

# SOLVING NONLINEAR LEAST-SQUARES REGRESSION PROBLEM THROUGH DIFFERENT PARADIGMS

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**Abstract** – This paper shows different methods for solving a nonlinear regression problem. The same dataset with 250 observations of a nonlinear SISO (single input, single output) system is used for the following methods: least-squares regressor by parts,  $k$ th order polynomial regressor, Mamdani fuzzy system, and 0-order Takagi-Sugeno fuzzy system. All models are analyzed via  $R^2$  for different hyperparameters (polynomial order, number of intervals, etc...). The best solutions' residues and scatter plots are analyzed and discussed.

**Keywords** – Nonlinear regression problem, Mamdani fuzzy system, Takagi-Sugeno fuzzy system, polynomial regressor, regression by parts.

## I. Least-Squares by parts

The Least-Squares (LS) method is an approximation technique for overdetermined systems that aims to minimize the squared value of the residuals. Such systems are characterized by having more equations than variables and are easily found in practice.

Consider the example of a discrete-time SISO system, where  $x_n, y_n \in \mathbb{R}$  are, respectively, its input and output values at the instant  $n \in \{1, 2, \dots, N\}$ . At each instant, one has an equation where the input and output are related through a set of  $k$  parameters,  $\theta \in \mathbb{R}^k$ . Mathematically, one can define the output variable as

$$y_n = f(x_n; \theta) \quad (1)$$

When  $f(\cdot)$  is a linear function, the LS problem is commonly called Ordinary Least-Square (OLS). The least-squares method aims to minimize the following cost function

$$J(\hat{\theta}) = \sum_{n=1}^N e_n^2, \quad (2)$$

where  $\hat{y}_n$  and  $\hat{\theta}$  are the estimates of  $y_n$  and  $\theta$ , respectively, and  $e_n = y_n - \hat{y}_n$ . Although the OLS method has no optimality associated with it, various practical problems, such as regression analysis, can be solved via OLS since no probabilistic assumptions need to be made about the data.

The linear regressor of the SISO system can be expressed as

$$\hat{y}_n = f(x_n; \hat{\theta}) = \hat{a}x_n + \hat{b}, \quad (3)$$

where  $\hat{\theta} = [\hat{a} \ \hat{b}]^T$ . By using the Equation (3), we can

rewrite the cost function as

$$J(\hat{\theta}) = \sum_{n=1}^N (y_n - \hat{a}x_n - \hat{b})^2. \quad (4)$$

The Equation (4) describes a convex function whose surface is a hyperparaboloid. The minimum value of the cost function corresponds to the set of coefficients sought. By calculating the derivative of  $J(\hat{\theta})$  with respect to  $\hat{a}$  and  $\hat{b}$ , we get

$$\frac{\partial J(\hat{\theta})}{\partial \hat{a}} = -2 \sum_{n=1}^N x_n (\hat{y}_n - \hat{a}x_n - \hat{b}) = 0 \quad (5)$$

and

$$\frac{\partial J(\hat{\theta})}{\partial \hat{b}} = -2 \sum_{n=1}^N (\hat{y}_n - \hat{a}x_n - \hat{b}) = 0, \quad (6)$$

respectively. The solution of this system of equations is given by

$$\hat{a} = \frac{\hat{\sigma}_{xy}}{\hat{\sigma}_x^2} \quad (7)$$

and

$$\hat{b} = \hat{\mu}_y - \hat{a}\hat{\mu}_x, \quad (8)$$

where  $\mu$  and  $\hat{\sigma}^2$  are the sample mean and sample variance with respect to its subscript, respectively, and  $\hat{\sigma}_{xy}$  is the estimate of the covariance of  $x_n$  and  $y_n$ .

