

SH2774 Numerical Methods in Nuclear Engineering

Project: Non-Linear Model Fitting

Aurora Jahan

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Abstract

This project focuses on the application of the Newton-Raphson method to perform non-linear least squares model fitting on power oscillations data from an accidental event that occurred in Oscarshamn-2 at a boiling water reactor in 1999.

The project begins with an exploration of linear least-squares problems and concepts such as the Pearson correlation coefficient, RMSE (Root Mean Square Error), RMSN (Root Mean Square Normalized), and CoD (Coefficient of Determination) to evaluate the performance of the fitted models. Then the project explores the Newton-Raphson method and its use in non-linear least square model fitting. Armed with the insights gained from these studies, the project progresses onto the main objective: to fit a non-linear model to the experimental power oscillation data.

First, the experimental data is preprocessed to remove a linear trend and to scale it with an appropriate scaling factor. Then its time evolution characteristics are examined in order to select an appropriate non-linear model- an exponentially decaying cosine function with four independent parameters. Analytical calculations are performed to obtain initial guesses for the parameters. Finally, the Newton-Raphson method is utilized to fit the non-linear model to the preprocessed data. To assess the quality of the fitted model, the decay ratio and RMSE are computed which provide insights into the model's capability to capture the dynamics of the power oscillations.

Keywords- Non-linear model fitting, least squares, Newton-Raphson method, power oscillations, Oscarshamn-2.

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Chapter 1

Introduction

Non-linear least squares model fitting is a powerful technique used in various fields of science and engineering to find the optimal parameters for a non-linear model that best describes a given set of data. Unlike linear least squares, which deals with linear relationships between variables, non-linear least squares allows for more flexible modeling of complex phenomena where the relationship between variables is non-linear. This method has proven to be particularly valuable in applications ranging from physics and chemistry to economics and data analysis.

In this project, we delve into the realm of non-linear least squares model fitting by applying it to power oscillation data from an accidental event that occurred in Oscarshamn-2, a boiling water reactor, in 1999. Power oscillations refer to fluctuations in the power output of a nuclear reactor caused by various factors, such as control system dynamics or disturbances in the core. Accurate modeling and understanding of power oscillations are essential for reactor safety and operational efficiency.

1.1 The preparatory work

Exploration of linear least squares model fitting

Our exploration began with a study of Cramer's rule, a simple but powerful mathematical tool that allows us to solve linear least-squares problems for small-scale systems. Additionally, we studied different performance evaluation metrics such as the Pearson correlation coefficient, RMSE, RMSN, and CoD. These metrics enabled us to quantitatively assess the quality of our fitted models and compare different models' performances.

Exploration of the Newton-Raphson method for non-linear least squares model fitting

To address non-linear least squares problems involving multidimensional overdetermined systems, we introduce the Newton-Raphson method. It is a powerful iterative algorithm that updates the parameter estimates based on the gradients of the model's objective function. By repeatedly refining the parameter values, the method converges towards an optimal solution that minimizes the sum of squared residuals between the model predictions and the actual data.

Initially, we studied the use of Newton-Raphson method in 2-parameter, 2-equation linear systems. Afterward, we also studied its usage in overdetermined systems involving more than 2 parameters.

1.2 The project

Fitting an appropriate non-linear model to the power oscillations data from the Oscarshamn-2 accidental event

We were provided with the power oscillation data from the Oscarshamn-2 reactor accident. This accidental event, which took place in 1999, resulted in significant power fluctuations. By analyzing and modeling this data, we aim to gain insights into the dynamics of the event and develop a fitting model that accurately captures the underlying behavior of the power oscillations.

First, we preprocessed the power oscillations data obtained from the accidental event in Oscarshamn-2. Preprocessing plays a crucial role in preparing the data for subsequent analysis and model fitting. We removed a linear trend from the raw data, scaled it up by a factor of the standard deviation, and adjusted the time scale to start from 0 seconds.

Next, we observed the time evolution characteristics of the power oscillations data, aiming to gain insights into its behavior and identify any discernible patterns or trends. We noticed that the power oscillation curve resembles a sine or cosine curve whose peaks grow as an exponential function. Thus, we chose an exponentially decaying (or growing, based on the sign of the decay constant) cosine function as our non-linear model. This function adequately encompasses the growth of the power oscillations over time by accurately capturing the interplay between the growing behavior and periodicity present in the power oscillations. Our chosen model involved four independent parameters- a constant coefficient a , the decay constant γ , the angular frequency ω , and the phase shift ϕ .

Then we analytically calculated initial guesses for the parameter values. These initial estimates provided a starting point for the iterative process of refining the parameter values to achieve the best fit between the model predictions and the preprocessed data.

Finally, we applied the Newton-Raphson algorithm to find the optimal values of the independent parameters. Upon finding our desired results, we evaluated the performance of our fitted model by calculating the decay ratio and the RMSE (Root Mean Square Error). The decay ratio provides insights into the rate at which the power oscillations grow over time, indicating the instability of the system. On the other hand, the RMSE quantifies the overall discrepancy between the model predictions and the observed data, allowing us to assess the accuracy of the fitted model. These evaluations provide valuable insights into the model's ability to replicate the underlying dynamics of the accidental event in Oscarshamn-2.

