

Method of mathematical model building with segmented parabolic regression usage

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Abstract

The paper is devoted to the analysis of different techniques of statistical data approximation for the best model building. Three approximation options (single and segmented cases) are investigated using a specific example. The paper presents the exact formula for the best segmented quadric regression. The connection of the segments was performed using Heaviside function. The problem of optimizing the abscissa of the segments connection point was solved to obtain the highest the accuracy of approximation. The advantages of using two-segmented regression are proved in terms of both approximation accuracy and prognostic properties based on the comparative statistical analysis.

Keywords

Approximation, segmented regression, least squares method, choosing the best model, accuracy of approximation

1. Introduction

The choice of the best mathematical becomes the urgent problem of scientific research [1]. The different assumptions can be applied individually or in some combination to perform the choice:

1. The minimum possible quantity of model coefficients for given margin of permissible error.
2. The simple form compatible with a permissible error.
3. Reasonable physical substantiation (derived from some law).
4. The minimum value of maximal deviation.
5. The coincidence with geometrical structure.
6. The minimum variance [2].

The various tools of the theory of the approximation theory are widely used to build mathematical models. Moreover, until the 80s of the twentieth century, Lagrange, Chebyshev and other high-order polynomials were often used. However, at present, when using the least squares method, polynomials above the third order are practically not used.

Recently, foreign researchers apply segmented regression approaches. This regression can contain linear or parabolic segments for data approximation in different ranges.

Regression analysis has become a modern research tool. The variety of methods have been synthesized to produce misleading results for empirical data samples [3].

The simplest model is linear (that contains only one independent variable) of following form

$$\psi = k_0 + k_1\theta + \tau,$$

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where ψ and θ are the dependent and independent variables, k_0 and k_1 are parameters which must be evaluated. Error of evaluation is represented by symbol τ (it tells about the absence of exact dependence between the dependent and independent variables) [3].

In practice, depending on the situation, parabolic, exponential and other types are also used for the construction of regression models.

2. Analysis of literature and problem statement

The analysis of literature [4 – 12] in the field of empirical data processing shows that for modern era of science and technology evolution, sufficient attention is paid to the problems of approximation. However, there are new tasks of optimizing the switching point abscissas between individual subsets of data when using segmented regressions [13 – 36]. These issues are not fully shown in the literature.

The calculation of the optimal values for location of the connection points will increase the approximation accuracy (for example, reduce the standard deviation) and generally improve the predictive properties [19].

This paper concentrates on the important scientific and practical task of empirical data approximation using segmented regression by the ordinary least squares (OLS) with the subsequent calculation of the optimal value of two segments (parabolas) connection point.

Consider the problem statement from a mathematical point of view. Assume that we observed two-dimensional dataset (θ_i, ψ_i) . Let different functions for approximation $\hat{\psi}_i = \Psi_l(\theta_i, \vec{k}_{m,l})$ exist, where $\vec{k}_{m,l}$ is a vector of m parameters for the approximation function, l is a total number of approximation options. Standard deviation σ between real values ψ_i and estimates $\hat{\psi}_i$ can be calculated for each approximation function. In this case, selection of the best model can be carried out according to the following formula

$$l = \inf(u \in N \forall t: \sigma(\Psi_u(\theta_i, \vec{k}_{m,s})) \leq \sigma(\Psi_t(\theta_i, \vec{k}_{m,t}))).$$

3. Polysegmented parabolic regression usage

Let us consider an example of the initial data given in [1]. These data characterize the dependence of the percentage y of defective goods on the percentage x of silicon in steel. The origin data are given in Table 1.

Table 1

Dependence of Percentage ψ of Rails Scrap on the Percentage θ of Silicon in Steel

The Percentage θ of Silicon in Steel	The Percentage ψ of Rails Scrap
0.04	15.38
0.08	7.27
0.12	4.38
0.16	3.16
0.2	2.93
0.24	4.33
0.28	4.99
0.32	8.22

Consider several possible options for building mathematical models, and then carry out comparative statistical analysis to choose the best of them.

