Introduction to iminuit

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- *iminuit* is a Python interface to the MINUIT2 C++ package (**standard tool at CERN**)
- Minimizes multi-variate function with optional box constraints
- **Uncertainty analysis**: Computes covariance matrix or profile likelihood contour
- [Part of Scikit-HEP Project (http://scikit-hep.org/)](http://scikit-hep.org/)
- [Latest version 1.3.7 on PyPI (https://pypi.org/project/iminuit/)](https://pypi.org/project/iminuit/)
- [Development version on GitHub (https://github.com/scikit-hep/iminuit)](https://github.com/scikit-hep/iminuit)
- [Documentation on ReadTheDocs (https://iminuit.readthedocs.io/en/latest/)](https://iminuit.readthedocs.io/en/latest/)

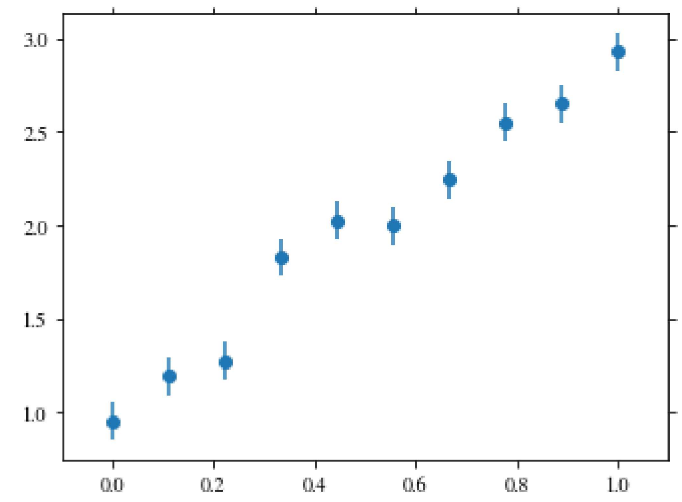
We are doing a gentle introduction on how to use *iminuit*. **Feel free to ask any questions!**

In [1]:
```
# basic setup of the notebook

# !pip install iminuit matplotlib numpy
%matplotlib inline
from matplotlib import pyplot as plt
plt.rcParams["font.size"] = 20
import numpy as np
```

Simple Fit: line model to scattered (x, y) data

- Line model has two parameters (a, b)

In [2]:
```
# let's make a line model
def line(x, a, b):
    return a + x * b

a_true = 1.0
b_true = 2.0

# let's make some data
x = np.linspace(0, 1, 10)

# precomputed random numbers from standard normal distribution
z = np.array([-0.49783783, -0.33041722, -1.71800806,  1.60229399,
                 1.36682387, -1.15424221, -0.91425267, -0.03395604,
                 -1.27611719, -0.7004073 ])

sigma_y = 0.1 * np.ones_like(x)
y = line(x, a_true, b_true) + sigma_y * z

plt.errorbar(x, y, sigma_y, fmt="o")
plt.xlim(-0.1, 1.1);
```



- Want to estimate parameters (a, b) of line model from data
- Need **score** which is minimal when model *best* agrees with data
  - Sum of residuals squared (least-squares method)
  - Negated sum of log-likelihood values (maximum-likelihood method)
- MINUIT always minimizes; negate score function to maximize
- Use *iminuit* to numerically minimize score as function of model parameters

In [3]:
```
# least-squares score function = sum of data residuals squared
def LSQ(a, b):
    return np.sum((y - line(x, a, b)) ** 2 / sigma_y ** 2)
```

In [4]:
```
# everything in iminuit is done through the Minuit object, so we import it
from iminuit import Minuit
```

In [5]:
```python
# create instance of Minuit and pass score function to minimize
m = Minuit(LSQ)
```

```
/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: Parameter
a does not have initial value. Assume 0.

/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: Parameter
a is floating but does not have initial step size. Assume 1.

/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: Parameter
b does not have initial value. Assume 0.

/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: Parameter
b is floating but does not have initial step size. Assume 1.

/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: errordef i
s not given. Default to 1.
```

- iminuit shows a lot of warnings to make us aware of additional settings
- things may work without, but it is better to set things up properly

Initial parameter values

- MINUIT searches for local minimum by gradient-descent method from starting point
- If function has several minima, minimum found will depend on starting point
- If function has only one minimum, iminuit will converge to it faster if started near minimum
- If no starting value is provided, iminuit uses 0 (which may be bad)

In [6]:
```python
# set start values via keywords for a and b
m = Minuit(LSQ, a=5, b=5)
```

```
/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: Parameter
a is floating but does not have initial step size. Assume 1.

/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: Parameter
b is floating but does not have initial step size. Assume 1.

/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: errordef i
s not given. Default to 1.
```

Notice how iminuit figured out that the arguments of LSQ are called "a" and "b". This is a cool gimmick of iminuit.

