Curve_fitting_Python

November 5, 2022

1 General information

- Author: Joris Busink, Junior Teacher Physics Education.
- Date: Fri, 4th Nov.
- About: Data-analysis and data-visualization using Python 3.

For questions and suggestions please email: J.Busink@vu.nl. Github

1.1 Structure of the notebook

Example 1, Curve_fit: 1. Load packages. 2. Model and mock data. 3. Plot data. 4. Fit data to model. 5. Plot residuals. 6. Calculate (reduced) χ^2. 7. Extra: confidence intervals.

Example 2, Lmfit: 8. Example: Lmfit.

2 Example: Analysis of a pendulum (SHO)

2.1 Load packages

I load the following packages: * Numpy, numerical Python. * Matplotlib.pyplot, for creating static, animated, and interactive visualizations in Python. * Pandas. A fast and efficient library to handle DataFrame objects.

[ ]:
```
import numpy as np
import matplotlib.pyplot as plt
import pandas as pd

np.set_printoptions(precision=4,threshold =9,suppress=True)  #Compact display.
```

2.2 Pendulum model and mock data

We are interested in x-position of the pendulum as a function of time. For abitrary (starting) angle $\theta(t)$ the system has a non-linear response. However, for small angles we can approximate $\sin(\theta(t)) \approx \theta$ and we have a linear system, thus:

$$x(t) = Ae^{-\gamma t}\sin(\omega t) \tag{1}$$

The harmonic response is given by $\sin(\omega t)$, with $\omega^2 = \frac{g}{l}$. A is the amplitude of the oscillation. g the gravitational acceleration and l the length of the cord. The damping term is modelled by an exponential decay $e^{-\gamma t}$, with γ a damping constant.

To start of, I create a mock-data set using the model of the simple pendulum (equation 1). The x-data is an array (a 'list' that allows nummerical manipulations) that represents the time-domain of the oscillator that ranges from 0 to 10, with $\delta t = 0.2$. The y-data is the x-position of the oscillator, we create this by evaluating the Simple Harmonic Oscillator model function using the following input parameters:

$$x(t) = 2e^{-0.2t}\sin(3t) + 0.2\sqrt{t}\zeta(t). \tag{2}$$

I included a stochastic term, $0.2\sqrt{t}\zeta(t)$, to make our data non-ideal/noisy. $\zeta(t)$ is a random uniform number (float) from -1 to 1. The exact details of the process are not important.

- Line 1: create random seed (to replicate noise).
- Line 3-4: generate t-data and yxdata.
- Line 5-6: noise in t-data and x-data.

[ ]:
```
np.random.seed(2) #initialize random number generator seed.

t = np.arange(0,10.2,0.2) # t-axis data, an array ('list') from [0,0.2...9.8,␣
↪10],
# this is equivalent to: t = np.array([ 0.,0.2 , 0.4 , ... , 9.8 ,  10.0])
x = 2*np.exp(-0.2*t)*np.sin(3*t) + 0.2*np.sqrt(t)*np.random.
↪uniform(-1,1,len(t)) # x-axis data.
terr = 0.1 # constant error in time.
xerr = 0*t +0.2 # The error in x-position, please note that the shape of xerr␣
↪must be of the same size as x.
```

2.2.1 Digital data

In case our data is only digital available (for example, as a .csv file), on option is to import the data as a DataFrame (df):

df = pd.read_csv('path\to\data.csv', delimiter='fill_in') Read_csv.

