SMD Hands-On Estimators / Fitting

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Least Squares

Analytic solution for linear combination of functions

(Analog to the exercise on the last sheet)

Here, we will fit a function of the form

$$f(x) = p_0 + p_1 \cdot \sin(x) + p_2 \cdot \cos(x)$$

to our data.

This function is a linear combination of basis functions:

$$f(x) = \sum_{i=0}^2 p_i f_i(x)$$

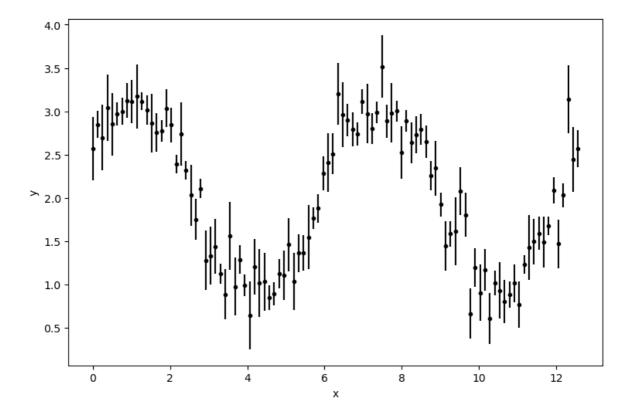
with

$$f_0(x) = 1, \quad f_1(x) = \sin(x), \quad f_2(x) = \cos(x)$$

In this case, we can use the analytic solution to the least squares optimization problem.

```
In [23]: def linear_combination(x, funcs, parameters):
              '''Evaluate a linear combination of basis functions
             Parameters
             x: number or np.ndarray
                 The point or points at which to evaluate
             funcs: iterable of callables
                 The basis functions
             parameters: iterable of numbers
                 The coefficients
             return np.sum([p * f(x) for p, f in zip(parameters, funcs, strict=True)], ax
In [24]: # define our linear model
         funcs = [np.ones_like, np.sin, np.cos]
In [25]: # create some randomized example data points
         rng = np.random.default_rng(1337)
         N = 100
         true_parameters = np.array([2, 1, 0.5])
         y_{unc} = rng.uniform(0.1, 0.4, N)
         x = np.linspace(0, 4 * np.pi, N)
         y = linear_combination(x, funcs, true_parameters)
         # add some noise for to simulate measurement uncertainty
         y += rng.normal(0, y_unc)
         plt.figure()
         plt.errorbar(x, y, yerr=y_unc, ls='', marker='.', color='k')
         plt.xlabel('x')
         plt.ylabel('y')
```

Out[25]: Text(0, 0.5, 'y')



Create the design matrix $oldsymbol{A}$

Define the weight matrix $\boldsymbol{W} = \operatorname{Cov}^{-1}(\boldsymbol{y})$ of the measurements.

Here we assume that all measured points do not have an uncertainty in x and that the y values are statistically independent (no off-diagonal entries in Cov(y)).

This is a very strong assumption.

The linear least squares method yields biased results if the Covariance is estimated from the data points themselves.

More on that further down in the muon example.

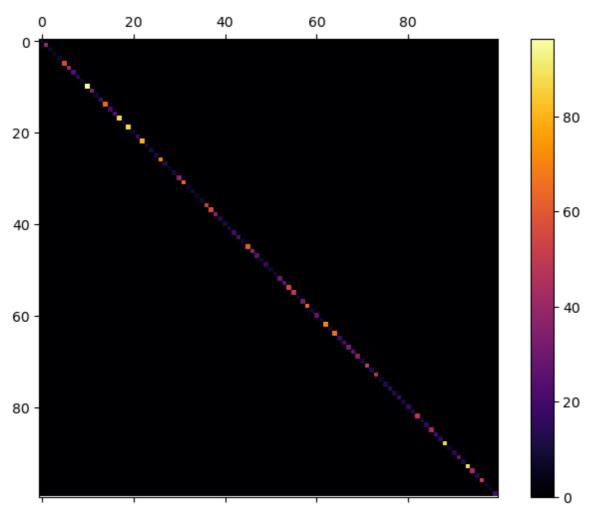
```
In [28]: # All measurements have a known uncertainty and no correlations
cov_y = np.diag(y_unc**2)

W = np.linalg.inv(cov_y)

fig, ax = plt.subplots()
```

```
plot = ax.matshow(W)
fig.colorbar(plot)
```