Although the solution of the SISO OLS method is rather straightforward, many input-output relationships found in practice have nonlinearities. In these cases, one can resort to applying a transformation to the data in order to linearize the problem. Another approach is to utilize the OLS method in intervals where the scatter plot behaves approximately linear, yielding a set of linear curves with their respective parameters for each path of the curve. It is also possible to exploit other nonlinear regression methods, such as polynomial regression. The scatter plot of the dataset, shown in Figure 1, suggests that the input-output relationship is severely nonlinear. Nonetheless, there are intervals where the function can be approximated to a linear curve. A natural hyperparameter arises in this approach: the number of intervals considered. The main trade-off is that the more intervals considered, the better the performance of the coefficient of determination tends to be. However, more parameters are needed to characterize the curve. The

best solution is to solve the nonlinear problem with as few parameters as possible.

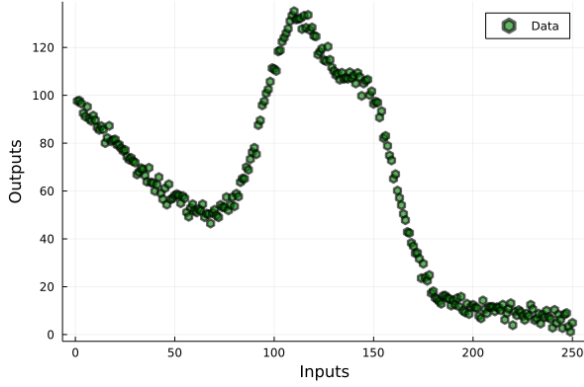


Fig. 1. Scatter plot of the dataset.

In this paper, the OLS algorithm by parts is implemented for different sets of curve intervals,  $\{R_i\}_{i=1}^I$ , where  $I \in \{4, 5, 6\}$  and  $R_i$  is the  $i$ th interval. Since it is obtained the coefficient of determination,  $R^2$ , for each interval, the mean,  $\mu_{R^2}$ , and the variance,  $\sigma_{R^2}^2$ , is analyzed for each configuration. The Figure 2 shows where the delimiters have been placed, in addition to the linear curves obtained by the OLS algorithm. The Algorithm 1 summarizes the behavior of the OLS algorithm by parts, and the Table I shows the performance for each value of  $I$ .

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**Algorithm 1:** OLS algorithm by parts

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**Input:**  $\{x_n\}_{n=1}^N$   
**1 for**  $I \in \{4, 5, 6\}$  **do**  
**2     for**  $i \in \{1, 2, \dots, I\}$  **do**  
**3         for**  $(x_n, y_n) \in R_i$  **do**  
**4** $\hat{\mu}_x \leftarrow \frac{1}{N_i} \sum x_n$   
**5** $\hat{\mu}_y \leftarrow \frac{1}{N_i} \sum y_n$   
**6** $\hat{\sigma}_{xy} \leftarrow \frac{1}{N_i} \sum x_n y_n - \hat{\mu}_x \hat{\mu}_y$   
**7** $\hat{\sigma}_x^2 \leftarrow \frac{1}{N_i} \sum x_n^2 - \hat{\mu}_x^2$   
**8** $\hat{a} \leftarrow \frac{\hat{\sigma}_{xy}}{\hat{\sigma}_x^2}$   
**9** $\hat{b} \leftarrow \hat{\mu}_y - \hat{a} \hat{\mu}_x$

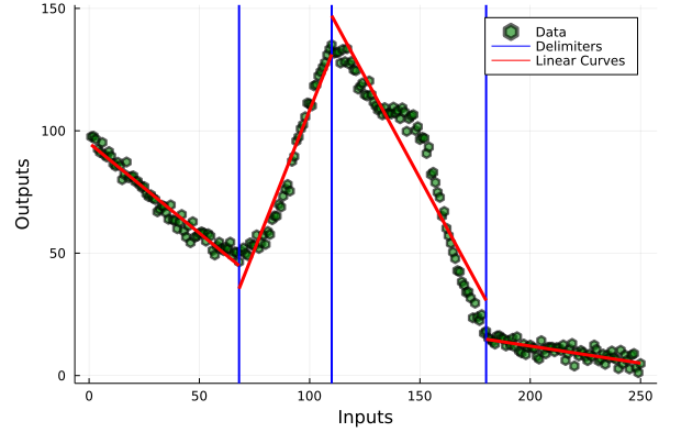
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**TABLE I**  
OLS by parts performance -  $R^2$