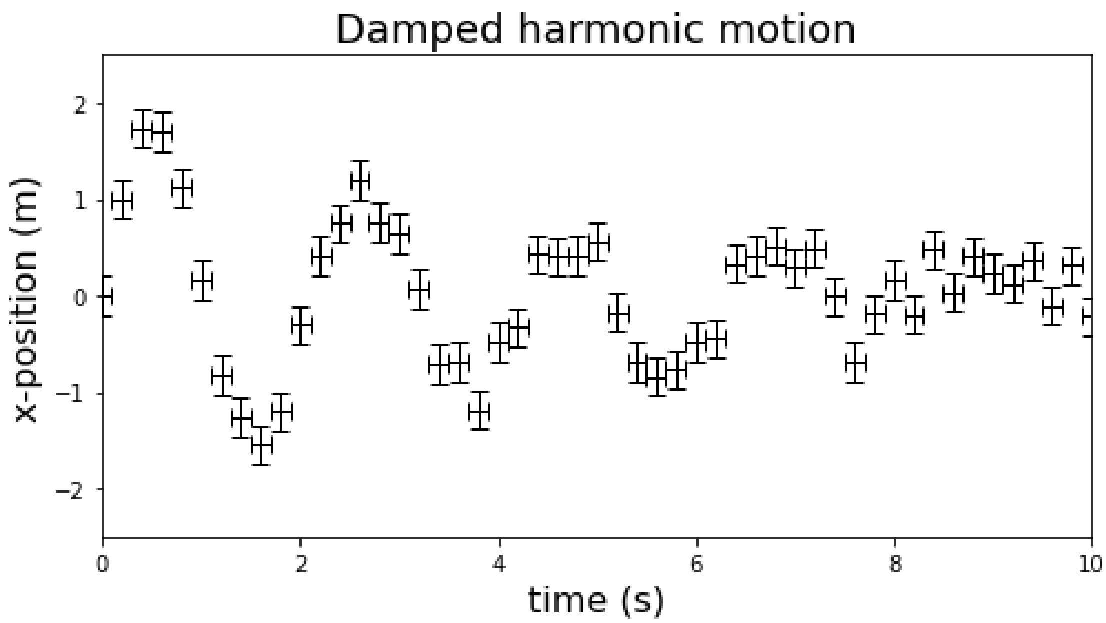
Another options is to use Numpy genfromtxt: data = genfromtxt('my_file.csv', delimiter=',')

2.3 plot the data

In the next lines of code I plot the data. Our data is 2 dimensional (x,y) and contains errors, so we use an errorbar plot.

- Line 1: create 1 figure (1 row and 1 column). Figure documentation
- Line 2: plot data using an errorbarplot. Errorbar documentation
- Line 3-8: optional commands.

[ ]:
```
fig, axes = plt.subplots(1,1,figsize=(8,4)) #Creates a single figure with dimensions (12 by 6 (inch))
axes.errorbar(t,x,xerr=terr,yerr=xerr,fmt='none',ecolor='black',capsize=4,elinewidth=1)
axes.set_title('Damped harmonic motion', fontsize=18)
axes.set_xlabel('time (s)',fontsize=16)
axes.set_ylabel('x-position (m)',fontsize=16)
axes.set_xlim(np.min(t),np.max(t))
axes.set_ylim(-2.5,2.5)
plt.show()
```



2.4 Fit data to model

We want to fit our model, equation 1, to our data, we use the scipy.optimize libary, and in particular we use the Curve_fit function.

- Line 1-2: Here we define our model (sinus_model()) using a Python function: a function starts with def and ends with return. Sinus_model() is our user defined model based on the theory. We vary the time coordinate (the independent variable, t) and the parameters (x_0, A, ω and ϕ) are determined by a fit. Be careful that the independent variable (t) must appear before the parameters, otherwise an error message will appear.
- Line 4: Apply a fit using the curve_fit function. Curve_fit documentation

Curve_fit asks for a minimum of three input arguments: (model, independent variable (time), dependent variable (x-coordinate)), more input arguments are optional. In our case, I provide an initial guess of the optimal parameters (p_0). Other options include: bounds, weights, method, etc. Note that providing a good initial guess of p_0 and apply parameter bounds significantly reduces the complexity of finding the optimal parameters, if possible, provided them! The output of Curve_fit are the optimal parameters popt and the covariance matrix $\mathcal{K}_{p_i p_j}$ pcov, where $\mathcal{K}_{p_i p_j}$ is defined as:

$$\mathcal{K}_{p_i p_j} = \begin{bmatrix} s_{p_a p_a} & s_{p_b p_a} \\ s_{p_a p_b} & s_{p_b p_b} \end{bmatrix} \tag{2}$$

For example, $s_{p_a p_a}$ is the (co)variance of parameter a. To obtain the standard deviation σ_a of parameter a we take the square root of the variance:

$$\sigma_a = \sqrt{s_{p_a p_a}} \tag{3}$$

- Line 6-8: Show the optimal fit values and corresponding standard deviations.

[ ]:
```python
from scipy.optimize import curve_fit

def sinus_model(t,A,gamma,omega,phi):
    return A*np.exp(-gamma*t)*np.sin(omega*t+phi)

popt, pcov = curve_fit(sinus_model,t,x,sigma = xerr,p0=[1,0.1,4.12,0.5])

parameter=['Amplitude (m)','Gamma (1/s)', 'Frequency (rad/s)', 'phase (rad)']
for i in range (4):
    print("The optimal value for ", parameter[i], 'is:', "{:.4f}".
 ↪format(popt[i]), '\u00B1', "{:.6f}".format(np.sqrt(pcov[i,i])))
```

```
The optimal value for  Amplitude (m) is: 2.0380 ± 0.144019
The optimal value for  Gamma (1/s) is: 0.2198 ± 0.023873
The optimal value for  Frequency (rad/s) is: 2.9934 ± 0.022534
The optimal value for  phase (rad) is: -0.0094 ± 0.063073
```

- Line 10-15: Make figure, plot the data (black) and the fit (orange).

We plot the fit by making a new dataset, called tfit. We evaluate the the function using the optimal parameters at the values of tfit.

- Line 17-25: Optional commands.

- Line 27-28: Save the figure.

Note that the figure is saved as a .svg extension. A .svg extension stands for Scalable Vector Image, the image is saved as an object (and not as a collection of pixels). One can import .svg picture in e.g. inkscape, powerpoint or adobe photoshop to manipulate these, try it!

[ ]:
```python
tfit = np.linspace(0,max(t),1000) #create new data for fit.

#Plot data + fit
fig,axes=plt.subplots(1,1,figsize=(8,4),sharex=True,sharey=True)
axes.plot(tfit,sinus_model(tfit,*popt), color ='darkorange', lw = 4,zorder =1)␣
 ↪#plot fit
```

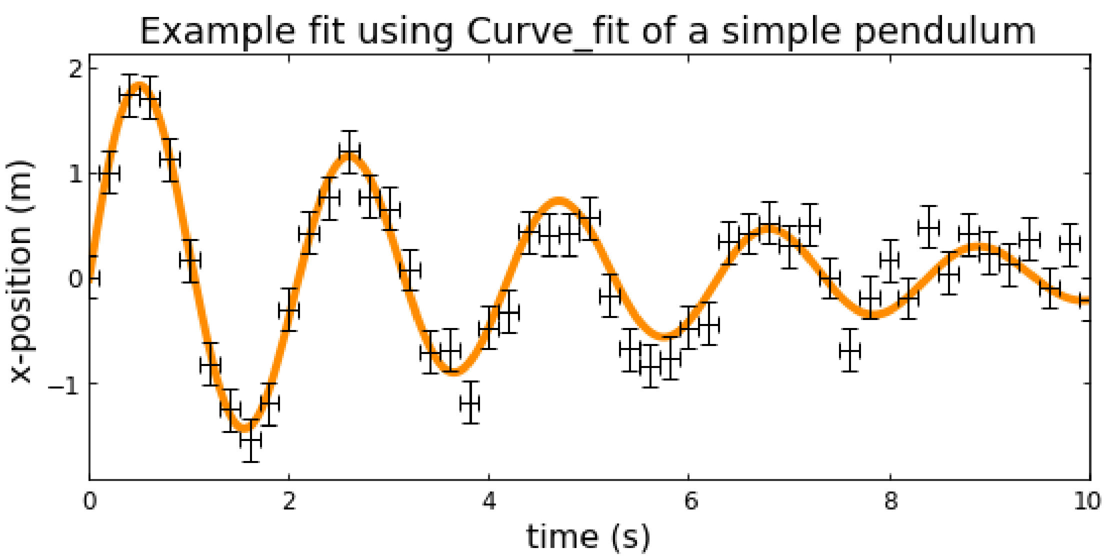
```
axes.
↪errorbar(t,x,xerr=terr,yerr=xerr,fmt='none',ecolor='black',capsize=4,elinewidth=1)

#plot axis labels and limits
axes.set_title('Example fit using Curve_fit of a simple pendulum',fontsize=18)
axes.set_xlabel('time (s)',fontsize=16)
axes.set_ylabel('x-position (m)',fontsize=16)
axes.set_xlim(0,10)

#Some plot settings
axes.tick_params(direction="in",labelsize=12,bottom = True,top = True,left=␣
↪True,right=True) #inward direction of tick-lines
plt.tight_layout() #creates optimal padding levels for figure (especially␣
↪usefull for side-by-side figures)

# location='Path' #Path to your prefered location, e.g. User/Downloads/
# plt.savefig(location+'simple_pendulum.svg') #Extension can be .png/.jpg/.etc␣
↪or .svg/.pdf (Vector Image)

plt.show()
```



2.5 Optional: Residuals

In the previous section we fit a model to our data. As expected, the sinusoidal model captures the data very well.

However, we might also be interested in the limitations of the model. To spot these limitations can be cumbersome, a elegant strategy is to calculate the difference between the data and the fit: the residuals. To visualize the residuals I will make an extra figure above the main panel. I use gridspec to create this extra panel. Using gridspec we can make two (or more) subfigures, a main figure and a sub (residuals) figure. In the main figure I plot the data and optimal fit. In the residuals plot I plot the difference between the data and the fit, the residuals ϵ of the data:

$$\epsilon = y_{data} - y_{model}. \tag{4}$$

The residual plot shows valuable information. For example, a systematic pattern in the residuals tells us that our model cannot capture the full data. In principle, when a systematic pattern in the residuals is visible, we should modify our model.

For a more extensive discussion about the meaning of a residual I refer to chapter 4.2 in An Introduction to Error Analysis, by John R. Taylor.

[ ]:
```
import matplotlib.gridspec as gridspec

fig = plt.figure(figsize=(8,8))
gs = gridspec.GridSpec(4, 4) #Creates a grid of 4 rows and 4 columns.
axes_main = plt.subplot(gs[1:4, :4]) #Main axis goes from row 1 to 4.
axes_residuals = plt.subplot(gs[0, :4],sharex=axes_main) #Residual axis is row␣
↪0.

axes_main.plot(tfit,sinus_model(tfit,*popt),color='darkorange', lw=4)
axes_main.
↪errorbar(t,x,xerr=terr,yerr=xerr,fmt='none',ecolor='black',capsize=4,elinewidth=1)

axes_main.set_xlabel('Time (s)',fontsize=16)
axes_main.set_ylabel('X-position (m)',fontsize=16)
axes_main.set_xlim(0,10)
axes_main.tick_params(axis='both',direction ='in',labelsize=12)

axes_residuals.
↪errorbar(t,x-sinus_model(t,*popt),xerr=terr,yerr=xerr,fmt='none',ecolor='black'
                        ,capsize=4,elinewidth=1)

axes_residuals.tick_params(axis='both',direction ='in',labelsize=12)
axes_residuals.hlines(0,np.min(t),np.max(t),color='black')
axes_residuals.set_ylabel(r'$\epsilon$ (m)',fontsize=16)
axes_residuals.set_xlim(0,10)

plt.tight_layout()
# plt.show()
plt.close()
```

2.6 reduced χ^2

In the previous figure we observed that our fit captures the data nicely. In the residuals we observe that after t $\approx$ 7 s, the noise starts to dominate. We quantify the deviation between the observed and expected data using a χ^2 analysis:

$$\chi^2 = \sum_1^N \frac{(y_i - f(x_i))^2}{\sigma_i^2} = \sum_1^N \frac{\epsilon_i^2}{\sigma_i^2}. \tag{5}$$

σ_i is the standard deviation 'error' on the observed datapoint y_i. Lastly, we should correct for the number of degrees of freedom. We have N data points and c parameters, so we have d = N - c degrees of freedom. We define the following:

$$\tilde{\chi}^2 = \frac{\chi^2}{d}, \tag{6}$$

$\tilde{\chi}^2$ is the reduced χ^2, it includes the effect of the degrees of freedom of the model. The value of $\tilde{\chi}^2$ is a measure of the deviation between the data and the model.

For a more general discussion about the significance and applicability of $\tilde{\chi}^2$ I refer to chapter 12 in An Introduction to Error Analysis by John R. Taylor.

[ ]:
```
chisq = np.sum(((x-sinus_model(t,*popt))/xerr)**2)
d = len(x) - len(popt)
red_chisq = chisq/d
print("chi-squared = %.4f" % chisq)
print("df = %d" % d)
print("Reduced chi-squared = %.4f" % red_chisq)
```

```
chi-squared = 60.3651
df = 47
Reduced chi-squared = 1.2844
```

2.7 Optional: Confidence Intervals

In the previous sections we calculated the optimal parameters, the errors on the optimal parameters and the $\tilde{\chi}^2$ value. Our model consists of 4 parameters and the error on the optimal parameter:

- The optimal value for A (m) is: 2.0137 $\pm$ 0.045014
- The optimal value for γ (1/s) is: 0.2087 $\pm$ 0.011162
- The optimal value for ω (rad/s) is: 2.9943 $\pm$ 0.010095
- The optimal value for ϕ (rad) is: 0.0010 $\pm$ 0.018336

Now we can ask ourself the question: how likely is it that my datapoint falls within n-standard deviations of my curve.

We answer this question by constructing confidence intervals (C.I.) around the optimal fit.

The C.I. is defined as,

$$\begin{aligned} Pr(\mu - 1\sigma \leq X \leq \mu + 1\sigma) &\approx 68.27\%, \\ Pr(\mu - 3\sigma \leq X \leq \mu + 3\sigma) &\approx 99.73\%, \\ Pr(\mu - n\sigma \leq X \leq \mu + n\sigma) &= erf(x/\sqrt{2}). \end{aligned}$$

The C.I. tells us how likely it is that our observation X is found within the interval, with μ the mean of the distribution X and σ the standard deviation of the distribution X.

We have 4 parameters, each with it's own deviation, constructing the C.I. is not trivial. For example, a (positive) deviation (from the mean) of the Amplitude can be mitigated by a (positive) deviation of the damping γ term.

However, the overall effect is a mean all parameters, we cannot simply add each individual contribution. To calculate the mean response and the C.I. we use a Monte-Carlo technique. We use repeated Gaussian sampling of the parameters to obtain a statistical mean response (the optimal fit) and we calculate the C.I. by the standard deviation of the mean response.

- Line 4-7: Random sampling around the optimal parameters.
- Line 8-11: Evaluate the model response of the random parameters 'ydata_random'.

Thus, ydata_random contains 1000 curves. Each curve has a (random) unique set of parameters around the optimal value. The mean of ydata_random is the optimal fit. The standard deviation (at each data point) of ydata_random is σ, this is the boundary of the C.I.

[ ]:

```
import matplotlib.gridspec as gridspec
import scipy.stats as st

popt0 = popt[0]+np.random.normal(0,1,size=1000)*np.sqrt(np.diag(pcov))[0]
popt1 = popt[1]+np.random.normal(0,1,size=1000)*np.sqrt(np.diag(pcov))[1]
popt2 = popt[2]+np.random.normal(0,1,size=1000)*np.sqrt(np.diag(pcov))[2]
popt3 = popt[3]+np.random.normal(0,1,size=1000)*np.sqrt(np.diag(pcov))[3]
ylist =[]
for i in range(0,1000,1):
    ydata_random = sinus_model(tfit,popt0[i],popt1[i],popt2[i],popt3[i])
    ylist.append(ydata_random)

fig = plt.figure(figsize=(8,8))
gs = gridspec.GridSpec(4, 4) #Creates a grid of 6 rows and 4 columns.
axes_main = plt.subplot(gs[1:4, :4]) #Main axis goes from row 1 to 6.
axes_residuals = plt.subplot(gs[0, :4],sharex=axes_main) #Residual axis is row 0.

axes_main.tick_params(axis='both',direction ='in',labelsize=12)
axes_main.errorbar(t,x,xerr=terr,yerr=xerr,fmt='none',ecolor='black',capsize=4,elinewidth=1,marker = 's',zorder=5) #fmt, ecolor and capsize can be personalized.
axes_main.plot(tfit,sinus_model(tfit,*popt),color='darkorange',ls='-',lw=2,zorder =5)

axes_main.fill_between(tfit,np.mean(ylist,axis=0)+3*np.std(ylist,axis=0),np.mean(ylist,axis=0)-3*np.std(ylist,axis=0),color='darkgray')
axes_main.fill_between(tfit,np.mean(ylist,axis=0)+1*np.std(ylist,axis=0),np.mean(ylist,axis=0)-1*np.std(ylist,axis=0),color='white')
axes_main.set_xlabel('Time (s)',fontsize=16)
```

```
axes_main.set_ylabel('x-position (m)',fontsize=16)
axes_main.set_xlim(0,10)

axes_residuals.errorbar(t,x-sinus_model(t,*popt),xerr=terr,yerr=xerr,
                        fmt='none',ecolor='black',capsize=4,elinewidth=1) #fmt, ecolor and capsize can be personalized.
# axes_residuals.hlines(0,np.min(t),np.max(t),color='black')

axes_residuals.tick_params(axis='both',direction ='in',labelsize=12)
axes_residuals.set_title('Confidence intervals',fontsize=18)
axes_residuals.set_ylabel(r'$\epsilon$ (m)',fontsize=16)
axes_residuals.set_xlim(0,10)

# plt.tight_layout()
# plt.show()
plt.close()
```

3 Example: fit data using lmfit

We can also use a package called 'lmfit' to fit our data to a model. On the canvas page there is an extensive document that guides you through the process of fitting using lmfit, for questions please visit the canvas page.

In the code below you find a minimum working example using lmfit:

- Line 4: define model using λ function.
- Line 7: Initialize model parameters system parameters (p_0).
- Line 10: Provide bound to e.g. amplitude parameter.
- Line 13: Apply fit.

[ ]:
```
from lmfit import models

#Define model:
model = models.Model(lambda t, Amplitude, Gamma, Omega,Phi:
    Amplitude * np.exp(-Gamma * t) * np.sin(Omega*t+Phi))

#Initialize parameters (p0)
params = model.make_params(Amplitude=2, Gamma=0.2, Omega=3,Phi=2)

#Provide bounds
params['Amplitude'].min = 0

#Fit data using model.fit
fit = model.fit(x, t=t, params=params,weights = 1/xerr)
```

We can show the fit using f.best_fit and show the fit statistics using fit.fit_report(). The fit_report() provides the optimal parameters, the error on each parameter and the $\tilde{\chi}^2$.

[ ]:
```
fig,axes=plt.subplots(1,1,figsize=(8,4),sharex=True,sharey=True)
axes.plot(t, fit.best_fit, color='darkorange',lw=4,zorder =1)#plot fit
axes.
 ↪errorbar(t,x,xerr=terr,yerr=xerr,fmt='none',ecolor='black',capsize=4,elinewidth=1)

#plot axis labels and limits
axes.set_title('Example fit using Lmfit',fontsize=18)
axes.set_xlabel('Time (s)',fontsize=16)
axes.set_ylabel('x-position (m)',fontsize=16)
axes.set_xlim(0,10)
# plt.show()
plt.close()
#print fit report
# print(fit.fit_report())
```

4 Your Experiment starts here

- Author: Student name.
- Date: Date.
- About: Your experiment.
- TA:

Please ask your TA if you need to hand in your code at the end of the practical course.

[ ]:
```
```