Out[28]: <matplotlib.colorbar.Colorbar at 0x7f09f8122080>



```
In [29]: W[:5, :5]
Out[29]: array([[ 7.571067 , 0. , 0.
                                                0.
                                                           0.
                                                                    ],
                       , 41.27194538, 0.
              [ 0.
                                                           0.
                                                0.
                                                         , 0.
              [ 0.
                          0.
                                     7.06318364, 0.
                                     0. ,
              [ 0.
                                                6.7827523 , 0.
                                                                    ],
              [ 0.
                                     0.
                                                     , 7.61618791]])
                          0.
                                                0.
```

Solve the linear least squares problem

```
In [30]: def solve_linear_least_squares(A, W, y):
    """Solve the linear least sqaures problem

Parameters
------
A: np.ndarray
    Design matrix
W: np.ndarray
    Weight matrix
y: np.ndarray
    Vector of y values
"""

cov = np.linalg.inv(A.T @ W @ A)
    parameters = cov @ A.T @ W @ y
```

```
return parameters, cov
         parameters, cov = solve_linear_least_squares(A, W, y)
         parameters, cov
Out[30]: (array([2.00565538, 0.97702516, 0.48411763]),
          array([[ 3.66470863e-04, -5.58492439e-05, -1.00389068e-05],
                  [-5.58492439e-05, 6.79396825e-04, 4.87671239e-05],
                  [-1.00389068e-05, 4.87671239e-05, 7.92958991e-04]]))
         Calculate the \chi^2 over the number of degrees of freedom:
In [31]: def chisquare_over_ndf(y, A, parameters):
             residuals = (y - A @ parameters)
             sum residuals = (residuals.T @ W @ residuals)
             ndf = len(y) - len(parameters)
             return sum residuals / ndf
         chisquare over ndf(y, A, parameters), chisquare over ndf(y, A, true parameters)
Out[31]: (0.9440998449492631, 0.9551361681741546)
         putting it all together:
In [32]: def linear_least_squares(x, y, funcs, cov_y=None):
             Perform a linear least squares fit.
             Parameters
             ------
             x : np.ndarray[ndim=1]
                 Vector of x values
             y : np.ndarray[ndim=1]
                 Vector of y values
             funcs : Sequence[Callable]
                 The basis functions
             cov_y : Optional[np.ndarray[ndim=2]]
                 The covariance matrix of the y values
             Returns:
             parameters : np.ndarray[ndim=1]
                 The estimated parameters
             cov : np.ndarray[ndim=2]
                 Covariance matrix of the parameters
             chisq ndf : float
                 The chisquare over the number of degrees of freedom
                 of the fit result.
             A = design_matrix(funcs, x)
             if cov_y is not None:
                 W = np.linalg.inv(cov_y)
             else:
                 W = np.eye(len(y))
             parameters, cov = solve linear least squares(A, W, y)
```

```
chisquare_ndf = chisquare_over_ndf(y, A, parameters)
return parameters, cov, chisquare_ndf
```

Result:

```
In [33]: parameters, cov, chisquare_ndf = linear_least_squares(x, y, funcs, cov_y)

In [34]: x_fit = np.linspace(0, 4 * np.pi, 1000)
    y_fit = linear_combination(x_fit, funcs, parameters)

    fig, ax = plt.subplots()

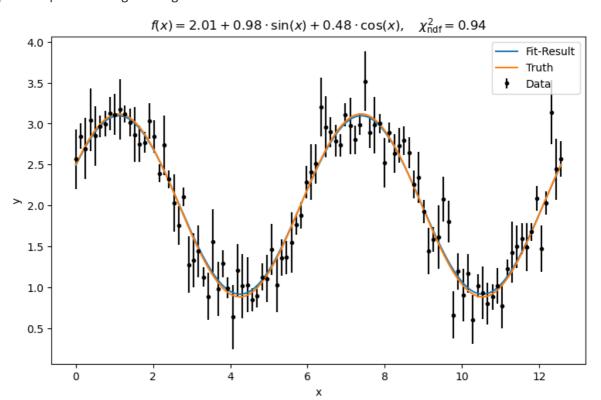
    ax.errorbar(x, y, yerr=y_unc, ls='', marker='.', label='Data', color='k')

ax.plot(x_fit, y_fit, label='Fit-Result')
    ax.plot(x_fit, y_truth, label='Truth')

ax.set(
    title=(
        rf'$f(x) = {parameters[0]:.2f} + {parameters[1]:.2f} \cdot \sin(x) + {parf', \quad \chi^2_\mathrm{{ndf}} = {chisquare_ndf:.2f}$'
    ),
        xlabel='x',
        ylabel='y',
    )
```