1.3 Organization of the report

Due to nature of the prompt for the project, the author has decided to divide the project into two major parts: preparatory work and the actual project work. Firstly, chapter 1 introduces the project. Then the theory, methodology, and results of the preparatory work is presented in chapter 2. Chapter 3 deals with the theory and methodology of the actual project while chapter 4 presents the results of the project. Lastly, chapter 5 includes a comprehensive discussion on the project.

Chapter 2

Theory, methodology, and results of the preparatory work (assignments 1 to 6 and 8)

2.1 Assignment 1: learning the Cramer's rule

Square of the total residuals can be written as-

$$R^2 = \sum_{i=1}^N (\alpha_0 + \alpha_1 x_i - y_i)^2$$

We can get our two equations by finding the minima of this equation w.r.t α_0 and α_1 , i.e. taking the derivatives of this equation with respect to α_0 and α_1 respectively and equating them to 0.

$$N\alpha_0 + \alpha_1 \sum x = \sum y \quad (2.1)$$

$$\alpha_0 \sum x + \alpha_1 \sum x^2 = \sum xy \quad (2.2)$$

If we put these two equations in a matrix form, we get

$$\begin{pmatrix} N & \sum x \\ \sum x & \sum x^2 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} \sum y \\ \sum xy \end{pmatrix} \quad (2.3)$$

Using the Cramer's rule, we can easily find

$$\alpha_1 = \frac{\begin{vmatrix} N & \sum y \\ \sum x & \sum xy \end{vmatrix}}{\begin{vmatrix} N & \sum x \\ \sum x & \sum x^2 \end{vmatrix}}$$
$$\Rightarrow \alpha_1 = \frac{N\sum xy - \sum x \sum y}{N\sum x^2 - (\sum x)^2}$$

And from here, we can find α_0 .

$$\alpha_0 = \frac{\sum y \sum x^2 - \sum x \sum xy}{N\sum x^2 - (\sum x)^2}$$

2.2 Assignment 2: solving a simple overdetermined system

Part a

Let us write down the simplest overdetermined system.

$$\begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

Part b

The normal equation is

$$\begin{aligned} A^T A \alpha &= A^T b \\ \Rightarrow \begin{pmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} &= \begin{pmatrix} 1 & 1 & 1 \\ x_1 & x_2 & x_3 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix} \\ \Rightarrow \begin{pmatrix} 3 & x_1 + x_2 + x_3 \\ x_1 + x_2 + x_3 & x_1^2 + x_2^2 + x_3^2 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} &= \begin{pmatrix} y_1 + y_2 + y_3 \\ y_1 x_1 + y_2 x_2 + y_3 x_3 \end{pmatrix} \\ \Rightarrow \begin{pmatrix} N & \sum x \\ \sum x & \sum x^2 \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} &= \begin{pmatrix} \sum y \\ \sum xy \end{pmatrix} \end{aligned}$$

So, the normal equation is the same as the equation found in assignment 1 (equation 2.3).

Part c

If we divide each side of the normal equation by N, we obtain

$$\begin{pmatrix} 1 & \bar{x} \\ \bar{x} & \overline{x^2} \end{pmatrix} \begin{pmatrix} \alpha_0 \\ \alpha_1 \end{pmatrix} = \begin{pmatrix} \bar{y} \\ \overline{xy} \end{pmatrix}$$

Part d

Using the Cramer's rule, we can easily find

$$\alpha_1 = \frac{\begin{vmatrix} 1 & \bar{y} \\ \bar{x} & \overline{xy} \end{vmatrix}}{\begin{vmatrix} 1 & \bar{x} \\ \bar{x} & \overline{x^2} \end{vmatrix}}$$

$$\Rightarrow \alpha_1 = \frac{\overline{xy} - \bar{x}\bar{y}}{\overline{x^2} - \bar{x}^2}$$

$$\Rightarrow \alpha_1 = \frac{\rho S_y}{S_x}$$

Part e

Using the first line of the normal equation and the value of α_1 , we can find

$$\alpha_0 = \bar{y} - \bar{x}\alpha_1$$

$$\Rightarrow \alpha_0 = \frac{\overline{x^2}\bar{y} - \bar{x}\overline{xy}}{S_x^2}$$

2.3 Assignment 3: fitting a linear model to a linear problem

Part a

We use the expressions for α_0 and α_1 that we previously found to calculate the values.

$$\alpha_0 = 11.395$$

$$\alpha_1 = 0.03$$

Part b

We plotted the regression line together with the experimental data in the same graph.

