Non-linear models

Non-Linear models are functions that are non-linear in their parameters

Exponential , power, Gaussian, Fourier etc.. functions, are non-linear because their coefficients are not linear

Exponential $y = yo \exp(-k x)$

Power $y = a x^b$

Examples of non-linear models and their applications:

https://acsess.onlinelibrary.wiley.com/doi/10.2134/agronj2012.0506

look at table1 for a summary of non-linear models

Fit non-linear models with SciPy

For non-linear models, we will use the scipy.optimize module, and in particular the curve_fit() function , which implements a non-linear least-squares procedure.

Import the curve_fit() in this way:

```
from scipy.optimize import curve_fit
```

```
popt, pcov = curve_fit(func, xarray, yarray, guess_array)
```

func - the fitting model function, which can be a custom function defined by def
xarray – array-like (1D array, Series) the independent variable
yarray – array-like (1D array, Series) the dependent variable
initial_guess – a list or 1D array containing the initial guess for each paramater
Useful when curve_fit() cannot calculate the covariance matrix.

The function returns:
popt array– fitting coefficients – 1D array
Optimal values for the parameters so that the sum of the square residuals is minimized.

pcov matrix – covariance matrix – 2D array NxN where N is the number of fitting parameters.

Calculate the Residuals for each point.

```
residuals = y_data - func(x_data, *popt)  #the * operator means all the elements in variable popt.
```

Calculate the standard error of the parameters

the square root of the diagonal elements of the covariance matrix gives the standard error for each parameter

```
perr = np.sqrt(np.diag(pcov))
```

Example – Fit a non-linear model with SciPy

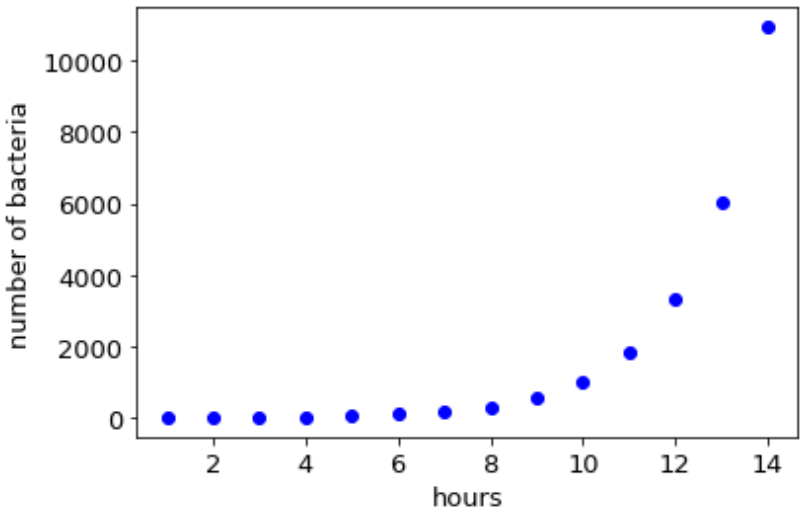
Download the data file bacteria.csv from Canvas DATA, which contains data on bacterial growth. The 1st field is the hours since observation and the 2nd field the number of bacteria in the sample. We will fit the data with an exponential growth model.

$$y = a\, e^{bx}$$

```
import numpy as np
import matplotlib.pyplot as plt
from scipy.optimize import curve_fit

data=np.loadtxt('bacteria.csv',delimiter=',')
x=data[:,0]  #hours since observation
y=data[:,1]  #number of bacteria


#plot row data
plt.rcParams['font.size']=13
fig, ax=plt.subplots()
ax.plot(x, y,'ob', label='data'
ax.set_xlabel('hours')
ax.set_ylabel('number of bacteria')
```



Example – Fit a non-linear model with SciPy


```
#fit with curve_fit
popt, pcov = curve_fit(mymodel, x, y)


#Sometimes an initial guess of the parameters is required for the
fitting method to work.
#popt, pcov = curve_fit(mymodel, x, y, [2.1, 0.3] ))#with an initial
guess


print(popt)
[2.49652581 0.59892497] # fitted parameters a and b


print(pcov) #covariance matrix
[[ 7.07224351e-05 -2.08093101e-06]
 [-2.08093101e-06  6.14351150e-08]]
```

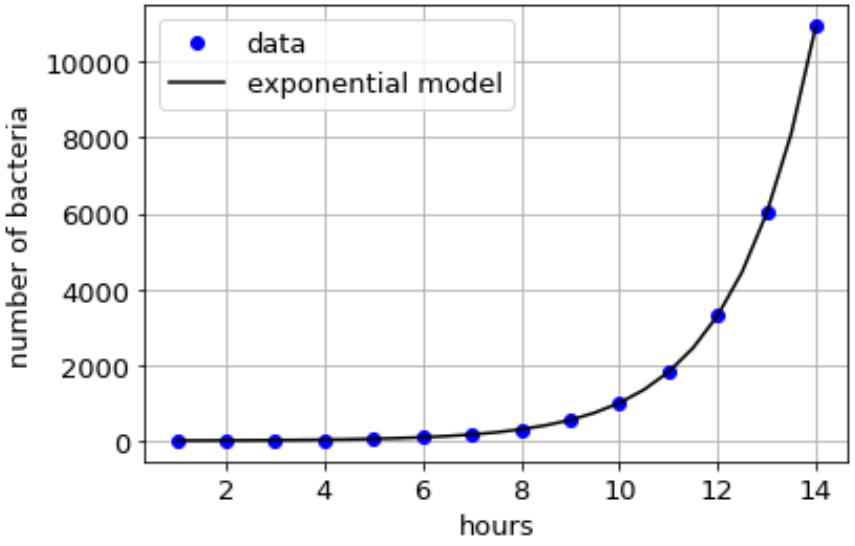
Example – Fit a non-linear model with SciPy

```
#Use the function to create an array containing the predicted values.

xsmall=np.arange(np.min(x),np.max(x)+0.1,0.5) #make more x values to smooth the model function

ypsmall=mymodel(xsmall,*popt) #the * operator means all the elements in variable popt.

#plot the fitted model.
ax.plot(xsmall,ypsmall,'k-',label='exponential model')
ax.grid()
ax.legend()
```



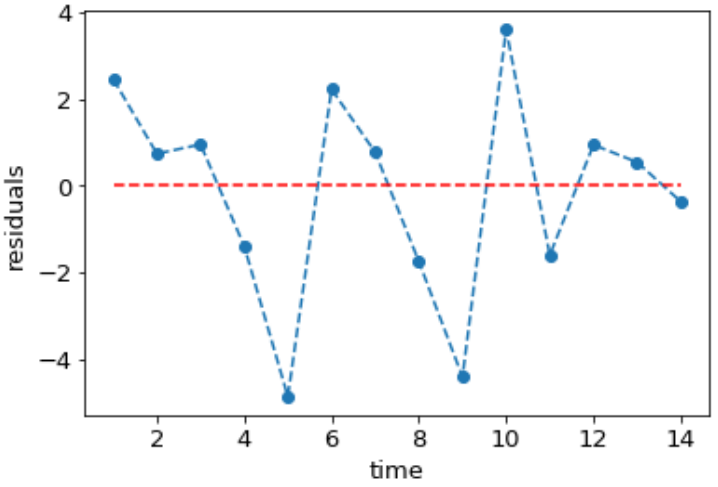
Non-linear models - Evaluating the fit

You can calculate the Residuals and make diagnostic plots.

```
#calculate and plot the residuals
yp=mymodel(x,*popt)
residuals = y - yp

fig1, ax1=plt.subplots()
ax1.plot(x, residuals,'o--')

#make and plot a line y=0
ax1.plot(x,np.zeros(x.size),'--r')
ax1.set_xlabel('time')
ax1.set_ylabel('residuals')
```



"good" fit: values are distributed randomly around 0, and there is no cluster of values all positive or all negative.

Non-linear models - Calculating standard errors of the parameters

The covariance matrix is:

```
print(pcov)
[[ 7.07224351e-05 -2.08093101e-06]
 [-2.08093101e-06  6.14351150e-08]]
```

To calculate the standard error for each parameter, we calculate the square root of the diagonal elements of the covariance matrix.

```
perr = np.sqrt(np.diag(pcov))
print(perr)
[0.00840966 0.00024786]
```

```
print("a=%.4f std_err=%.4f" %(popt[0],perr[0]))
print("b=%.4f std_err=%.4f" %(popt[1],perr[1]))
a=2.4965 std_err=0.0084
b=0.5989 std_err=0.0002
```

The estimated parameters are:

a=2.4965±0.0084

b=0.5989±0.0002

Make predictions

We can calculate how many bacteria are expected after 15 hours.

```
xpred=15
ypred=mymodel(xpred,*popt)

ax.plot(xpred,ypred,'dg', label='prediction')
ax.legend()

plt.show()
```