

# Computational Physics: Model Fitting

## UCT- PHY2004W

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# 1 Introduction

In this Computational Physics Report, we take a deeper look into the concept of Least-Square Fitting. The Least-Square line appears when we try to come up with a model for a certain phenomenon or observation. The process of fitting a line of least squares is achieved by comparing the model's 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 nonlinear models to data containing uncertainties

## 3 Theory

The chi value is given by

$$\chi^2 = \sum_{i=0}^{N-1} \frac{(y_i - f(t_i; [p]))^2}{u_i^2}$$

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  $t_i$  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 minimize the chi-square and determine the parameters that will optimize our best fit.

For the purpose of this report we are consider 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

Python can provide 'best fit' values for the parameters of our model, this is a procedure of 'Curve Fitting'. In 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 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

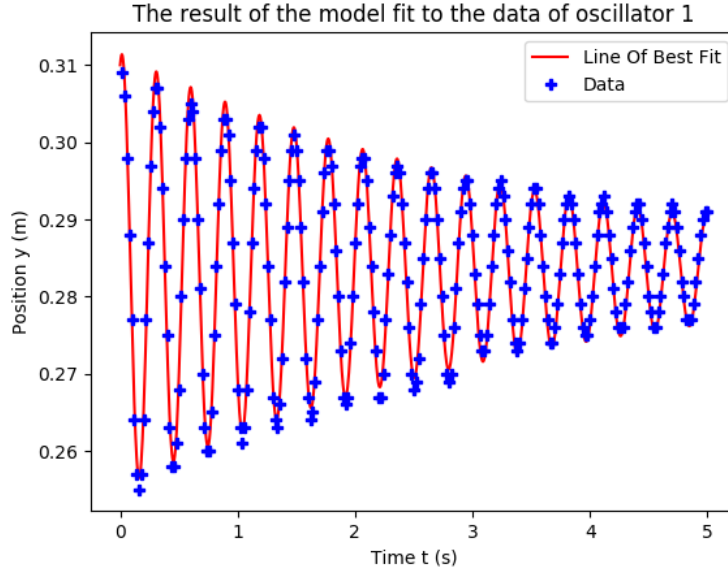


Figure 3: Weighted Model Fitted To Oscillator Data

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  $A = 0.288379 \pm 0.000064$ ,  $B = -0.028149 \pm 0.000247$ ,  $\gamma = 0.281214 \pm 0.004662$ ,  $\omega = 21.462276 \pm 0.004662$ ,  $\alpha = 3.470977 \pm$

0.0008869. It is 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.