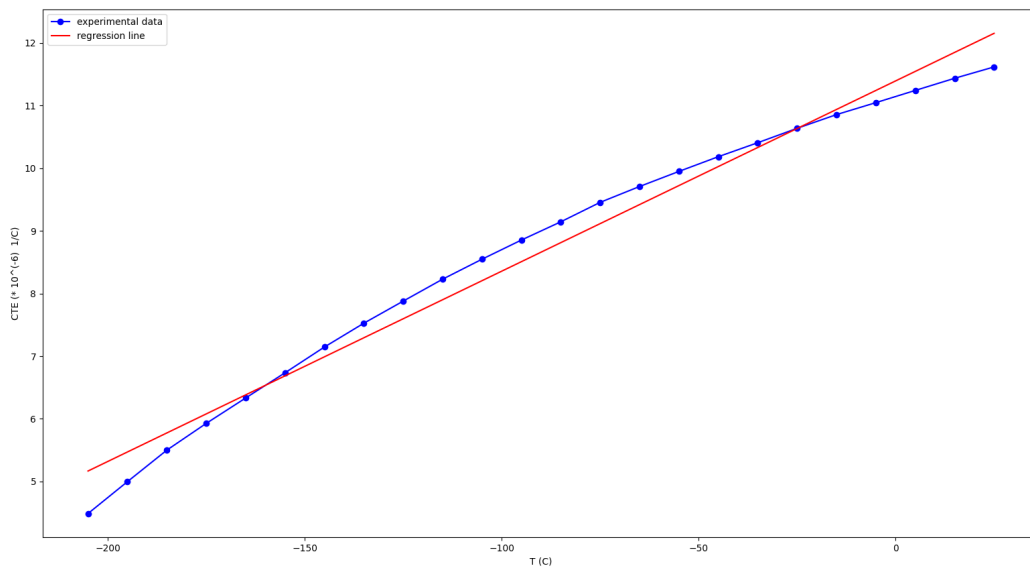


Figure 2.1: The regression line together with the experimental data.

Part c

We determined how well the regression line predicts the CTE coefficient by evaluating the following

$$\text{Pearson correlation coefficient} = \sqrt{\text{CoD}} = 0.989$$

$$\text{RMSE} = 0.308$$

$$\text{RMSN} = 0.145$$

$$\text{CoD} = 0.979$$

2.4 Assignment 4: fitting a linear model to a non-linear problem

Part a

We plotted the scattered data y vs r .

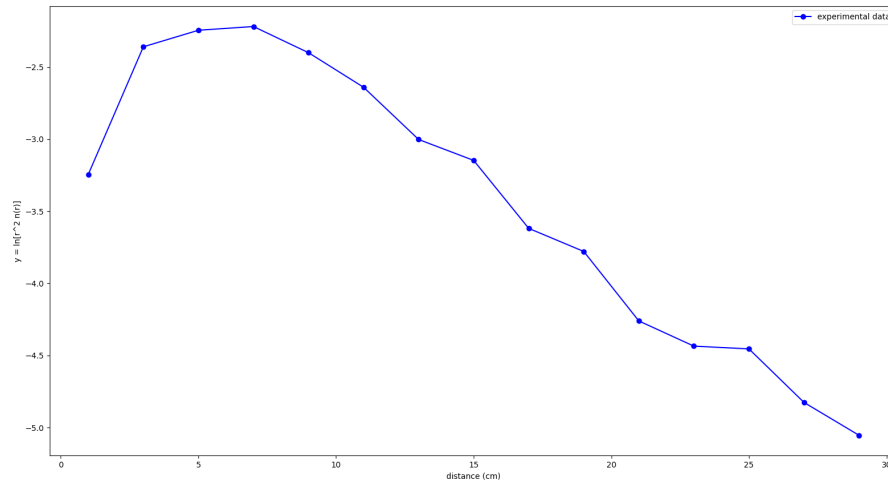


Figure 2.2: Scattered data containing outliers.

Part b

We identified that the first two data points do not agree with the linear trend. Thus we considered them to be outliers and eliminated them. Then plotted the scattered data y vs r again.

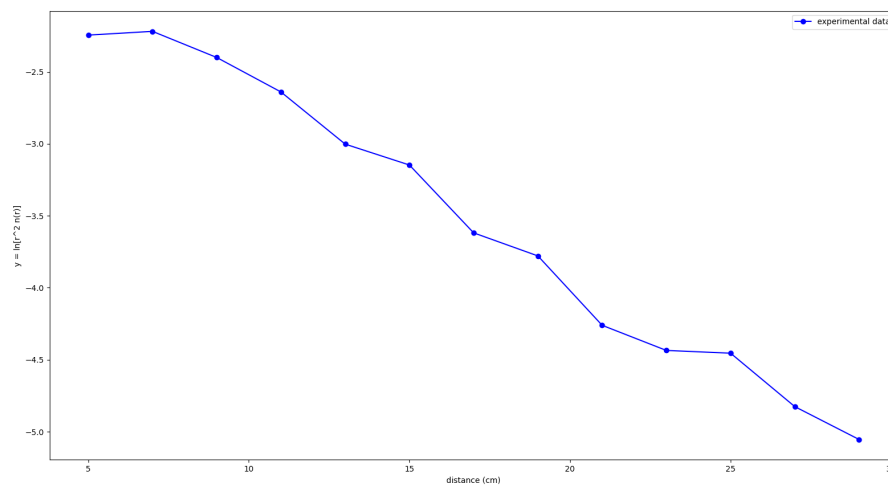


Figure 2.3: Scattered data without the outliers.