Out[34]: <matplotlib.legend.Legend at 0x7f09f0a64130>

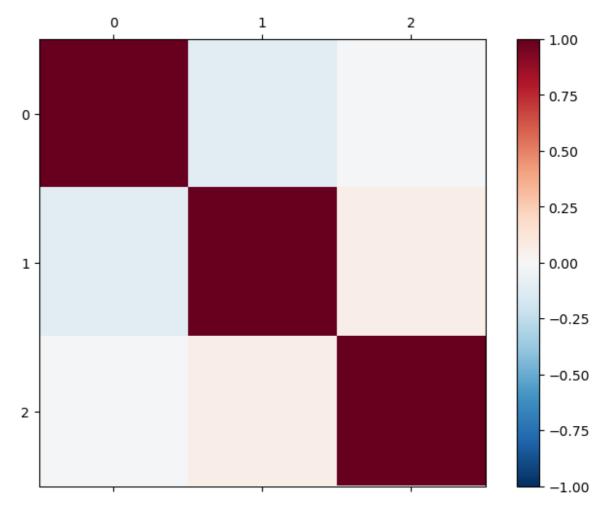
ax.legend()



```
In [35]: corr = cov_to_corr(cov)

fig = plt.figure(constrained_layout=True)
ax = fig.add_subplot(1, 1, 1)
m = ax.matshow(corr, cmap='RdBu_r', vmin=-1, vmax=1)
fig.colorbar(m)
```

Out[35]: <matplotlib.colorbar.Colorbar at 0x7f09f093b250>



Numerical solution for non-linear functions

If the function is not a linear combination of basis functions, the solution can only be found numerically.

From the lab courses, you probably know the scipy.optimize.curve_fit function, which does exactly this.

The Nelder-Mead-Algorithm use by curve_fit has the nice property that it is guaranteed to find the analytical solution, if it exists.

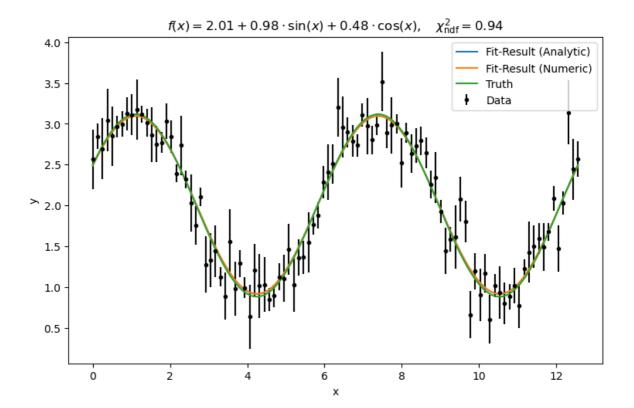
• https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.curve_fit.html

Example application to our linear problem

```
In [36]: from scipy.optimize import curve_fit
```

```
def func(x, p1, p2, p3):
             return p1 + p2 * np.sin(x) + p3 * np.cos(x)
         # absolute_sigma prevents scaling of errors to match χ²/ndf=1
         parameters_numeric, cov_numeric = curve_fit(
             func, x, y,
             sigma=np.full(N, y_unc),
             absolute_sigma=True,
         )
         print(parameters, parameters_numeric, cov, cov_numeric, sep='\n')
        [2.00565538 0.97702516 0.48411763]
        [2.00565538 0.97702516 0.48411763]
        [[ 3.66470863e-04 -5.58492439e-05 -1.00389068e-05]
        [-5.58492439e-05 6.79396825e-04 4.87671239e-05]
        [-1.00389068e-05 4.87671239e-05 7.92958991e-04]]
        [[ 3.66470865e-04 -5.58492426e-05 -1.00389039e-05]
         [-5.58492426e-05 6.79396818e-04 4.87671238e-05]
         [-1.00389039e-05 4.87671238e-05 7.92959005e-04]]
In [37]: x_{fit} = np.linspace(0, 4 * np.pi, 1000)
         y_fit = func(x_fit, *parameters)
         y num = func(x fit, *parameters numeric)
         y_truth = func(x_fit, *true_parameters)
         fig, ax = plt.subplots()
         ax.errorbar(x, y, yerr=y_unc, ls='', marker='.', label='Data', color='k')
         ax.plot(x_fit, y_fit, label='Fit-Result (Analytic)')
         ax.plot(x_fit, y_num, label='Fit-Result (Numeric)')
         ax.plot(x_fit, y_truth, label='Truth')
         ax.set(
             title=(
                 rf'$f(x) = {parameters[0]:.2f} + {parameters[1]:.2f} \cdot \sin(x) + {parameters[1]:.2f}
                 rf', \quad \chi^2_\mathrm{{ndf}} = {chisquare_ndf:.2f}$'
             ),
             xlabel='x',
             ylabel='y',
         ax.legend()
```