Initial step sizes

- iminuit computes gradients numerically from finite differences over some step size
- step size should be
  - small compared to the curvature of the function $\mathrm{d}^2 f/\mathrm{d}a^2$, $\mathrm{d}^2 f/\mathrm{d}b^2$
  - large compared to numerical resolution (about 1e-14)
- iminuit very tolerant to step sizes and optimizes step size while it is running
- converge rate theoretically faster with optimal step size, but little impact in practice

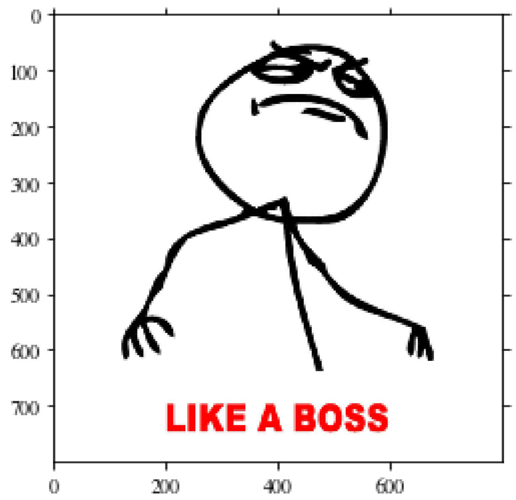
In [7]:
```python
# set step size with error_<name>=... keyword
m = Minuit(LSQ, a=5, b=5, error_a=0.1, error_b=0.1)
```

```
/Users/hdembins/Code/iminuit/py37/lib/python3.7/site-packages/ipykernel_launcher.py:2: InitialParamWarning: errordef i
s not given. Default to 1.
```

"Error definition"

- difficult to explain quickly (ask me and I will try), so just remember rule for 1 sigma uncertainties
  - `errordef=1` for least-squares score function
  - `errordef=0.5` for maximum-likelihood score function
- only changes uncertainty computation (no effect on minimization)

```python
# set errordef=1 for least-squares score function
m = Minuit(LSQ, a=5, b=5, error_a=0.1, error_b=0.1, errordef=1)

# no more warnings! :-D

# fast alternative: just silence all warnings
m = Minuit(LSQ, pedantic=False)

import matplotlib.image as mpimg
img = mpimg.imread("img/trollface.png")
plt.imshow(img);
```




```python
# check current parameter state (do this at any time)
m.get_param_states()
```

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	0.0	1.0					
1	b	0.0	1.0					

Parameters with limits

- Model parameters often have physical or mathematical limits, e.g. $x \geq 0$ in $\sqrt{x}$
- iminuit allows you to set a one-sided and two-sided limit for each parameter
- iminuit will never leave range bounded by limits
- slow convergence for parameters close to limit

```python
# one-sided limit a > 0, two-sided limit 0 < b < 10
m = Minuit(LSQ, a=5, b=5,
           error_a=0.1, error_b=0.1,
           limit_a=(0, None), limit_b=(0, 10),
           errordef=1)

m.get_param_states()
```

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	5.00	0.10			0		
1	b	5.00	0.10			0	10	

(Initially) Fixing parameters

- for complex model with many parameters, may want to fix some parameters initially
- release fixed parameters when other parameters are close to optimal
- also useful for systematic checks

```python
# fix parameter a
m = Minuit(LSQ, a=2, b=5, fix_a=True,
           error_a=0.1, error_b=0.1,
           errordef=1)

m.get_param_states()
```

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	2.00	0.10					yes
1	b	5.00	0.10					

Now let's minimize that #$%@ function

In [12]:
```python
# run migrad; will not vary a because we fixed it, only b
m.migrad()
```