Part c

The coefficients of the regression line are

$$\alpha_0 = -1.366$$

$$\alpha_1 = -0.128$$

Part d

We can write

$$y = \ln A - \frac{r}{\lambda}$$

From here, we can identify that

$$\alpha_1 = -\frac{1}{\lambda}$$

$$\Rightarrow \lambda = 7.803$$

Part e

We plotted the regression line together with the filtered data in the same graph.

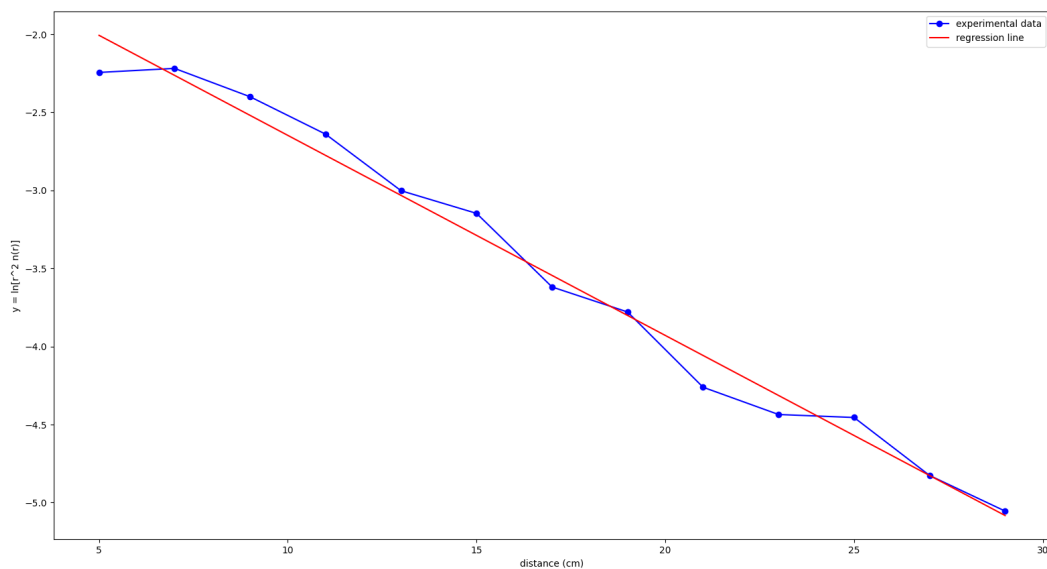


Figure 2.4: The regression line together with the filtered data.

Part f

We determined how well the regression line represents the quantity y by evaluating the following

$$\text{Pearson correlation coefficient} = \sqrt{\text{CoD}} = 0.992$$

$$\text{RMSE} = 0.120$$

$$\text{RMSN} = 0.125$$

$$\text{CoD} = 0.984$$

2.5 Assignment 5: Newton-Raphson method for 2 variables

Part a

We plotted the two curves determined by the two equations.

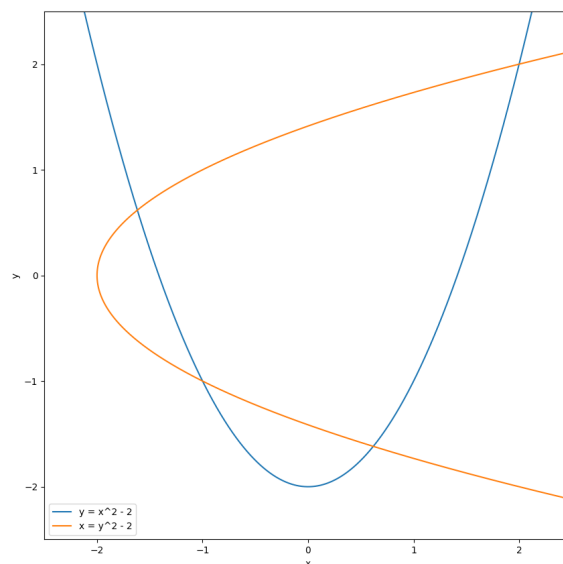


Figure 2.5: The two curves determined by the two equations.

