Innovative Journal of Mathematics
v. 1 no. 3, 1-8, (2022)
doi: 10.55059/ijm.2022.1.3/49

ISSN 2790-3370 (print)
ISSN 2790-3389 (online)

Nonlinear models by parameters and their transformation

Research Article

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Abstract: The development of nonlinear models is presented as a need to carry out various researches that cannot be achieved through the linear models. Some of the concepts that will be elaborated are the meaning of the nonlinear regression, the general form of the nonlinear models, the separation of the nonlinear models and some applications of the nonlinear models through SPSS. We will also explain the way of realizing the transformation of the nonlinear models in simpler and more convenient forms of the work.

Keywords: Nonlinear regression • Nonlinear models • Essential linear and nonlinear patterns • Sum of squares of residuals

Received 2022-06-13; Accepted 2022-07-12; Published 2022-07-14

1. Introduction

Solving and analyzing the various problems whether in the business world or even in general, it requires the knowledge of mathematics and for this purpose statistics comes to our aid. Linear models are preferred so that calculations such as hypothesis testing and parameter estimation can be done more easily. The linear model works well in many cases, but in some cases, this is not possible. It cannot be said that the relationship can be best expressed by a linear model. Therefore, it can be decided even more accurately by trying non-linear models as well as linear models. Various estimation methods have been developed in linear and non-linear regression models. The ordinary least squares (OLS) method is one of the most widely used methods in the regression analysis. Therefore, the OLS method plays an important role in teaching the regression analysis.

The purpose of this paper is to elaborate on how through the nonlinear regression we will come to the conclusion about the dependence of two variables for which we cannot reach a more specific conclusion using the linear regression. Nonlinear regression is a statistical method to adapt the nonlinear models to

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types of data sets that have nonlinear relationships between independently and dependent variables. The main advantages of nonlinear models are parsimony, interpretability, and prediction. In general, nonlinear models are capable of accommodating a vast variety of mean functions, although each individual nonlinear model can be less flexible than linear models (i.e., polynomials) in terms of the variety of data they can describe; however, nonlinear models appropriate for a given application can be more parsimonious (i.e., there will be fewer parameters involved) and more easily interpretable. Interpretability comes from the fact that the parameters can be associated with a biologically meaningful process. One problem with nonlinear regression is that it works iteratively: we need to provide initial guesses for model parameters and the algorithm adjusts them step by step, until it (hopefully) converges on the approximate least square's solution. To my experience, providing initial guesses may be troublesome. The use of nonlinear models is more complex, therefore we will explain the transformation into linear models and the use of SPSS statistical program to facilitate work with nonlinear models, respectively realization of nonlinear regression.

2. Materials and Methods

2.1. Nonlinear Regressions

Regression is a statistical measurement used in finance, investment, and other disciplines by performing a set of processes to evaluate the relationship between a dependent variable which that often called the conclusive variable and one or more independent variables often called variables. predictive and as a final result a regression equation is obtained.

The two basic types of regression are linear regression and multiple linear regression. In addition to linear regression in mathematical modeling statistics there are also nonlinear regression methods that are used for more complex data and analysis.

Nonlinear regression is a common form of regression analysis in which the observed data are modeled by a function that is a nonlinear combination of parameters and depends on one or more independent variables.

The use of data will often lead to the construction of a model system led by nonlinear models. The most general class of nonlinear models in parameters allows the mean of the dependent variable to be expressed through some function $f(x_i;\theta)$. The model has the form:

$$y_i = f(x_i;\theta) + \varepsilon_i \qquad (1)$$

where: $f(x_i;\theta)$ is the nonlinear function related to $E(Y)$ of the independent variable,

x_i is the consecutive vector of observations in independent k-variables for the i-observation unit, and

θ vector of i with p-parameters.

Nonlinear models are usually chosen because they are more realistic or because the functional form of the model allows the results to be better specified, and are models for structuring mathematical functions such as exponential, logarithmic, trigonometric, etc.

Nonlinear models are divided into two categories:

i. Essential linear models

ii. Essential nonlinear models

Essential linear models include nonlinear models which can be transformed into linear models by means of appropriate transformations in the dependent variable. An example of essential linear models is:

$$Y = \frac{\theta_0 X}{\theta_1 + X} \tag{2}$$

This model can be transformed into a linear model with simple transformations.

The group of nonlinear essential models includes models that cannot be transformed by simple transformations, but special methods must be used.
Nonlinear models are chosen because they provide better and more realistic approximations but their use is sometimes extremely difficult without the help of statistical program SPSS, programming languages such as PYTHON or R.

Some of these models are:

- Exponential model
- Power model or log-log
- Logistic model
- Weibull model

Let's see the implementation of any of the nonlinear models with the help of the SPSS statistical program.