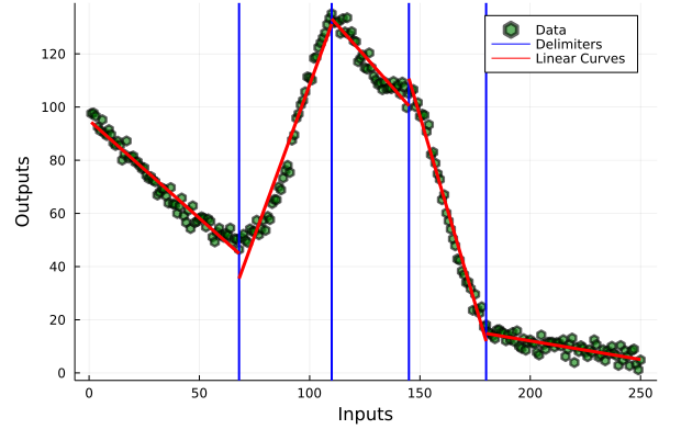
$I$	$i = 1$	$i = 2$	$i = 3$	$i = 4$	$i = 5$	$i = 6$	$\mu_{R^2}$	$\sigma_{R^2}^2$
4	0.962	0.952	0.911	0.627	NaN	NaN	0.863	0.018
<b>5</b>	<b>0.962</b>	<b>0.952</b>	<b>0.895</b>	<b>0.985</b>	<b>0.627</b>	<b>NaN</b>	<b>0.884</b>	<b>0.017</b>
6	0.962	0.952	0.876	0.314	0.985	0.627	0.786	0.059

The best solution is found for  $I = 5$ , highlighted in the Table I. Although it is expected to achieve better performance as it is increased the number of intervals, there are few data in the new interval when  $I = 6$  since it is too short, which decreases  $R^2$ , making it worse when compared with the case where  $I = 5$ .

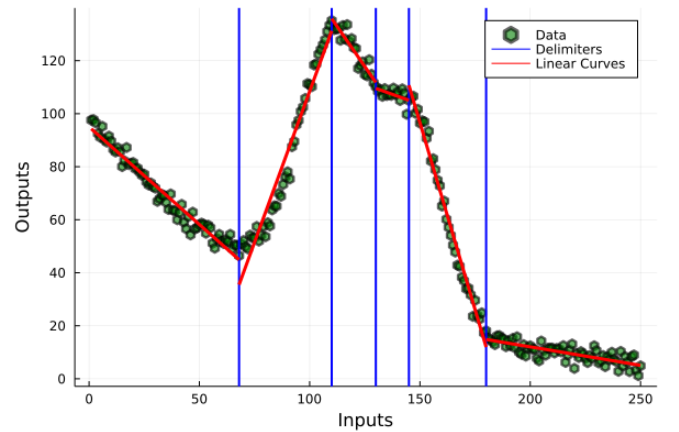
In addition to the regressor performance, one can analyze the distribution of the residuals. Let  $\xi_n$  be the normalized residual value, that is,  $\xi_n = e_n / \sigma_e$ . For a good placement of the intervals, the normalized residual distribution approximates



(a)  $I = 4$



(b)  $I = 5$



(c)  $I = 6$

Fig. 2. The position of the delimiters considered in this article.