Part b

We conjectured that two obvious solutions would be $(-1, -1)$ and $(2, 2)$. It is simple to show that they are correct.

$$\begin{aligned}(-1)^2 - 2 &= -1 \\ \text{and } 2^2 - 2 &= 2\end{aligned}$$

Part c

First, we analytically obtained the following

$$\begin{aligned}f_1 &= x^2 - y - 2 ; \partial_x f_1 = 2x ; \partial_y f_1 = -1 \\ f_2 &= y^2 - x - 2 ; \partial_x f_2 = -1 ; \partial_y f_2 = 2y\end{aligned}$$

Next, we wrote a computer program to solve the following iterative scheme

$$\begin{pmatrix} \partial_x f_1^{(k)} & \partial_y f_1^{(k)} \\ \partial_x f_2^{(k)} & \partial_y f_2^{(k)} \end{pmatrix} \begin{pmatrix} \Delta x^{(k)} \\ \Delta y^{(k)} \end{pmatrix} = - \begin{pmatrix} f_1^{(k)} \\ f_2^{(k)} \end{pmatrix}$$
$$\begin{pmatrix} x^{(k+1)} \\ y^{(k+1)} \end{pmatrix} = \begin{pmatrix} x^{(k)} \\ y^{(k)} \end{pmatrix} + \begin{pmatrix} \Delta x^{(k)} \\ \Delta y^{(k)} \end{pmatrix}$$

Part d

We numerically obtained two more solutions: (-1.618, 0.618) and (0.618, -1.618).

Part e

If we start from the initial guesses $x_0 = 0.5$ and $y_0 = 0.5$, the Jacobian matrix becomes a singular matrix and its determinant becomes 0. So the equation cannot be solved in a determinant sense.

2.6 Assignment 6: analytical work in preparation for the project

Part a

The model equation is

$$y(t) = ae^{-\gamma t} \cos(\omega t + \phi)$$

Now, let us first find where the peaks of this equation occurs. Clearly, the equation has an exponentially growing or decaying (depending on the value of γ) amplitude while its periodicity is given by the cosine factor. Thus, we can conclude that even though the value of the peaks will be determined by the exponential factor, the peaks will actually occur when the value of the cosine factor is the highest.

With this hypothesis, we proceed to find the values of t that gives the highest values of the cosine. To that end, we first remember that the highest value of cosine is 1. So, if t_{mn} is the time at which the n -th maxima occurs, we can write

$$\begin{aligned} \cos(\omega t_{mn} + \phi) &= 1 \\ \implies \omega t_{mn} + \phi &= 2n\pi \\ \implies t_{mn} &= \frac{2n\pi - \phi}{\omega} \end{aligned}$$

Now, it is simple to calculate the decay ratio.

$$\begin{aligned} \frac{a_2}{a_1} &= \frac{e^{-\gamma t_{m2}}}{e^{-\gamma t_{m1}}} \\ \implies \text{DR} &= e^{-\frac{2\pi\gamma}{\omega}} = e^{-\gamma T} \end{aligned}$$

where T is the time period.

Part b

To calculate the phase difference ϕ , we again use the time when the peaks occur. We know that at such time instances, we will have

$$\begin{aligned} \omega t_{mn} + \phi &= 2n\pi \\ \implies \phi &= 2n\pi - \omega t_{mn} \\ \implies \phi &= 2\pi(n - \frac{t_{mn}}{T}) \end{aligned}$$

2.7 Assignment 8: analytical work on the Jacobian matrix

We analytically calculated the first row corresponding to $i = 1$, $t = 230$ seconds.

$$\partial_a f_1(\alpha) = e^{-230\gamma} \cos(230\omega + \phi)$$

$$\partial_\gamma f_1(\alpha) = -230ae^{-230\gamma} \cos(230\omega + \phi)$$

$$\partial_\omega f_1(\alpha) = -230ae^{-230\gamma} \sin(230\omega + \phi)$$

$$\partial_\phi f_1(\alpha) = -ae^{-230\gamma} \sin(230\omega + \phi)$$

Chapter 3

Theory and methodology of the project (assignments 7, 9, and 10)

3.1 Assignment 7: preprocessing the experimental data

We began by removing a linear rising trend from the data. Then we rescaled the de-trended data by the standard deviation. We also readjust the time axis so that the data began from 0 seconds. Finally, we plotted the raw data and the preprocessed data.