Out[37]: <matplotlib.legend.Legend at 0x7f09f0838160>



Why not simply always chose the numerical solution then?

```
In [38]: %%timeit
linear_least_squares(x, y, funcs)

42.8 \mus \pm 2.62 \mus per loop (mean \pm std. dev. of 7 runs, 10,000 loops each)

In [39]: %%timeit
curve_fit(func, x, y)

285 \mus \pm 38.8 \mus per loop (mean \pm std. dev. of 7 runs, 1,000 loops each)
```

Example with non-linear function

From the lab courses: single slit diffraction

```
In [40]: df = pd.read_csv('resources/spalt.csv')

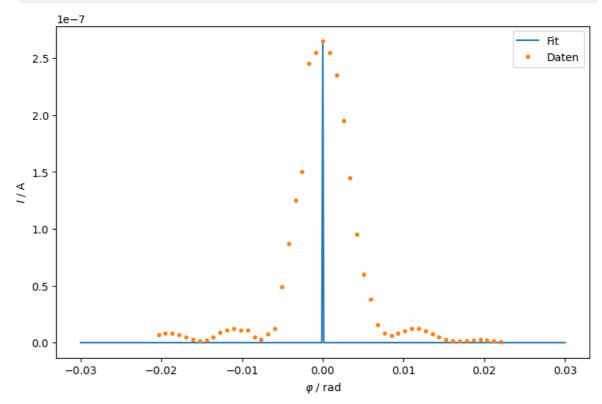
LASER_WAVELENGTH_NM = 632.8e-9

def theory(phi, A0, b):
    return (A0 * b * np.sinc(b * np.sin(phi) / LASER_WAVELENGTH_NM))**2

# first try with default initial guess (1 for every parameter)
p0 = None

# now with an "educated guess" based on the data and knowledge of the
# order of magnitude of the slit size
# p0 = [np.sqrt(df['I'].max()) / 1e-4, 1e-4]

params, cov = curve_fit(theory, df['phi'], df['I'], p0=p0)
```



Maximimum-Likelihood-Method

Unbinned Fit of Probability Densities

Strongly simplified example of a CERN-Like analysis.

We are looking for the mass-peak of a (normally distributed) particle.

We also observed a background, which in this simplified example is assumed to be exponentially distributed.

We create a simple "Toy"-Dataset using Monte Carlo methods:

```
In [41]: rng = np.random.default_rng(42)
E_MIN = 75
```

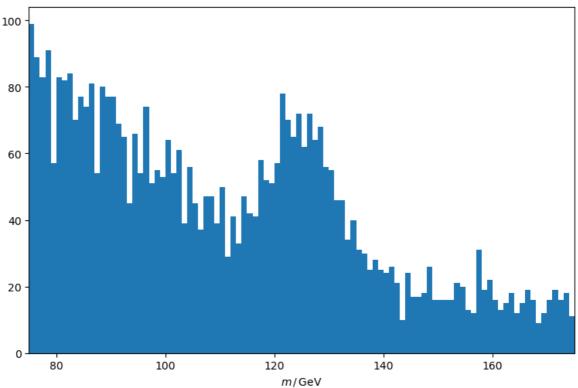
```
# normally distributed signal
higgs_signal = np.random.normal(126, 5, 500)

# exponentially distributed background
background = np.random.exponential(50, size=20000)

# combine signal and background
measured = np.append(higgs_signal, background)

# remove events outside of "detector range"
in_range = (E_MIN <= measured) & (measured <= E_MAX)
measured = measured[in_range]

fig, ax = plt.subplots()
ax.hist(measured, bins=100)
ax.set_xlabel('$m \,/\, \mathrm{GeV}$')
ax.margins(x=0)
None</pre>
```



Definition of the negative Log-Likelihood

We create a superposition of two probability densities, each with a proportion of p and 1-p respectively.

We also need to normalize the densities to the observed interval.