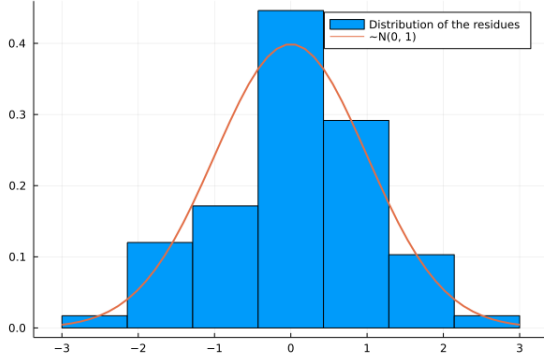


Fig. 3. Distribution of the residuals.

to a zero-mean Gaussian distribution with unitary variance, i.e.,  $\xi_n \sim N(0, 1)$ . The Figure 3 shows the distribution of the residuals along with the Gaussian distribution.

## II. Polynomial Regression

The Polynomial regression is a nonlinear method which extends the concept of the SISO OLS algorithm. At the moment  $n$ , the input  $x_n$  is utilized to generate the tuple  $(h_{n,1}, h_{n,2}, \dots, h_{n,K})$ , where  $h_{n,k} = x_n^k$ ,  $\forall k \in \{1, 2, \dots, K\}$ . Therefore, the SISO model is transformed into a MISO (Multiple Input, Single Output) model, where the  $k$ th input  $x_n$  to the power  $k$ . Note that, albeit this model is not linear with relation to  $x_n$ , it is with relation to  $h_{n,k}$ , i.e.,

$$\begin{aligned} y_n &= f(x_n; \hat{\boldsymbol{\theta}}) = \mathbf{h}_n^T \hat{\boldsymbol{\theta}} \\ &= \hat{\theta}_0 + \hat{\theta}_1 h_{n,1} + \hat{\theta}_2 h_{n,2} + \dots + \hat{\theta}_K h_{n,K}, \end{aligned} \quad (9)$$

where  $\hat{\boldsymbol{\theta}} = [\hat{\theta}_0 \ \hat{\theta}_1 \ \dots \ \hat{\theta}_K]^T \in \mathbb{R}^{K+1}$  and  $\mathbf{h}_n = [1 \ h_{n,1} \ h_{n,2} \ \dots \ h_{n,K}]^T \in \mathbb{R}^{K+1}$ . The matricial notation for all  $N$  observations is given by

$$\hat{\mathbf{y}} = \mathbf{H} \hat{\boldsymbol{\theta}} \quad (10)$$

where  $\mathbf{y} = [y_1 \ y_2 \ \dots \ y_N]^T \in \mathbb{R}^N$  and

$$\mathbf{H} = \begin{bmatrix} 1 & h_{1,1} & h_{1,2} & \dots & h_{1,K} \\ 1 & h_{2,1} & h_{2,2} & \dots & h_{2,K} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & h_{N,1} & h_{N,2} & \dots & h_{N,K} \end{bmatrix} \in \mathbb{R}^{N \times K} \quad (11)$$

The cost function is given by

$$\begin{aligned} J(\hat{\boldsymbol{\theta}}) &= (\mathbf{y} - \mathbf{H} \hat{\boldsymbol{\theta}})^T (\mathbf{y} - \mathbf{H} \hat{\boldsymbol{\theta}}) \\ &= \mathbf{y}^T \mathbf{y} - 2\mathbf{y}^T \mathbf{H} \hat{\boldsymbol{\theta}} + \hat{\boldsymbol{\theta}}^T \mathbf{H}^T \mathbf{H} \hat{\boldsymbol{\theta}} \end{aligned} \quad (12)$$

By differentiating the Equation (12) with respect to  $\hat{\boldsymbol{\theta}}$  and setting its result to zero, we get

$$\begin{aligned} \frac{\partial J(\hat{\boldsymbol{\theta}})}{\partial \hat{\boldsymbol{\theta}}} &= -2\mathbf{H}^T \mathbf{y} + 2\mathbf{H}^T \mathbf{H} \hat{\boldsymbol{\theta}} = 0 \\ \therefore \hat{\boldsymbol{\theta}} &= \mathbf{H}^\dagger \mathbf{y}, \end{aligned} \quad (13)$$

where  $\mathbf{H}^\dagger = (\mathbf{H}^T \mathbf{H})^{-1} \mathbf{H}^T$  is the pseudoinverse of  $\mathbf{H}$ , also called left inverse since  $\mathbf{H}$  is a tall matrix ( $N > K$ ). The fact that  $\mathbf{H}$  is full rank ( $\text{rank}(\mathbf{H}) = K$ ) guarantees the invertibility of  $\mathbf{H}^T \mathbf{H}$  [1].