One of the nonlinear models is the Weibull model which that has the form:

$$Y_i = \alpha \left[1 - e^{-\left(\frac{x_i}{\delta}\right)^{\gamma}}\right] \tag{3}$$

2.2. Transformation of nonlinear models

As mentioned above nonlinear models can be transformed or transformed into linear models by means of corresponding transformations.

The reasons why nonlinear to linear models are transformed are:

1. Simpler relationships are easier to understand and easier to explain
2. In statistical models, models that have fewer parameters are considered simpler
3. Relationships expressed in straight lines are simpler than those expressed in curves
4. Finally, linear models in parameters are considered simpler than nonlinear models

Some nonlinear models can be transformed with simple conversions while some may not be so easily transformed.

The purpose of the transformation in this case is to transform the nonlinear model into a form that is linear with parameters and for which the principle of smaller squares can be used.

One of the nonlinear models that can be transformed is:

$$y = \theta_0 X^{\theta_1} \tag{4}$$

which is linearized by taking the natural logarithm side by side, and we get:

$$Ln(Y) = Ln(\theta_0 X^{\theta_1}) \tag{5}$$

$$Ln(Y) = Ln(\theta_0) + Ln(X^{\theta_1}) \tag{6}$$

$$Ln(Y) = Ln(\theta_0) + \theta_1 Ln(X) \tag{7}$$

If we receive replacements:

$$Ln(Y) = Y^* \qquad Ln(\theta_0) = {\theta_0}^*; \qquad Ln(X) = X^* \tag{8}$$

We will get the linearized model according to the parametersθ_0 and θ_1 between X^* and Y^*:

$$Y^* = \theta_0 + \theta_1 X^* \tag{9}$$

The evaluation of the parameters is done using the principle of the smallest squares. We now turn to nonlinear models which that cannot be linearized.

Let it:

$$Y_i = f(x_i'; \theta) + \varepsilon_i \tag{10}$$

where ε_i- are independent and each of them has normal distribution with mathematical expectation 0 and variance σ^2, i.e., $N(0, \sigma^2)$.

In these cases, we can rely on some of the principles of smaller squares. The principle of smaller squares is used similarly to linear models to evaluate parameters.

The estimator by the method of the smallest squares for the parameter θ will be denoted by $\hat{\theta}$ and is the solution of the parameters that minimizes the sum of the error squares (residues).

Thus:

$$SER = \sum_{1}^{n} \left[Y_i - f(x_i'; \hat{\theta})\right]^2 \tag{11}$$

Then, the estimator of θ will be:

$$\hat{\theta} = \min_{\theta} S \tag{12}$$

Which we find this way:

First, we find the partial derivatives of SER according to θ, then we equate the partial derivatives with 0 and then the parameters θ_i will be replaced by $\hat{\theta}_i$, that is, normal equations p are obtained.

Every normal equation has this general form:

$$\frac{\partial\{SER\}}{\partial\hat{\theta}_i} = -\sum_{i=1}^{n}\left[Y_i - f(x_i^{'};\hat{\theta})\right]\cdot\frac{\partial f(x_i^{'};\hat{\theta})}{\partial\hat{\theta}_i} \qquad (13)$$

However, the functions to be solved are nonlinear according to the parameters $\hat{\theta}_i$ and are often difficult to solve even in the simplest case, therefore iterative numerical methods are often used.

These methods require initial assumptions, or initial values for the parameters. Initial values are denoted by θ^0. The initial assumptions are substituted instead of θ to calculate the sum of the squares of error (deviation) and to calculate the approximation of θ^0 that reduce or reduce the sum of the squares of error hoping that θ^0 will bring us closer to the solution of the smallest square. New parameter estimates are used to repeat the process until a better approximation is made at each step. If this happens, we say that the process converges to the solution.

With the help of various computer programs such as SPSS, PYTHON, R several methods have been used to find solutions to normal nonlinear equations of error squares and find the most realistic value of parameter estimators and find the regression equation.

3. Results

Assuming that the best approximation for this case is made by the Weibull model find the predicted estimators and write the equation that gives the connection between the suspension of calcium moles depending on time! For this study, an example is taken in which the data of the radioactive amount of calcium (nmol / mg) are given, which amount is related to the suspension of hot calcium over periods of time (minutes). Data were obtained in 27 independent mixtures lasting from 0.45 to 15.00 minutes. The obtained data are given in the following table:

Table 1. Sample data

Nr. Suspension	Time	Calcium (nmol/mg)
1	0.45	0.3417
2	0.45	-0.00438
3	0.45	0.82531
4	1.3	1.77967
5	1.3	0.95384
6	1.3	0.6408
7	2.4	1.75136
8	2.4	1.27497
9	2.4	1.17332
10	4.0	3.12273
11	4.0	2.60858
12	4.0	2.57429
13	6.1	3.17881
14	6.1	3.00782
15	6.1	2.67061

16	8.05	3.05959
17	8.05	3.94321
18	8.05	3.43726
19	11.15	4.80735
20	11.15	3.35583
21	11.15	2.78309
22	13.15	5.13825
23	13.15	4.70274
24	13.15	4.25702
25	15.0	3.60407
26	15.0	4.15029
27	15.0	3.42484