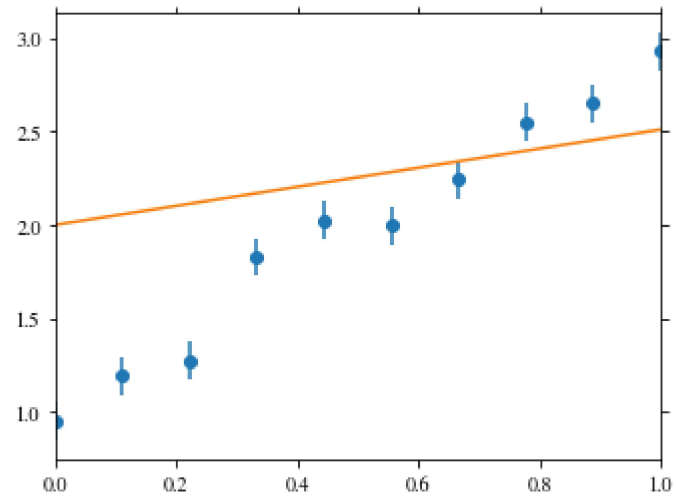
Out[12]:

FCN = 305.1		Ncalls = 13 (13 total)	
EDM = 2.33E-16 (Goal: 1E-05)		up = 1.0	
Valid Min.	Valid Param.	Above EDM	Reached call limit
True	True	False	False

Hesse failed	Has cov.	Accurate	Pos. def.	Forced
False	True	True	True	False

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	2.00	0.10					yes
1	b	0.51	0.05					

In [13]:
```python
# get parameter values
a_fit = m.values["a"]  # m.values[0] also works
b_fit = m.values["b"]  # m.values[1] also works

plt.errorbar(x, y, sigma_y, fmt="o")
plt.plot(x, line(x, a_fit, b_fit));
```



In [14]:
```python
# release fix on "a" and minimize again
m.fixed["a"] = False  # m.fixed[0] = False also works
m.migrad()
```

Out[14]:

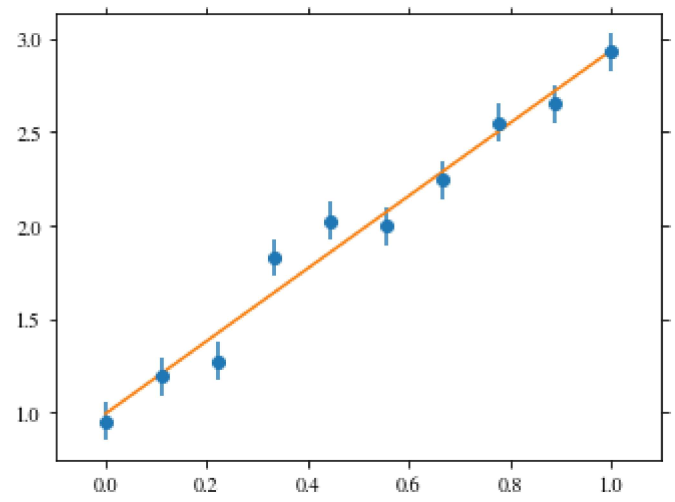
FCN = 10.39		Ncalls = 29 (42 total)	
EDM = 2.06E-14 (Goal: 1E-05)		up = 1.0	
Valid Min.	Valid Param.	Above EDM	Reached call limit
True	True	False	False

Hesse failed	Has cov.	Accurate	Pos. def.	Forced
False	True	True	True	False

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	0.99	0.06					
1	b	1.94	0.10					

- iminuit can fail, so carefully check Migrad status report
  - green is good, red is bad
  - Ncalls should not be too large
  - EDM should be small
- Common reasons for failures
  - score function evaluates to NaN because Migrad tries invalid parameters
  - score function is not analytical
    - discontinuous in value
    - discontinuous in first and/or second derivative
- Acceptable issues
  - "Accurate" is False
  - Call `m.hesse()` to repair this
- Possibly tolerable issues (but indicate that something is fishy)
  - "Pos. def." == False
  - "Forced" == True

In [15]:
```
# get better parameter values
a_fit = m.values["a"]
b_fit = m.values["b"]

plt.errorbar(x, y, sigma_y, fmt="o")
plt.plot(x, line(x, a_fit, b_fit))
plt.xlim(-0.1, 1.1);
```



Fit of model with flexible number of parameters

- Sometimes model has large or variable number of parameters
- Example: fit a polynomial of degree 2, 3, 4, ... ?
- iminuit has alternative interface which passes parameters as numpy array to score function

In [16]:
```
def LSQ_numpy(par):  # par is numpy array here
    ym = np.polyval(par, x)  # for len(par) == 2 this is a line
    return np.sum((y - ym) ** 2 / sigma_y ** 2)
```