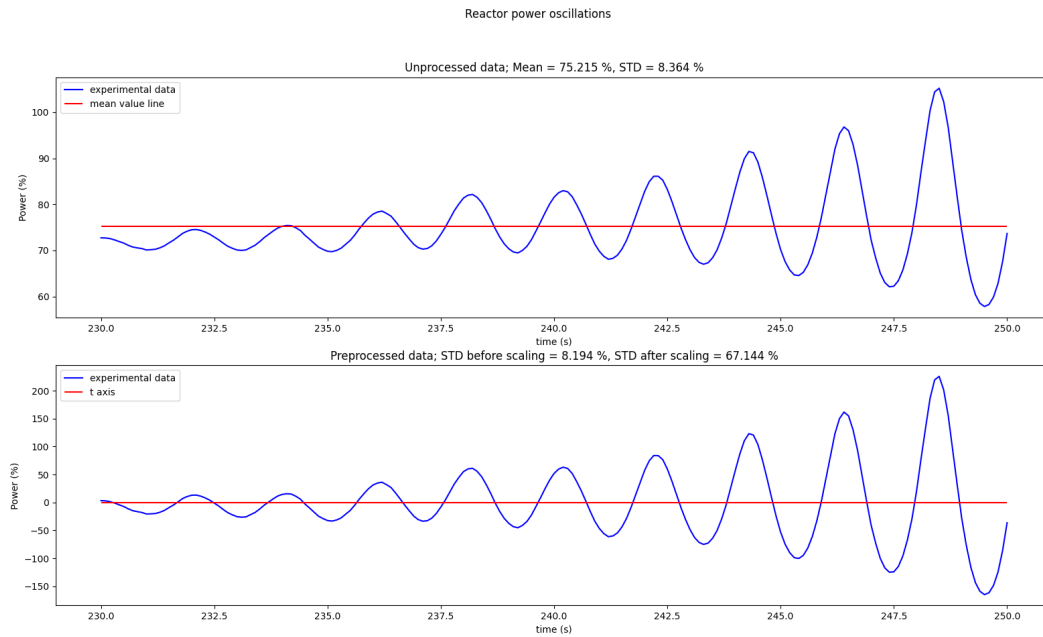


Figure 3.1: The raw data and the preprocessed data along with the mean and the standard deviation values.

3.2 Choosing an appropriate non-linear model function

First, we observed the time evolution characteristics of the power oscillations.

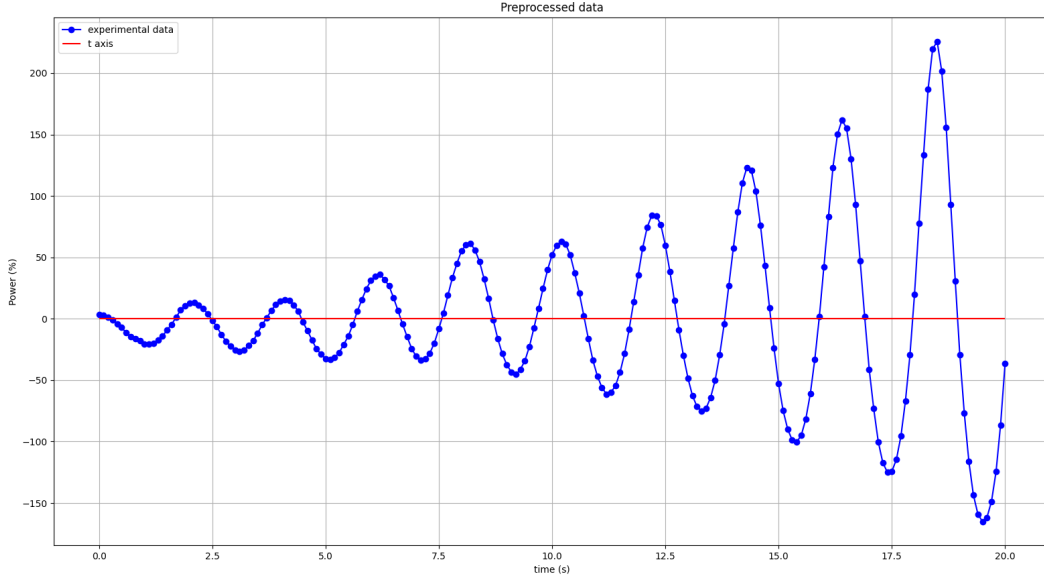


Figure 3.2: Time evolution characteristics of the power oscillations.

Here, we can identify that the preprocessed data has a general tendency to oscillate like a sinusoidal function but the amplitude of this function grows exponentially with time. Thus, we conclude that a function of the following form would be appropriate to model this power oscillation behavior

$$f(t) = ae^{-\gamma t} \cos(\omega t + \phi)$$

In this model, the exponential factor provides the growing tendency of the oscillation peaks while the cosine factor provides the periodicity. The model has four independent parameters: a , a constant coefficient to scale the function up (or down, depending on the final outcome) to the appropriate magnitude, the decay constant γ , the angular frequency ω , and the phase difference ϕ . From our previous studies, we identified that we can use the Newton-Raphson method for an overdetermined system to find the optimal values of these parameters.