The results show that the equation of the Weibull model examining growth is given:

$$Y_i = \alpha\left[1 - e^{-\left(\frac{X_i}{\delta}\right)^{\gamma}}\right] \tag{14}$$

where in the concrete case Y_i represent the moles of calcium while X_i the time in minutes:

To find the estimators of the parameters α, γ, δ the normal form equation must be minimized:

$$\frac{\partial\{SER\}}{\partial\hat{\theta}_i} = -\sum_{i=1}^{n}\left[Y_i - f(x_i^{\prime};\hat{\theta}\right] \cdot \frac{\partial f\left(x_i^{\prime};\hat{\theta}\right)}{\partial\hat{\theta}_i} \tag{15}$$

Consequently, we have to find the partial derivatives and the obtained equations to be equal to zero and then solve them according to the respective parameters.

Since in this case we will get equations that are difficult to solve so to find the parameter evaluators we will use the statistical program SPSS and we will have:

Table 2. Calculation of assessors in SPSS and iterative method steps

Iteration Number[a]	Residual Sum of Squares	Parameter A	D	G
1.0	61.994	3.900	.500	1.000
1.1	217.338	3.403	1.150	-1.050
1.2	43.448	3.790	.609	.601
2.0	43.448	3.790	.609	.601
2.1	31.843	3.643	.868	.281
3.0	31.843	3.643	.868	.281
3.1	26.570	3.473	1.028	.431
4.0	26.570	3.473	1.028	.431
4.1	19.317	3.358	1.559	.675
5.0	19.317	3.358	1.559	.675
5.1	10.727	3.757	2.916	.837
6.0	10.727	3.757	2.916	.837
6.1	7.613	4.339	4.880	.906
7.0	7.613	4.339	4.880	.906
7.1	7.466	4.260	4.660	1.013
8.0	7.466	4.260	4.660	1.013
8.1	7.463	4.284	4.735	1.015
9.0	7.463	4.284	4.735	1.015
9.1	7.463	4.284	4.733	1.016
10.0	7.463	4.284	4.733	1.016
10.1	7.463	4.284	4.733	1.016

Table 3. Calculation of confidence interval in SPSS

Parameter	Estimate	Std. Error	95% Confidence Interval Lower Bound	Upper Bound
A	4.284	.475	3.304	5.263
D	4.733	1.271	2.109	7.357
G	1.016	.227	.547	1.485

So, from the results of the above table we see that the estimators for the parameters that in SPSS we have taken as A instead of α, G for γ and D for δ then:

$$\hat{\alpha} = 4.284\ ; \qquad \hat{\gamma} = 1.016; \qquad \hat{\delta} = 4.733 \tag{16}$$

These are the most approximate estimators of the parameter 3.12273 that is obtained at the time 4 min in the result of the 10 realizations made.

The confidence intervals for the parameters, and are respectively:

- For $\hat{\alpha}$ is (3.304, 5.265),
- For $\hat{\gamma}$ is (2.109, 7.357)
- For $\hat{\delta}$ is (0.547, 1.485)

Since the deviation of the parameter 3.2273 with the parameter is large, we see that the parameter 3.2273 does not belong to the interval (0.547, 1.485), which is also seen from the standard error which is 0.227.

And finally, the equation that according to Weibull gives the best approximation is:

$$\hat{y} = 4.284\left[1 - e^{-\left(\frac{x_i}{4.733}\right)^{1.016}}\right] \tag{17}$$

From the table above, it can be seen that the standard errors of the parameters are small and this shows that the dependence between the moles of calcium suspension and time is strongly positive (increasing).

4. Conclusion

During the elaboration of the paper the main goal was to clarify as clearly as possible the concepts related to nonlinear regression, nonlinear models and the transformation of nonlinear models.

The findings of our study were carried out in the laboratories of the Faculty of Natural Mathematical Sciences at the University of Tetovo with the students of the chemistry and physics study programs. Since it is the first time dealing with such problems with students from our side, we think that in the future, after the results we will get from another source, we will also make comparisons between them.

Therefore, as it was explained, nonlinear models are much more complex than the cases of linear study and the relations between the error (avoidance) and the independent variable cannot be given with a simple function, because of the complexity there is a need to transform them into linear models with mathematical operations and these models are called essential linear models. We used the statistical program SPSS.

In this study, novelty is introduced in our work because we take a new look at nonlinear regression in testing estimators for parameters and develop new methods to improve its accuracy and predictive ability for a variety of statistical data.

Funding

This study did not receive any specific grant from funding agencies in the public, commercial, or not-for-profit sectors.

Competing Interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Statements and Declarations

No funding was received to assist with the preparation of this manuscript.

Acknowledgements

I would like to express our great appreciation to the team during the planning and development of this research.

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