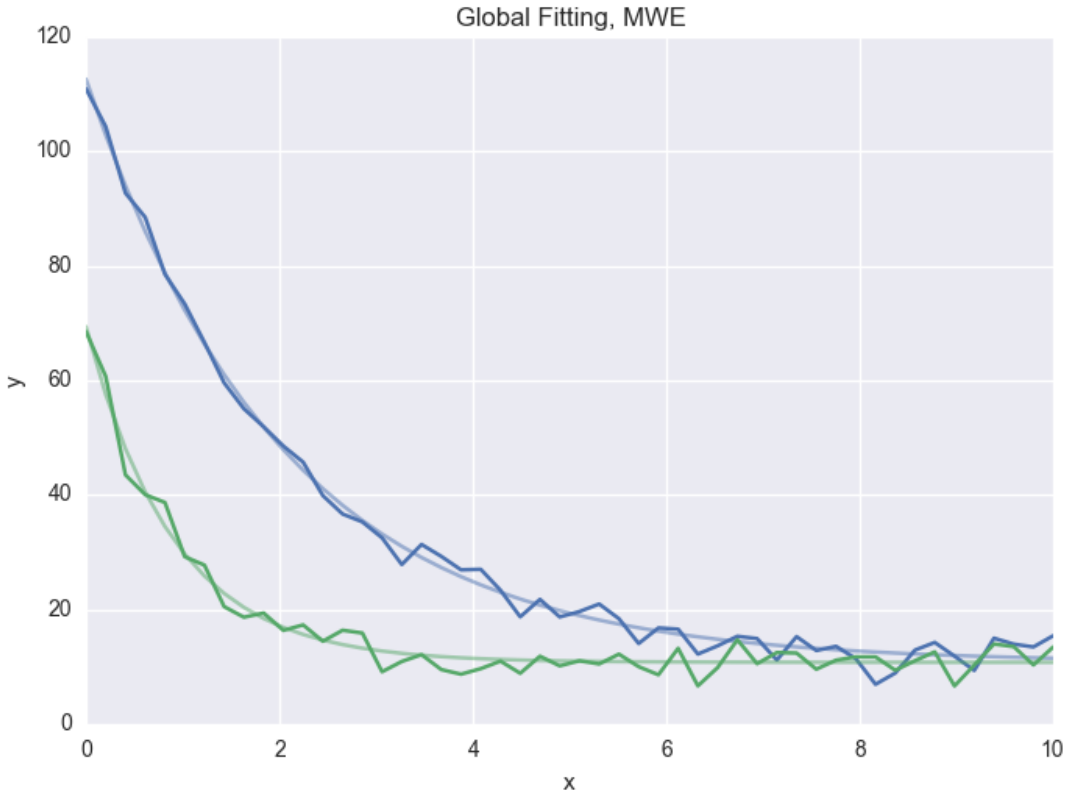
In order to fit to this, we define the following model:

```
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 coeeficient 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`.



4.6.1 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(', '.join('z_{}'.format(i) for i in range(6)))
a, b = parameters('a, b')

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

4.7 How Does `Fit` Work?

How does `Fit` get from a (named) model and some data to a fit? Consider the following example:

```
from symfit import parameters, variables, Fit

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

fit = Fit(model, x=x_data, y=y_data, sigma_y=sigma_data)
fit_result = fit.execute()
```

The first thing `symfit` does is build χ^2 for your model:

```
chi_squared = sum((y - f)**2/sigmas[y]**2 for y, f in model.items())
```

In this line `sigmas` is a dict which contains all vars that where given a value, or returns 1 otherwise.

This χ^2 is then transformed into a python function which can then be used to do the numerical calculations:

```
vars, params = seperate_symbols(chi_squared)
py_chi_squared = lambdify(vars + params, chi_squared)
```

We are now almost there. Just two steps left. The first is to wrap all the data into the `py_chi_squared` function using `partial` into the function to be optimized:

```
from functools import partial

error = partial(py_chi_squared, **data_per_var)
```

where `data_per_var` is a dict containing variable names: value pairs.

Now all that is left is to call `leastsqbound` and have it find the best fit parameters:

```
best_fit_parameters, covariance_matrix = leastsqbound(
    error,
    self.guesses,
    self.eval_jacobian,
    self.bounds,
)
```

That's it! Finally there are some steps to generate a FitResult object, but these are not important for our current discussion.

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 unambiguis way using this ordering. In the above example:

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

CHAPTER 5

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 multidimentional data using ordered arguments can become ambiguous and it even appears there is a difference in interpretation between py2 and py3. To prevent such ambiguity and to make sure your code is transportable, always use named models. And the result is more readable anyway right?

- When evaluating models use tuple-unpacking:

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

  and not:

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

  or something similar.

CHAPTER 6

Technical Notes

Essays on mathematical and implementation details.

6.1 On Likelihood Fitting

The *Likelihood* object is a subclass of *Maximize*. The *error_func* and *eval_jacobian* definitions have been changed to facilitate what one would expect from Likelihood fitting:

error_func 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 entirely 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 σ. 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 σ 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 +- 1.000000e-01 when `sigma_y` is provided. This matches the analytical prediction.
- a = 5.102056e-02 +- 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 +- 9.897135e-03 when `sigma_y` is provided. This matches the analytical prediction.
- a = 5.102056e-03 +- 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.py`, `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 area's 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.

CHAPTER 7

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.

CHAPTER 8

Module Documentation

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

8.1 Fit

class `symfit.core.fit.`**`BaseFit`**(*model*, **ordered_data*, ***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<https://github.com/sympy/sympy/wiki/Faq>'_**.

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.

bounds

Returns List of tuples of all bounds on parameters.

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.

class symfit.core.fit.**ConstrainedNumericalLeastSquares**(*model*, **args*, ***kwargs*)
Bases: *symfit.core.fit.Minimize*, *symfit.core.fit.HasCovarianceMatrix*

This object performs χ^2 minimization, subject to constraints. As an example, 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 = ConstrainedNumericalLeastSquares(
        model=model,
        a_i=data[0],
        b_i=data[1],
        c_i=data[2],
        constraints=[Equality(a + b + c, 180)]
    )
    fit_result = fit.execute()
```

Unlike *NumericalLeastSquares*, it also supports vector components of unequal length and is therefore preferred for Global Fitting problems.

In order to perform minimization, this object is a subclass of *Minimize*, and the output might therefore deviate slightly from the MINPACK result given by the more traditional *NumericalLeastSquares* object.

error_func(*p*, *independent_data*, *dependent_data*, *sigma_data*, *flatten_components=True*)
Returns χ^2, summing over all the vector components and data indices.

This function now supports setting variables to None. Needs mathematical rigor!

Parameters

- **p** – array of floats for the parameters.
- **data** – data to be provided to `Variable`'s.
- **flatten_components** – If `True`, χ^2 is returned. If `False`, the χ^2 per vector component is returned.

eval_jacobian(*p*, *independent_data*, *dependent_data*, *sigma_data*)
Evaluates the jacobian of χ^2, summing over all the vector components and data indices.

Returns array of len(self.model.params) containing the components of the Jacobian.

execute(**args*, ***kwargs*)
This wraps the execute of 'Minimize' with the calculation of the covariance matrix. Read *Minimize.execute* for a more general description.

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.

constraint_type
alias of Equality

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*, ***named_data*)
Bases: *symfit.core.fit.NumericalLeastSquares*

Wrapper for NumericalLeastSquares to give it a more appealing name. In the future I hope to make this object more intelligent so it can search out the best fitting object based on certain qualifiers and return that instead.

Therefore do not assume this object to always behave as a certain fitting type! If it matters to you to have for example NumericalLeastSquares or NonLinearLeastSquares for your problem, use those objects directly. What of course will not change, is the API.

execute(**options*, ***kwoptions*)
Execute Fit, giving any options and kwoptions to NumericalLeastSquares.

class symfit.core.fit.**FitResults**(*params*, *popt*, *pcov*, *infodic*, *mesg*, *ier*, *ydata=None*, *sigma=None*)
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. - parameters + stdev - R squared (Regression coefficient.) - fitting status message

This object is made to behave entirely read-only. This is a bit unnatural to enforce in Python but I feel it is necessary to guarantee the integrity of the results.

__init__(*params*, *popt*, *pcov*, *infodic*, *mesg*, *ier*, *ydata=None*, *sigma=None*)
Excuse the ugly names of most of these variables, they are inherited from scipy. Will be changed.

Parameters

- **params** – list of Parameter's.
- **popt** – best fit parameters, same ordering as in params.
- **pcov** – covariance matrix.
- **infodic** – dict with fitting info.
- **mesg** – Status message.
- **ier** – Number of iterations.
- **ydata** –

__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.

infodict
Read-only Property.

iterations
Read-only Property.

params
Read-only Property.

r_squared
r_squared Property.

Returns Regression coefficient.

status_message
Read-only Property.

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.

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.**Likelihood**(*model*, **args*, ***kwargs*)
Bases: *symfit.core.fit.Maximize*

Fit using a Maximum-Likelihood approach. This object maximizes the log-likelihood function.

error_func(*p*, *independent_data*, *dependent_data*, *sigma_data*)
Error function to be maximised(!) in the case of log-likelihood fitting.

Parameters

- **p** – guess params
- **data** – xdata

Returns scalar value of log-likelihood

eval_jacobian(*p*, *independent_data*, *dependent_data*, *sigma_data*)
Jacobian for log-likelihood is defined as $\nabla_{\vec{p}}(\log(L(\vec{p}|\vec{x})))$.

Parameters

- **p** – guess params
- **data** – data for the variables.

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

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) -> 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 χ^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.**Maximize**(*model*, **args*, ***kwargs*)
Bases: *symfit.core.fit.Minimize*

Maximize a model subject to constraints. Simply flips the sign on error_func and eval_jacobian in order to maximize.

class symfit.core.fit.**Minimize**(*model*, **args*, ***kwargs*)
Bases: *symfit.core.fit.BaseFit*

Minimize a model subject to constraints. A wrapper for `scipy.optimize.minimize`.