In this special case, we ignore this for the normal distribution, assuming that it is fully contained in the measurement interval.

$$P_1 = N(\mu, \sigma) \tag{1}$$

$$P_2 = \frac{1}{\exp(-E_{\min}/\tau) - \exp(-E_{\max}/\tau)} \exp(-E/\tau)$$
 (2)

$$P(E|p, \mu, \sigma, \tau) = p \cdot P_1(E, \mu, \sigma) + (1 - p)P_2(E|\tau)$$
(3)

$$\mathcal{L}(p,\mu,\sigma,\tau) = \prod_{i} P(E_i|p,\mu,\sigma,\tau) \tag{4}$$

$$-\log \mathcal{L}(p, \mu, \sigma, \tau) = -\sum_{i} \log(P(E_i|p, \mu, \sigma, \tau))$$
 (5)

In code, using the distribution classes from scipy.stats, it looks like this:

```
In [42]: from scipy.stats import norm, expon

def pdf(x, mean, std, tau, p):
    mass_peak = p * norm.pdf(x, mean, std)

expon_norm = np.exp(-E_MIN / tau) - np.exp(-E_MAX / tau)
    background = (1 - p) / expon_norm * expon.pdf(x, scale=tau)

return mass_peak + background
```

Solution using scipy.optimize.minimize und numdifftools.Hessian

Using scipy.optimize.minimize, we can minimize arbitrary functions.

The functions need to have an array of the fit parameters as first argument.

Further arguments can be passed using the args argument of minimize.

Naïvely, our negative Log-Likelihood for use with scipy looks like this:

```
In [43]: def neg_log_likelihood(parameters, data):
    # we add an epsilon to avoid inf in case of p=0
    return -np.sum(np.log(pdf(data, *parameters) + 1e-30))
```

Naïve, because often, analytic simplifications of the log-likelihood are possible!

Analytic simplifications both benefit numerical precision and evaluation speed.

It is almost always a good idea, to write down the likelihood on paper and simplify analytically as far as possible.

We find a minimum (and hopefully the global one) using scipy.optimize.minimize.

As known from the previous lecture, we can estimate the covariance matrix of the parameters from the inverse of the Hessian matrix of the negative log-likelihood, evaluated at the found minimum.

The Hessian matrix needs to be determined numerically. scipy.optimize.minimize returns a rough estimate, but this is borderline unusable.

We use numdifftools. Hessian to get the Hessian numerically.

scipy.optimize.minimize can use multiple algorithms each with benefits and drawbacks under the hood. For more information, see

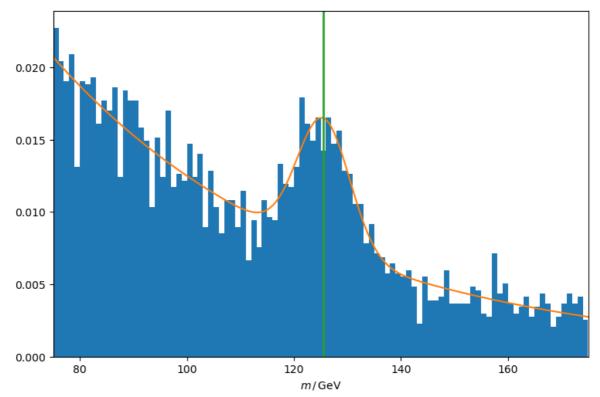
- https://docs.scipy.org/doc/scipy/reference/generated/scipy.optimize.minimize.html
- https://docs.scipy.org/doc/scipy/reference/optimize.minimize-lbfgsb.html

```
In [44]: from scipy.optimize import minimize
         # a very small number to achive > 0 instead of >= 0
         eps = np.finfo(np.float64).eps
         result = minimize(
             neg_log_likelihood,
             args=(measured, ),
             x0=[130, 2, 30, 0.2], # here, the initial guess is required
             bounds=[
                 (0, None), # mean >= 0
                 (eps, None), \# std > 0
                 (eps, None), # tau > 0
                 (0, 1), \# 0 \le p \le 1
             ],
         result
Out[44]: message: CONVERGENCE: REL_REDUCTION_OF_F_<=_FACTR*EPSMCH</pre>
           success: True
            status: 0
               fun: 19420.7016916766
                 x: [ 1.255e+02 4.926e+00 4.953e+01 1.112e-01]
               nit: 31
               jac: [-7.276e-04 1.091e-03 -7.276e-04 -4.584e-02]
              nfev: 200
              njev: 40
          hess inv: <4x4 LbfgsInvHessProduct with dtype=float64>
In [45]: from numdifftools import Hessian
         hesse = Hessian(neg_log_likelihood)
         cov = np.linalg.inv(hesse(result.x, measured))
In [46]: higgs_mass = result.x[0]
         higgs_mass_unc = np.sqrt(cov[0, 0])
         print(f'Higgs mass is {higgs_mass:.2f} ± {higgs_mass_unc:.2} GeV')
       Higgs mass is 125.52 \pm 0.43 GeV
In [47]: e = np.linspace(E_MIN, E_MAX, 1000)
```

fig, ax = plt.subplots()

```
ax.hist(measured, bins=100, density=True)
ax.plot(e, pdf(e, *result.x))
ax.axvline(result.x[0], color='C2', lw=2)

ax.set_xlabel('$m \,/\, \mathrm{GeV}$')
ax.margins(x=0)
```