3.3 Assignment 9: calculating the initial guesses of the optimal parameters

Part a

We plotted the preprocessed data along with the grid lines

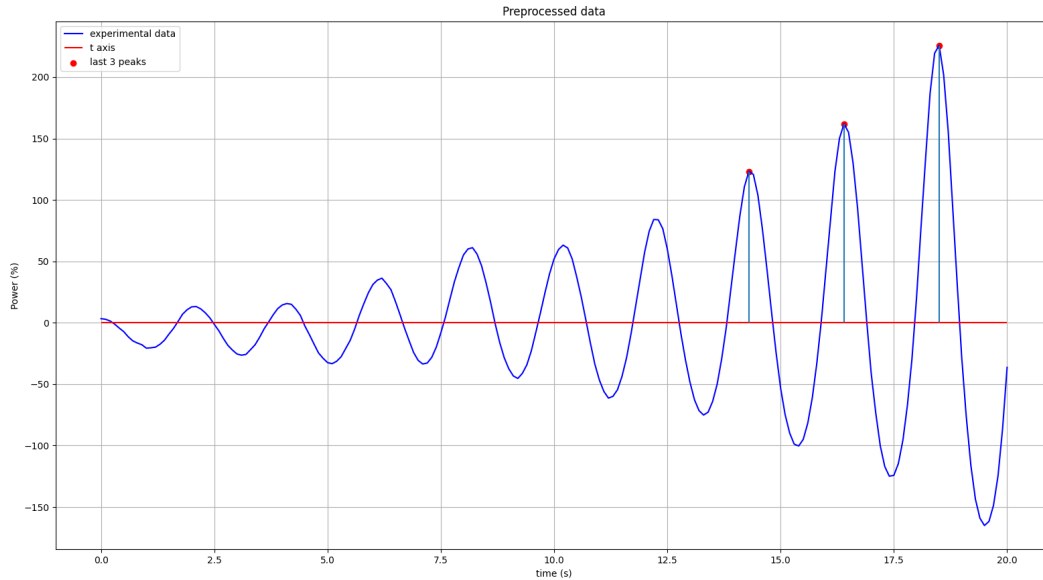


Figure 3.3: The preprocessed data along with the grid lines.

Part b

We found the last 3 successive peaks. Then we calculated the following

$$T = 2.1 \text{ s}$$

$$\text{FR} = 0.476 \text{ s}^{-1}$$

$$\omega = 2.992 \text{ rad s}^{-1}$$

Part c

We calculated the last 3 peaks.

$$p_1 = 123.266 \text{ \% power}$$

$$p_2 = 161.956 \text{ \% power}$$

$$p_3 = 225.87 \text{ \% power}$$

Then we calculated the decay ratios.

$$\text{DR}_1 = 1.314$$

$$\text{DR}_2 = 1.395$$

$$\text{DR}_3 = 1.354$$

Part d

We calculated the decay constant γ .

$$\gamma = -\text{FR} \times \ln(\text{DR})$$

$$\implies \gamma = -0.144 \text{ s}^{-1}$$

We also estimated $a = 15.472 \%$ power.

Part e

Finally, we estimated the phase difference, ϕ .

$$\phi_1 = 1.197 \text{ rad}$$

$$\phi_2 = 1.197 \text{ rad}$$

$$\phi_3 = 1.197 \text{ rad}$$

3.4 Assignment 10: Fitting the model to the experimental data

We first analytically obtained the following

$$\begin{aligned}
 f_i &= ae^{-\gamma t_i} \cos(\omega t_i + \phi) \\
 \partial_a f_i &= e^{-\gamma t_i} \cos(\omega t_i + \phi) \\
 \partial_\gamma f_i &= -t_i a e^{-\gamma t_i} \cos(\omega t_i + \phi) \\
 \partial_\omega f_i &= -t_i a e^{-\gamma t_i} \sin(\omega t_i + \phi) \\
 \partial_\phi f_i &= -a e^{-\gamma t_i} \sin(\omega t_i + \phi)
 \end{aligned}$$

Next, we wrote a computer program to solve the following iterative scheme

$$\begin{pmatrix} \partial_a f_1^{(k)} & \partial_\gamma f_1^{(k)} & \partial_\omega f_1^{(k)} & \partial_\phi f_1^{(k)} \\ \partial_a f_2^{(k)} & \partial_\gamma f_2^{(k)} & \partial_\omega f_2^{(k)} & \partial_\phi f_2^{(k)} \\ \vdots & \vdots & \vdots & \vdots \\ \partial_a f_N^{(k)} & \partial_\gamma f_N^{(k)} & \partial_\omega f_N^{(k)} & \partial_\phi f_N^{(k)} \end{pmatrix} \begin{pmatrix} \Delta a^{(k)} \\ \Delta \gamma^{(k)} \\ \Delta \omega^{(k)} \\ \Delta \phi^{(k)} \end{pmatrix} = - \begin{pmatrix} f_1^{(k)} \\ f_2^{(k)} \\ \vdots \\ f_N^{(k)} \end{pmatrix}$$

$$\begin{pmatrix} \Delta a^{(k+1)} \\ \Delta \gamma^{(k+1)} \\ \Delta \omega^{(k+1)} \\ \Delta \phi^{(k+1)} \end{pmatrix} = \begin{pmatrix} a^{(k)} \\ \gamma^{(k)} \\ \omega^{(k)} \\ \phi^{(k)} \end{pmatrix} + \begin{pmatrix} \Delta a^{(k)} \\ \Delta \gamma^{(k)} \\ \Delta \omega^{(k)} \\ \Delta \phi^{(k)} \end{pmatrix}$$

in a least squares sense. We used the values of a , γ , ω , and ϕ calculated in assignment 9 as the initial guesses.

Chapter 4

Results of the project

4.1 Part a: necessary number of iterations

Our code needed 6 iterations to converge to the predefined accuracy level.

