Activity – fitting a non-linear model

In this exercise you will replicate a Nonlinear Least Square Regression analysis performed by the NIST, the National Institute of Standards and Technology (NIST), which is one of the US oldest physical science laboratories, specialized in advancing measurement science, standards, and technology.

The data provided in **Chwirut1.txt**, are the result of a NIST study involving ultrasonic calibration. Here more information.

Below are reported some information on the data set, the fitting model and procedure, and certified parameters.

```
Procedure:      Nonlinear Least Squares Regression

Description:    These data are the result of a NIST study involving
                ultrasonic calibration.  The response variable is
                ultrasonic response, and the predictor variable is
                metal distance.

Data:           1 Response Variable  (y = ultrasonic response)
                1 Predictor Variable (x = metal distance)
                214 Observations

Model:          Exponential Class
                3 Parameters (b1 to b3)

                y = exp[-b1*x]/(b2+b3*x)


      Starting values

  b1 =   1.9027818370E-01
  b2 =   6.1314004477E-03
  b3 =   1.0530908399E-02



Parameter                 Certified Values
                  Estimate                    Std. Error
     b1        1.9027818370E-01        2.1938557035E-02
     b2        6.1314004477E-03        3.4500025051E-04
     b3        1.0530908399E-02        7.9281847748E-04

Sum of Squares Residuals          2.3844771393E+03
```

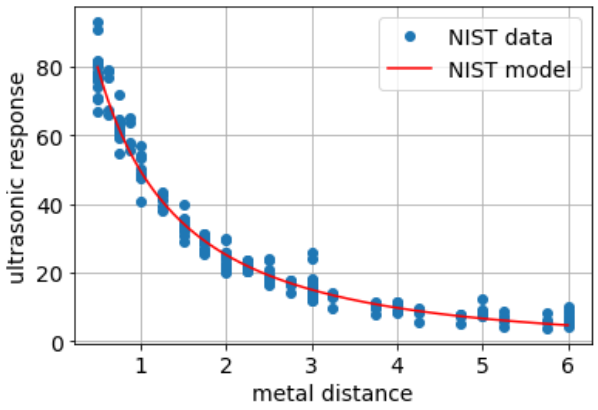
In a script called **A22-nist.py** do the following:

Use NumPy, Matplotlib, and SciPy for fitting.

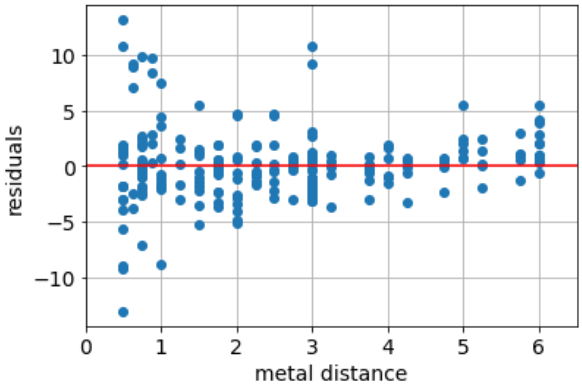
Q1 Create the variables x and y, to store the data for the metal distance and ultrasonic response, respectively, for the fit. Use NumPy.loadtxt() only one time.

Q2 Fit the data to estimate the fitting parameters, b1, b2 and b3. Use the *Starting Values* reported above, as initial guess.

Q3 Plot the data and the model. Label the axis, make the legend, set font size to 14figure size to (6,4) and add the grid to match the graph below. You should smooth the model line by increasing the number of points in the x axis.



Q4 Plot the residuals vs the x data (metal distance).
Then write in a comment line – use triple double quotes - the reason why this model is a good model, based on the residuals.



Q5 Calculate the Sum of Squares Residuals and print to screen this formatted output:

```
Sum of Squares Residuals 2.38448e+03
```

Q6 Print to screen the fitted parameters:

```
[0.19027818 0.0061314  0.01053091]
```

Q7 Calculate the standard errors of the fitted parameters and store them in a variable. Print it to screen.

```
[0.02193856 0.000345   0.00079282]
```

Q8 Write the fitted parameters and their standard errors in a file called **results.csv.** The file should contain the following:

```
# b1,b2,b3
1.9028e-01,6.1314e-03,1.0531e-02
2.1939e-02,3.4500e-04,7.9282e-04
```

Use NumPy savetxt().
Hint: stack the two 1D arrays to make a 2D array.
Use the header parameter of savetxt() to make the header line of the file.

Submit A22-NIST.py to A22.