Solution using iminuit

Iminuit provides python bindings for the Minuit minimization package from the ROOT framework.

It does not require a full ROOT installation.

"Minuit" is held to be – at least among particle physisicists – as non-plus-ultra of mimimizers.

iminuit provides the minimizers and several helper classes for loss functions. This makes it much simpler to perform fits.

It can also use likelihood ratio tests via the minos interface to estimate parameter uncertainties. (More on that in the next lectures).

For starters, let's solve the same problem as above, this time using iminuit:

```
In [48]: from iminuit import Minuit
from iminuit.cost import UnbinnedNLL

# minuit's UnbinnedNLL takes directly the pdf and the observed data
loss = UnbinnedNLL(measured, pdf)

m = Minuit(loss, mean=130, std=2, tau=30, p=0.2)
```

```
# set bounds
m.limits['mean'] = (0, None) # >= 0
m.limits['std'] = (eps, None) # > 0
m.limits['tau'] = (eps, None) # > 0
m.limits['p'] = (0, 1)

# perform minimization
m.migrad()

# perform likelihood scan for confidence intervals
m.minos()
```

Out[48]: Migrad

FCN = 3.884e+04 Nfcn = 327

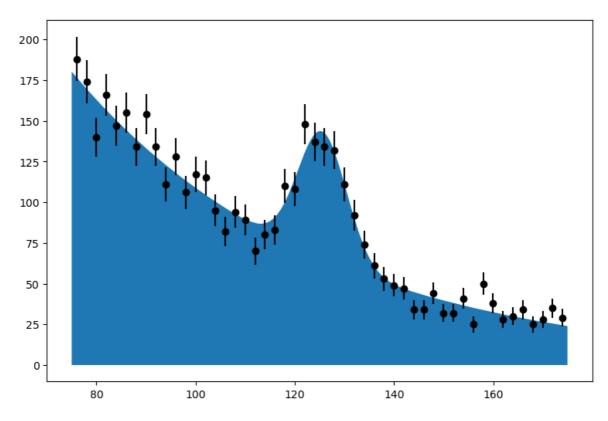
EDM = 4.21e-06 (Goal: 0.0002)

Valid Mini	No Parameters at limit			
Below EDM thresh	Below call limit			
Covariance	Hesse ok	Accurate	Pos. def.	Not forced

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	mean	125.5	0.4	-0.4	0.4	0		
1	std	4.9	0.4	-0.4	0.4	2.22E-16		
2	tau	49.5	1.6	-1.5	1.6	2.22E-16		
3	р	0.111	0.009	-0.009	0.009	0	1	

	me	ean	std		tau		р	
Error	-0.4	0.4	-0.4	0.4	-1.5	1.6	-0.009	0.009
Valid	True	True						
At Limit	False	False						
Max FCN	False	False						
New Min	False	False						

	mean	std	tau	р
mean	0.186	0.00 (0.013)	-0.05 (-0.078)	-0.10e-3 (-0.026)
std	0.00 (0.013)	0.148	-0.11 (-0.173)	1.62e-3 (0.463)
tau	-0.05 (-0.078)	-0.11 (-0.173)	2.54	-3.86e-3 (-0.266)
р	-0.10e-3 (-0.026)	1.62e-3 (0.463)	-3.86e-3 (-0.266)	8.26e-05



```
In [49]: higgs_mass = m.values['mean']
higgs_mass_unc = m.errors['mean']
print(f'Higgs mass is {higgs_mass:.2f} ± {higgs_mass_unc:.2} GeV')
```

Higgs mass is 125.52 ± 0.43 GeV

Poisson-Likelihood-Fit using a binned Event Distribution

If the single observations are not accessible or the runtime of the analysis is critical for large amounts of data, a so-called "binned" fit is also possible.

In a binned fit, we estimate the parameters of the distributions from a histogram.