1. The usage of quadratic regression.

To build this model, a parabola of the second order as an approximating function was used:

$$\psi(\theta) = k_0 + k_1\theta + k_2\theta^2,$$

where k_0 , k_1 and k_2 are coefficients of parabola.

2. The usage of cubic regression.

To build this model, a parabola of the third order as an approximating function was used:

$$\psi(\theta) = k_0 + k_1\theta + k_2\theta^2 + k_3\theta^3,$$

where k_0, k_1, k_2 and k_3 are coefficients of parabola.

Table 2
Deviations of the Approximated Value from the Empirical

The Percentage θ of Silicon in Steel	Deviations
0.04	1.432
0.08	-1.624
0.12	-0.899
0.16	0.057
0.2	0.564
0.24	1.261
0.28	-0.22
0.32	-0.57

The formulas for unknown coefficients

$$k_0 = \frac{\Delta_1}{\Delta},$$

$$k_1 = \frac{\Delta_2}{\Delta},$$

$$k_2 = \frac{\Delta_3}{\Delta},$$

$$k_3 = \frac{\Delta_4}{\Delta},$$

where

$$\Delta = \det \begin{pmatrix} n & \sum_{i=1}^n \theta_i & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 \\ \sum_{i=1}^n \theta_i & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 \\ \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 \\ \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 & \sum_{i=1}^n \theta_i^6 \end{pmatrix},$$

$$\Delta_1 = \det \begin{pmatrix} \psi_1 & \sum_{i=1}^n \theta_i & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 \\ \psi_2 & \sum_{i=1}^n \theta_i & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 \\ \psi_3 & \sum_{i=1}^n \theta_i & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 \\ \psi_4 & \sum_{i=1}^n \theta_i & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 \end{pmatrix},$$

$$\Delta_2 = \det \begin{pmatrix} \psi_1 & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 \\ \psi_2 & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 \\ \psi_3 & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 \\ \psi_4 & \sum_{i=1}^n \theta_i^2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 \end{pmatrix},$$

$$\Delta_3 = \det \begin{pmatrix} \psi_1 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 \\ \psi_2 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 \\ \psi_3 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 \\ \psi_4 & \sum_{i=1}^n \theta_i^3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 \end{pmatrix},$$

$$\Delta_4 = \det \begin{pmatrix} \psi_1 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 & \sum_{i=1}^n \theta_i^6 \\ \psi_2 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 & \sum_{i=1}^n \theta_i^6 \\ \psi_3 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 & \sum_{i=1}^n \theta_i^6 \\ \psi_4 & \sum_{i=1}^n \theta_i^4 & \sum_{i=1}^n \theta_i^5 & \sum_{i=1}^n \theta_i^6 \end{pmatrix}.$$

The OLS method is implemented to compute the unknown coefficients.

After calculations, the equation of the following form for the data of Table 1 can be obtained:

$$\psi(\theta) = 25.151 - 302.823\theta + 1253\theta^2 - 1487\theta^3.$$

The same equation as the approximating one was chosen in [1].

A graphical representation of the initial data and their approximation using a third order parabola are shown in Fig. 2.