`Minimize` itself doesn't work when data is provided to its Variables, use one of its subclasses for that.

__init__(*model*, **args*, ***kwargs*)
Because in a lot of use cases for Minimize no data is supplied to variables, all the empty variables are replaced by an empty np array.

Constraints constraints the minimization is subject to.

error_func(*p*, *independent_data*, *dependent_data*, *sigma_data*)
The function to be optimized. Scalar valued models are assumed. For Minimize the thing to minimize is simply *self.model* directly.

Parameters

- **p** – array of floats for the parameters.
- **data** – data to be provided to `Variable`'s.

eval_jacobian(*p*, *independent_data*, *dependent_data*, *sigma_data*)
Takes partial derivatives of model w.r.t. each `Parameter`.

Parameters

- **p** – array of floats for the parameters.
- **data** – data to be provided to `Variable`'s.

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

scipy_constraints
Read-only Property of all constraints in a scipy compatible format.

Returns dict of scipy compatible statements.

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 χ^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 χ^2

chi_squared_jacobian

Return a symbolic jacobian of the χ^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 lambda functions of the jacobian matrix of the function, which can be used in numerical optimization.

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_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.

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. 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 itterations. 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.`**NumericalLeastSquares**(*model*, **ordered_data*, ***named_data*)
Bases: *symfit.core.fit.BaseFit*

Solves least squares numerically using leastsqbounds. Gives results consistent with MINPACK except when borders are provided.

error_func(*p*, *independent_data*, *dependent_data*, *sigma_data*, *flatten=True*)
Returns the value of the square root of χ^2, summing over the components.

This function now supports setting variables to None. Needs mathematical rigor!

Parameters

- **p** – array of parameter values.
- **independent_data** – Data to provide to the independent variables.
- **dependent_data** –
- **sigma_data** –
- **flatten** – If True, summing is performed over the data indices (default).

Returns $\sqrt(\chi^2)$

execute(**options*, ***kwoptions*)

Parameters

- **options** – Any postional arguments to be passed to leastsqbound
- **kwoptions** – Any named arguments to be passed to leastsqbound

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** –
- **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.

__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

class symfit.core.fit.**ParameterDict**(*params*, *popt*, *pcov*, **args*, ***kwargs*)
Bases: `object`

Container for all the parameters and their (co)variances. Behaves mostly like an OrderedDict: can be **-ed, allowing the sexy syntax where a model is called with values for the Variables and **params. However, under iteration it behaves like a list! In other words, it preserves order in the params.

__getattr__(*name*)
A user can access the value of a parameter directly through this object.

Parameters **name** – Name of a `Parameter`. Naming convention: let a = Parameter(). Then: .a gives the value of the parameter. .a_stdev gives the standard deviation.

__getitem__(*param_name*)
This method allows this object to be addressed as a dict. This allows for the ** unpacking. Therefore return the value of the best fit parameter, as this is what the user expects.

Parameters **param_name** – Name of the `Parameter` whose value your interested in.

Returns the value of the best fit parameter with name 'key'.

__iter__()
Iteration over the `Parameter` instances. :return: iterator

__len__()
Length gives the number of `Parameter` instances.

Returns len(self.__params)

covariance_matrix
Returns the covariance matrix.

get_stdev(*param*)
Deprecated. :param param: `Parameter` instance. :return: returns the standard deviation of param :raises: DeprecationWarning

get_value(*param*)
Deprecated. :param param: `Parameter` instance. :return: returns the numerical value of param :raises: DeprecationWarning

keys()

Returns All `Parameter` names.

stdev(*param*)

Parameters **param** – `Parameter` instance.

Returns returns the standard deviation of param

value(*param*)

Parameters **param** – `Parameter` instance.

Returns returns the numerical value of param

class symfit.core.fit.**TakesData**(*model*, **ordered_data*, ***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*, ***named_data*)

Parameters

- **model** – (dict of) sympy expression or `Model` object.
- **bool** (*absolute_sigma*) – 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.

dependent_data
Read-only Property

Returns Data belonging to each dependent variable.

Return type OrderedDict with variable names as key, data as value.

independent_data
Read-only Property

Returns Data belonging to each independent variable.

Return type OrderedDict with variable names as key, data as value.

initial_guesses

Returns Initial guesses for every parameter.

sigma_data
Read-only Property

Returns Data belonging to each sigma variable.

Return type OrderedDict with variable names as key, data as value.

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 NonLinearLeastSquares. 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 :math:‘

ec{p}‘ and :math:‘ ec{p_0}‘

around which to expand, but params should only give :math:‘

ec{p}‘. To get a mapping to the :math:‘

ec{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 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 immidiately.

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.
- Perhaps in the future I will make this inspect-compatible so then we come full circle.

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

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')

8.5 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.

CHAPTER 9

Indices and tables

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Bibliography

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