In [17]:
```
# pass starting values and step sizes as numpy arrays
m = Minuit.from_array_func(LSQ_numpy, (5, 5), error=(0.1, 0.1), errordef=1)

# automatic parameter names are assigned x0, x1, ...
m.get_param_states()
```

Out[17]:

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	x0	5.00	0.10					
1	x1	5.00	0.10					

In [18]:
```
# can easily change number of fitted parameters and assign names
m = Minuit.from_array_func(LSQ_numpy, (2, 1, 3, 5), error=0.1,
                           name=("a", "b", "c", "d"), errordef=1)

m.get_param_states()
```

Out[18]:

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	2.00	0.10					
1	b	1.00	0.10					
2	c	3.00	0.10					
3	d	5.00	0.10					

In [19]:
```
# fit the thing
m.migrad()
```

Out[19]:

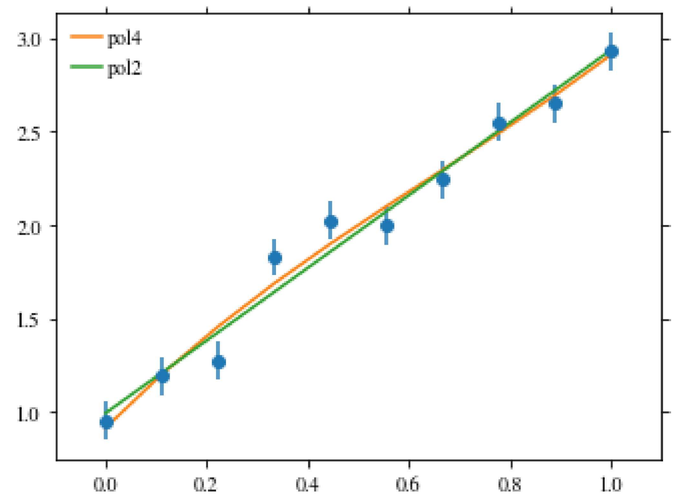
FCN = 9.033			Ncalls = 96 (96 total)	
EDM = 4.37E-13 (Goal: 1E-05)			up = 1.0	
Valid Min.	Valid Param.	Above EDM	Reached call limit	
True	True	False	False	
Hesse failed	Has cov.	Accurate	Pos. def.	Forced
False	True	True	True	False

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	0.8	1.3					
1	b	-1.5	2.0					
2	c	2.7	0.8					
3	d	0.91	0.09					

In [20]:
```python
# can also use score function with scipy.optimize.minimize-like interface
from iminuit import minimize  # has same interface as scipy.optimize.minimize
minimize(LSQ_numpy, (5, 5, 5, 5))
```

Out[20]:
```
      fun: 9.033192085977742
 hess_inv: array([[ 1.72052069, -2.58078004,  0.97920889, -0.05947462],
       [-2.58078004,  3.99542986, -1.59307405,  0.10762097],
       [ 0.97920889, -1.59307405,  0.69138171, -0.05716727],
       [-0.05947462,  0.10762097, -0.05716727,  0.00823772]])
  message: 'Optimization terminated successfully.'
   minuit: <iminuit._libiminuit.Minuit object at 0x7fd98c3a8840>
     nfev: 104
     njev: 0
  success: True
        x: array([ 0.7654755 , -1.50304927,  2.73544024,  0.91193726])
```

In [21]:
```python
# get parameter values as arrays
par_fit = m.np_values()

plt.errorbar(x, y, sigma_y, fmt="o")
plt.plot(x, np.polyval(par_fit, x), label="pol4")
plt.plot(x, line(x, a_fit, b_fit), label="pol2")
plt.legend()
plt.xlim(-0.1, 1.1);
```



In [22]:
```python
# check reduced chi2, goodness-of-fit estimate, should be around 1
m.fval / (len(y) - len(m.values))
```

Out[22]: 1.5055320143296989

Parameter uncertainties

- iminuit can compute symmetric uncertainty intervals ("Hesse errors")
  - automatically done during standard minimisation
  - to make sure you get accurate errors, call `m.hesse()` explicitly after `m.migrad()`
  - slow, computation time scales with N_{par}^2
- iminuit can also compute asymmetric uncertainty intervals ("Minos errors")
  - need to explicitly call `m.minos()`
  - very slow, computation time scales with N_{par}^2