Since a histogram is a counting experiment, the single event numbers in each bin each follow a Poisson distribution.

The cumulative probability function yields together with the total number of observed events the expected value in each histogram bin, dependent on the fit parameters θ .

$$\mathcal{L} = \prod_{i=1}^N \mathcal{P}(k=H_i, \lambda=\lambda_i(oldsymbol{ heta}))$$

with

$$\lambda_i = N_{ ext{total}} \cdot (ext{CDF}(b_i, oldsymbol{ heta}) - ext{CDF}(a_i, oldsymbol{ heta}))$$

Here, a_i und b_i are the bin edges of the i-th bin. We then integrate the PDF in each bin and multiply with the total number of events.

Example from "Lifetime of cosmic Muons" (Lab Course Experiment V01)

The experimental setup of this lab course experiment directly produces a histogram of observed decay times in hardware.

We thus cannot perform an unbinned fit, the single values are simply not available.

The lab course instruction ask for a least squares fit to the bin heights.

This method yields an unbiased estimator but with non-optimal spread, as long as an unweighted fit is performed.

In the past, it was recommended to perform a weighted fit assuming $\sigma_i = \sqrt{H_i}$.

This is wrong! This method consistently yields biased results, due to under-fluctuations being weighted more strongly than over-fluctuations of the same amount.

The correct method is the binned Poisson-likelihood fit as discussed here or the iterative least squares method discussed in SMD-2.

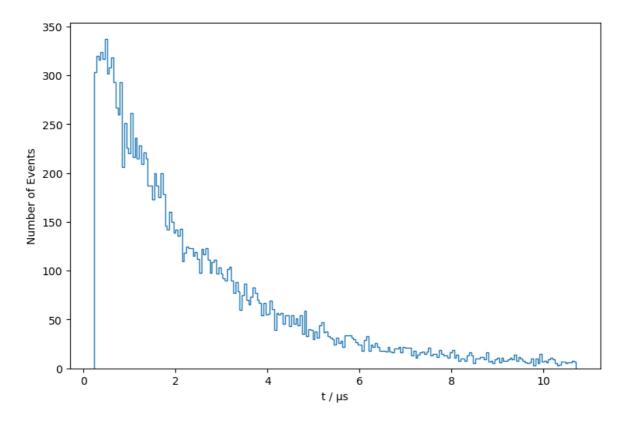
A comparison of the different methods is available here: https://gist.github.com/maxnoe/41730e6ca1fac01fc06f0feab5c3566d

In the experiment, there is an additional uniformly distributed background from non-decaying, coincident muons.

```
In [50]: N = np.genfromtxt("resources/muon_data.txt")
t = np.arange(len(N) + 1) / 21.48

t = t[5:]
N = N[5:]

plt.figure()
plt.stairs(values=N, edges=t)
plt.xlabel('t / \mus')
plt.ylabel('Number of Events')
None
```



Iminuit provides the BinnedNLL loss function for this use cases.

```
In [51]: from iminuit.cost import BinnedNLL
         from scipy.stats import uniform
         T_MIN, T_MAX = t[0], t[-1]
         def cdf(x, tau, p):
             # normalize to 1 in histogram range
             cdf_min, cdf_max = expon.cdf([T_MIN, T_MAX], scale=tau)
             norm = 1 / (cdf_max - cdf_min)
             signal = p * expon.cdf(x, scale=tau) * norm
             background = (1 - p) * uniform.cdf(x, T_MIN, T_MAX)
             # combine exponential signal with uniform background
             return signal + background
         # histogram counds, histogram edges and cumulative distribution function
         loss = BinnedNLL(N, t, cdf)
         m = Minuit(loss, tau=2, p=0.99)
         m.limits['tau'] = (eps, None)
         m.limits['p'] = (0, 1)
         m.migrad()
         m.minos()
```

Out[51]: Migrad

FCN = 247.5 (χ^2 /ndof = 1.1) Nfcn = 103

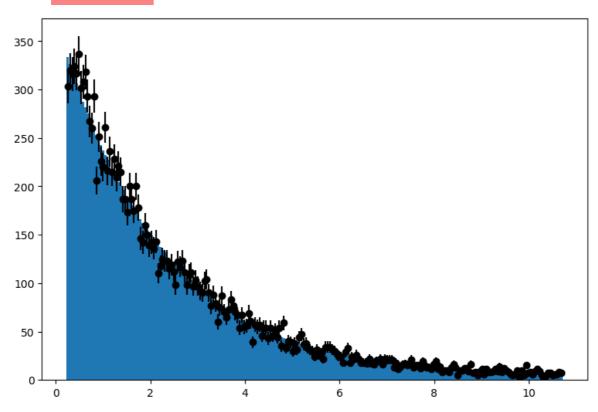
EDM = 1.62e-08 (Goal: 0.0002)