## III. ORGANIZATION OF THE PAPER

This section presents the main issues for editing the manuscript.

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At the end of these guidelines, there is an example of how the references should be inserted ?, ?, ?, ?, ?, ?, ?.

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On the last page of the paper, the authors should distribute the contents evenly, using both columns, in a way that both end in a parallel manner.

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Tables and figures (drawings or pictures) should be inserted in the text right after they are mentioned for the first time, as long as they fit the size of the columns; if necessary, use the whole page. Figures resolution should be at least 300 dpi and vector files should be preferably used for better print quality. Table captions should be above the tables and figure captions should be below the figures. The tables should have titles and they are designated by the word Table, being numbered in sequence by Roman numerals. Table captions must be centered and in bold.

Figures also need captions and they are designated by Figure in the text (Fig. in the caption itself), numbered with Arabic numerals in a sequenced manner, left- and right-

justified, as shown in the example. The designation of the parts of a figure is done by adding lowercase letters to the numbers of the figures starting with the letter a, e.g. Figure 1(a).

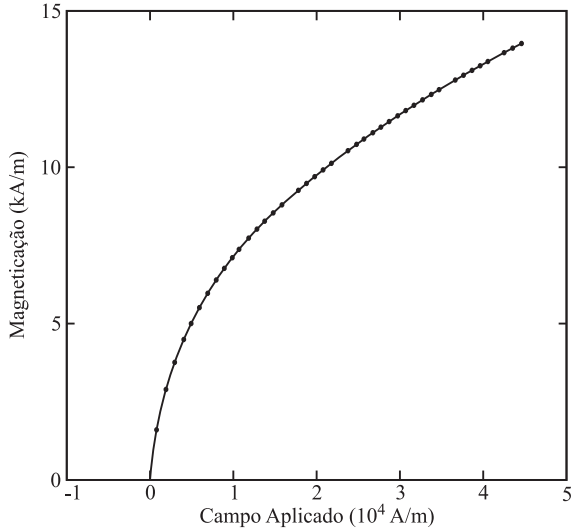


Fig. 4. Magnetization as a function of applied field. (Note that “Fig.” is abbreviated and there is a period after the figure number followed by two spaces.)

To better understand graphs, the definition of their axes should be done with words not letters, except when referring to waveforms and phase planes. The units should be between parentheses. For example, use the denomination “Magnetization (A/m)”, instead of “M (A/m)”.

Figures and tables should be positioned preferably in the beginning or the end of the column, avoiding putting them in the middle. Avoid tables and figures whose sizes exceed the size of the columns. The figures should preferentially be in black, with a white background, since the printed version of the journal is in black and white. Their lines should be thick, so the impression is readable.

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Number equations consecutively with equation numbers in parentheses flush with the right margin, as in (1). The equations should be written in a compact form, centered in the column. If a nomenclature section is not included in the beginning of the text, the quantities should be defined right after the equation, such as:

$$\Delta I_L = I_o + \frac{\sqrt{3}}{2} \frac{V_i}{Z} \quad (14)$$

where:

- $\Delta I_L$  - resonant inductor peak current;
- $I_o$  - load current;
- $V_i$  - source voltage;
- $Z$  - characteristic impedance.

## V. CONCLUSIONS

This paper was fully written in accordance with the guidelines for submissions of papers in English.

## ACKNOWLEDGEMENTS

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## REFERENCES

- [1] G. Strang, G. Strang, G. Strang, G. Strang, *Introduction to linear algebra*, vol. 3, Wellesley-Cambridge Press Wellesley, MA, 1993.