Covariance and correlation matrix from Hesse

In [23]:
```python
# calling hesse explicitly
m.hesse()
```

Out[23]:

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	0.8	1.3					
1	b	-1.5	2.0					
2	c	2.7	0.8					
3	d	0.91	0.09					

In [24]:
```python
# get full correlation matrix (automatically prints nicely in notebook)
m.matrix(correlation=True)
```

Out[24]:

	a	b	c	d
a	1.00	-0.98	0.90	-0.50
b	-0.98	1.00	-0.96	0.59
c	0.90	-0.96	1.00	-0.76
d	-0.50	0.59	-0.76	1.00

In [25]:
```python
# or get covariance matrix
m.matrix()
```

Out[25]:

	a	b	c	d
a	1.721	-2.581	0.979	-0.059
b	-2.581	3.995	-1.593	0.108
c	0.979	-1.593	0.691	-0.057
d	-0.059	0.108	-0.057	0.008

In [26]:
```python
# or get matrix as numpy array
m.np_matrix()
```

Out[26]:
```
array([[ 1.72054192, -2.58081288,  0.979222  , -0.05947552],
       [-2.58081288,  3.99548068, -1.59309437,  0.10762237],
       [ 0.979222  , -1.59309437,  0.69138984, -0.05716783],
       [-0.05947552,  0.10762237, -0.05716783,  0.00823776]])
```

In [27]:
```python
# access individual elements of matrices
corr = m.np_matrix(correlation=True)
print(corr[0, 1])
print(corr[0, 3])
```

```
-0.9843269379727133
-0.4995753625986588
```

Asymmetric uncertainty intervals from Minos

In [28]:
```python
m.minos()
```

Out[28]:

a		Valid
Error	-1.3	1.3
Valid	True	True
At Limit	False	False
Max FCN	False	False
New Min	False	False

b		Valid
Error	-2.0	2.0
Valid	True	True
At Limit	False	False
Max FCN	False	False
New Min	False	False

c		Valid
Error	-0.8	0.8
Valid	True	True
At Limit	False	False
Max FCN	False	False
New Min	False	False

d		Valid
Error	-0.09	0.09
Valid	True	True
At Limit	False	False
Max FCN	False	False
New Min	False	False

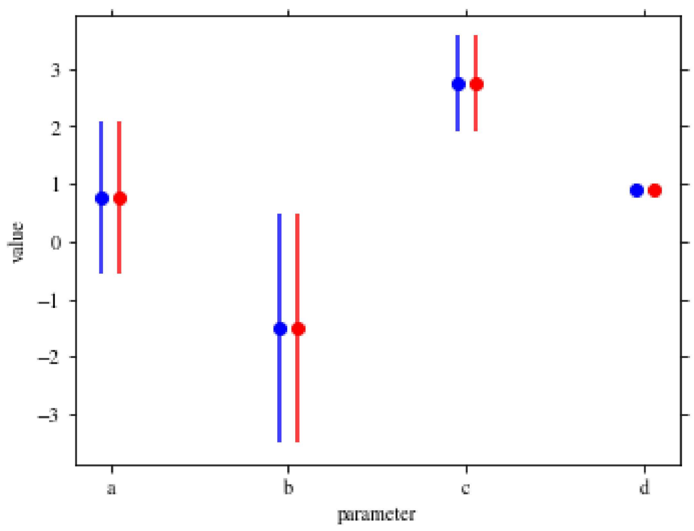
- Minos can fail, check messages:
  - "Valid": everything is chipper
  - "At Limit": Minos hit parameter limit before finishing contour
  - "Max FCN": Minos reached call limit before finishing contour
  - "New Min": Minos found a new minimum while scanning

In [29]:
```python
# Minos errors now appear in parameter table
m.get_param_states()
```

Out[29]:

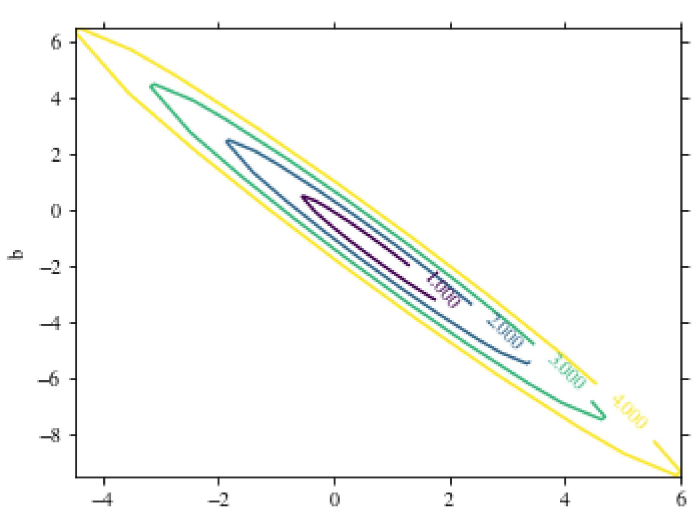
	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	a	0.8	1.3	-1.3	1.3			
1	b	-1.5	2.0	-2.0	2.0			
2	c	2.7	0.8	-0.8	0.8			
3	d	0.91	0.09	-0.09	0.09			

In [30]:
```python
# plot parameters with errors
v = m.np_values()
ve = m.np_errors()
vm = m.np_merrors()

npar = len(v)
indices = np.arange(npar)

# plot hesse errors
plt.errorbar(indices - 0.05, v, ve, fmt="ob")

# plot minos errors
plt.errorbar(indices + 0.05, v, vm, fmt="or")

# make nice labels
plt.xticks(indices, m.values.keys())
plt.xlim(-0.2, indices[-1] + 0.2)
plt.xlabel("parameter")
plt.ylabel("value");
```

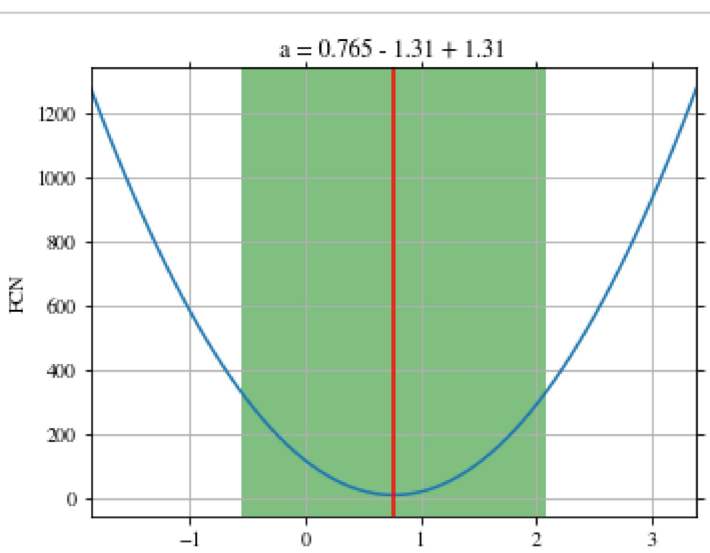


Builtin plotting

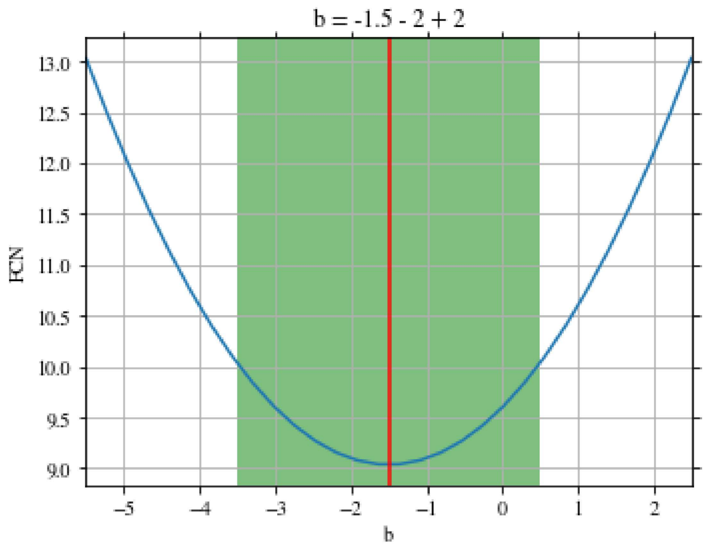
In [31]:
```python
m.draw_mncontour('a','b', nsigma=4);  # nsigma=4 says: draw four contours from sigma=1 to 4
```



In [32]:
```python
m.draw_profile("a");
```



In [33]:
```
m.draw_mnprofile("b");
```



In [34]:
```
# get scan data to plot it yourself
px, py = m.profile('a', subtract_min=True)
plt.plot(px, py);
```