4.2 Part b: optimal values of the independent parameters

From our code, we obtained the following values of the optimal parameters.

Table 4.1: Found values of the optimal parameters up to 6 decimal places

	a	λ	ω	ϕ	DR	RMSE
Guess	15.472000	-0.144000	2.992000	1.197000	1.354000	23.746693
Found	15.586833	-0.131192	3.043562	0.358970	1.311059	12.211063

4.3 Part c: comparison of the fitted model with the experimental data

We plotted the model function along with the de-trended original signal.

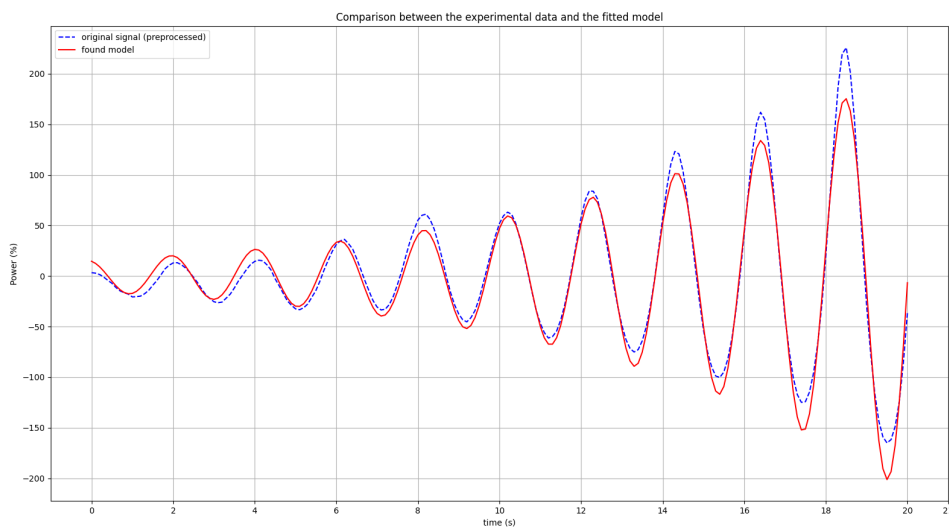


Figure 4.1: The model function along with the de-trended original signal.

Chapter 5

Discussion on the project

In this numerical methods project, through a series of steps involving preprocessing, model selection, parameter estimation, and performance evaluation, we have successfully captured the underlying dynamics of the power oscillations and developed a fitting model that accurately represents the experimental data.

5.1 General discussion

The preprocessing step was crucial in preparing the power oscillations data for analysis. By de-trending the original data of a linear rising behavior, we managed to vastly simplify the complexity of the modeling function. Without this step, we would have had to add a linear function to the model and that would have increased the number of independent parameters by 2. However, after de-trending the experimental data using a built-in function, the magnitude of the oscillations became undesirably low. Thus, we scaled the de-trended data up by a factor of the standard deviation. Additionally, we adjusted the time data to begin from 0 seconds to simplify calculations.

After observing the time evolution characteristics, we gained valuable insights into the behavior of the oscillations. This understanding guided our selection of an exponentially decaying cosine function as the non-linear model to fit the data. This choice was motivated by the exponential growth of the amplitude of oscillations over time, which was a prominent feature in the observed behavior along with a periodic behavior with a cosine factor successfully imitated.

The next step involved analytically calculating initial guesses for the parameters and utilizing the Newton-Raphson method for estimation of the optimal values of these parameters. This method proved to be effective in iteratively refining the parameter values to minimize the sum of squared residuals between the model predictions and the preprocessed data. This iterative process allowed us to converge to an optimal solution that provided the best fit to the observed data.

The evaluation of the performance of our fitted model was carried out by calculating the decay ratio and the RMSE. The decay ratio provided valuable insights into the rate at which the power oscillations decreased over time. By examining this ratio, we could assess the stability and behavior of the system, gaining a deeper understanding of the underlying dynamics. Furthermore, the RMSE served as a comprehensive measure of the overall discrepancy between the model predictions and the experimental data. A low RMSE indicated a close alignment between the model and the observed behavior, validating the effectiveness of our fitted model.

Overall, our project successfully demonstrated the power and utility of non-linear least squares model fitting in capturing complex phenomena such as power oscillations in nuclear reactors. By combining analytical techniques, numerical methods, and data analysis, we were able to develop a fitting model that accurately represented the underlying dynamics.

5.2 Limitations

It is important to acknowledge the limitations and assumptions of our project. The accuracy and reliability of the fitted model are contingent on the quality of the experimental data. Factors such as measurement errors, system noise, and unaccounted external influences can introduce uncertainties. Furthermore, the choice of the specific non-linear model and the initial guesses for the parameters may have inherent biases and limitations.

5.3 Future work

To enhance the robustness of our model and address these limitations, future work could involve incorporating additional data sources, refining the model structure, and considering alternative optimization algorithms. Additionally, conducting sensitivity analyses and uncertainty quantification would provide a more comprehensive understanding of the model's performance and reliability.