Valid Mini	No Parameters at limit			
Below EDM thresh	Below call limit			
Covariance	Hesse ok	Accurate	Pos. def.	Not forced

	Name	Value	Hesse Error	Minos Error-	Minos Error+	Limit-	Limit+	Fixed
0	tau	2.169	0.034	-0.034	0.035	2.22E-16		
1	р	0.958	0.007	-0.007	0.007	0	1	

	ta	u	p)
Error	-0.034 0.035		-0.007	0.007
Valid	True	True	True	True
At Limit	False	False	False	False
Max FCN	False	False	False	False
New Min	False	False	False	False

	tau	р
tau	0.00119	0.20e-3 (0.790)
р	0.20e-3 (0.790)	5.47e-05



```
In [52]: muon_lifetime = m.values['tau']
    muon_lifetime_unc = m.errors['tau']
    pdg_reference = 2.1969811
    pdg_reference_unc = 0.0000022

    print(f'Fit: \tau = \{\text{muon_lifetime:.3f}\} \tau \{\text{muon_lifetime_unc:.3f}\} \text{ \musin s'}\}
    print(f'Lit: \tau = \{\text{pdg_reference:.7f}\} \tau \{\text{pdg_reference_unc:.7f}\} \text{ \musin s'}\}

    Fit: \tau = 2.169 \tau 0.034 \text{ \musin s}
    Lit: \tau = 2.1969811 \tau 0.0000022 \text{ \musin s}

    Likelihood-Scan for uncertainty intervals:

In [53]: tau, ts, valid = m.mnprofile('tau', size=100)

In [54]: plt.figure()
    plt.axvline(m.values['tau'], color='C1')
    plt.plot(m.values['tau'], m.fval. color='C1', marker='o', zorder=3)
```

```
In [54]: plt.figure()

plt.axvline(m.values['tau'], color='C1')

plt.plot(m.values['tau'], m.fval, color='C1', marker='o', zorder=3)

plt.axvline(m.values['tau'] + m.merrors['tau'].lower, color='C2')

plt.axvline(m.values['tau'] + m.merrors['tau'].upper, color='C2')

plt.axvline(m.fval + 1, color='C3')

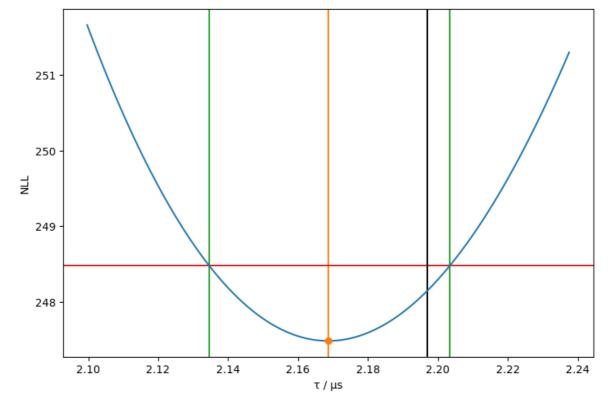
plt.axvline(pdg_reference, color='k', label='PDG')

plt.plot(tau, ts)

plt.xlabel('t / \mus')

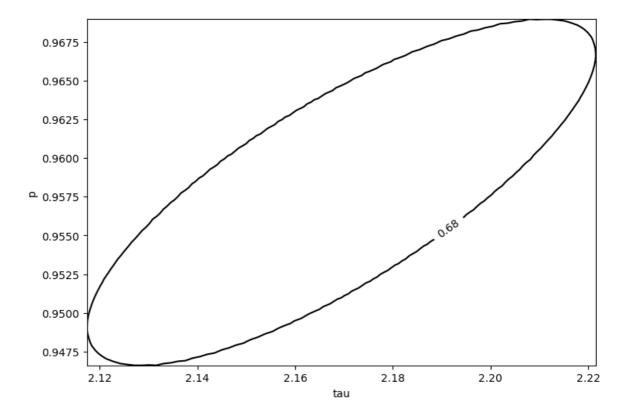
plt.ylabel('NLL')

None
```



```
In [55]: plt.figure()
m.draw_mncontour('tau', 'p', size=250)
```

Out[55]: <matplotlib.contour.ContourSet at 0x7f09e9e56380>



In []: