Advanced Model Fitting and Plotting in Python

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February 29, 2020

1 Introduction

In this Computational Physics Report we take a deeper look into the concept of Least-Square Fitting. The Least-Sqaure line appears when we try to come up with a model for a certain phenomena or observation. The process of fitting a line of least squares is achieved by comparing the models values with the actual observed value and then trying to minimize the variations between the two, This is known as "curve fitting". The measure of how well a least-square fits its actual data is called the "chi square" value.

2 Aim

To fit linear and non linear models to data containing uncertainties

3 Theory

The chi value is given by

$$X^2 = \Sigma_{i=0}^{N-1} \frac{(y_i - f(t_i : [p]))^2}{u_i^2}$$

where i runs over the data points (N of them), y_i is the value of the data at t_i and $f(t_i; [p])$ is the model value which depends on ti and a set of parameters [p].

$$\frac{(y_i - f(t_i; [p]))^2}{u_i}$$

is known as the weight least squares.

The Levenberg - Marquardt algorithm will be used to minimized the chi square and the determine the parameters of that will optimize our best fit.

For the purpose of this report we are consider the the position as a function of time for an under-damped oscillator which can be modeled as :

$$y(t) = A + Be^{-\gamma t} cos(\omega t - \alpha)$$

4 Data

Pyhton can provide 'best fit' values for the parameters of our model, this is procedure of 'Curve Fitting'. In the the figure 1 these values are shown with the corresponding uncertainty for each parameter.

	Parameter	Best Fit value	Uncertainty of Parameter (+/-)
0	A	0.28379	0.000064
1	B	-0.028149	0.000247
2	gamma	0.281214	0.004608
3	omega	21.462276	0.004662
4	alpha	3.470977	0.0008869

Figure 1: Fitted parameters with 68 % C.I.

After acquiring these values it is necessary to think about how well these values 'blend' with each other. To do this the correlation matrix is used.This specialized matrix displays the the correlation coefficients between variables.

	A	B	gamma	omega	alpha
A	1				
B	0.00039	1			
gamma	0.002733	-0.77047	1		
omega	-0.04291	0.023301	-0.01492	1	
alpha	-0.04432	0.032423	-0.02329	0.774365	1

Figure 2: Correlation Matrix of Under-Damped Oscillator

Only half of the correlation is displayed as it is symmetric about the main diagonal.

5 Results

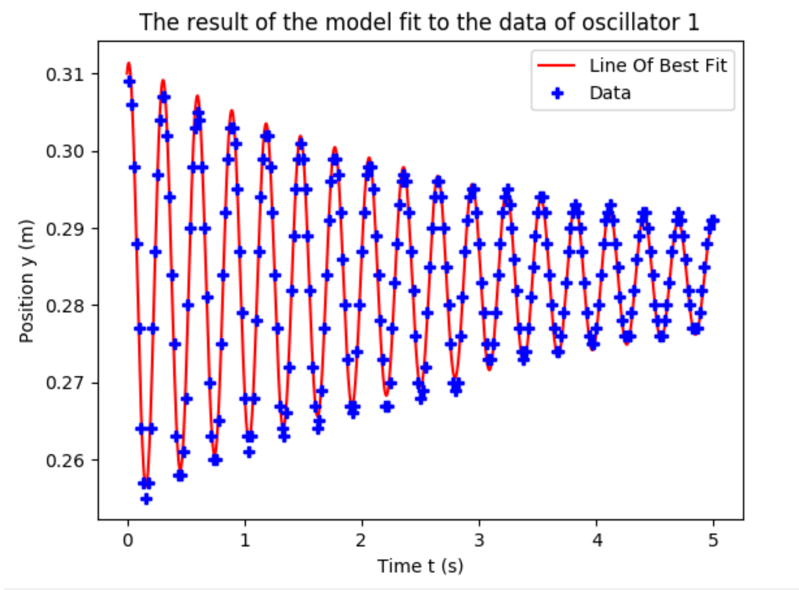

Figure 3: Weighted Model Fitted To Oscillator Data

Variable	Value
Chi squares	252.731847
No. of Degrees of Freedom (dof)	245
Chi square per dof	1.031558559
m	0.0037
c	0.282508

Figure 4: Calculated Values

6 Conclusion

The best fit parameters are A = 0.288379 ± 0.000064, B = -0.028149 ± 0.000247, $\gamma = 0.281214 \pm 0.004662, \omega = 21.462276 \pm 0.004662, \alpha = 3.470977 \pm$

0.0008869. It safe to assume that these parameters are appropriate as the value of Chi square per dof is approximately one (= 1.037558559). Additionally a rather good correlation and anti-correlation can be observed from the parameters $\alpha \& \omega$ and $\gamma \& B$ respectively.