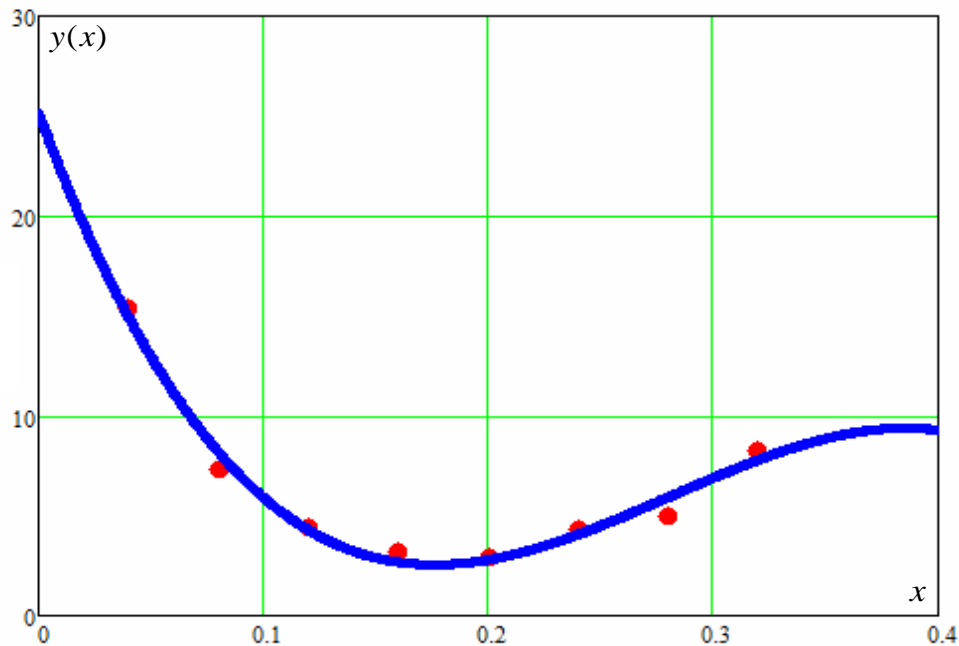


Figure 2: Approximation of empirical data by a parabola of third order

Let us analyze the deviations and variances for this approximation option. The deviation values are given in Table 3.

Table 3
Deviations of the Approximated Value from the Empirical

The Percentage θ of Silicon in Steel	Deviations
0.04	0.433
0.08	-0.911
0.12	0.1
0.16	0.485
0.2	0.135
0.24	0.262
0.28	-0.933
0.32	0.429

The variance is 0.601. The obtained result was a prerequisite for choosing a cubic function as approximating in [1], because variance is 2.5 times less than with quadratic approximation.

According to this article authors opinion, the choice of a cubic function is unsuccessful because this function has a maximum at an abscissa $\theta = 0.385$, and then has a monotone decreasing character. This property of the function does not allow it to be used as a predictor.

Therefore, it is necessary to consider a more rational approximation.

3. The usage of two-segmented parabolic regression.

Alternative option to build mathematical model is usage of two branches of a second order parabola as an approximating function. The equation in this case has the form:

$$\psi(\theta) = k_0 + k_1\theta + k_2\theta^2 + k_3(\theta - \theta_{sw})^2H(\theta - \theta_{sw}),$$

where θ_{sw} is switching (connection) point of parabola segments, $H(\theta - \theta_{sw})$ is Heaviside function.

The formulas for unknown coefficients

$$K = \theta^{-1}\Phi,$$

$$K = (k_0 \ k_1 \ k_2 \ k_3), \quad \Phi = \left(\sum_{i=1}^n \psi_i \sum_{i=1}^n \theta_i \psi_i \sum_{i=1}^n \theta_i^2 \psi_i \sum_{i=i_{sw}}^n (\theta_i - \theta_{sw})^2 \psi_i \right),$$

$$\theta = \left(n \sum_{i=1}^n \theta_i \sum_{i=1}^n \theta_i^2 \sum_{i=i_{sw}}^n (\theta_i - \theta_{sw})^2 \sum_{i=1}^n \theta_i \sum_{i=1}^n \theta_i^2 \sum_{i=1}^n \theta_i^3 \sum_{i=i_{sw}}^n \theta_i (\theta_i - \theta_{sw})^2 \sum_{i=1}^n \theta_i^2 \sum_{i=1}^n \theta_i^3 \sum_{i=1}^n \theta_i^4 \sum_{i=i_{sw}}^n \theta_i^2 (\theta_i - \theta_{sw})^2 \sum_{i=i_{sw}}^n (\theta_i - \theta_{sw})^2 \sum_{i=i_{sw}}^n \theta_i (\theta_i - \theta_{sw})^2 \sum_{i=i_{sw}}^n \theta_i^2 (\theta_i - \theta_{sw})^2 \sum_{i=i_{sw}}^n (\theta_i - \theta_{sw})^4 \right),$$

where i_{sw} is a sample number of order statistic that corresponds to abscissa of switching point.

In case of segmented regression utilization, uncertainty arises. This uncertainty is associated with determining the rational position of the segments switching points. This uncertainty can be eliminated by optimizing the abscissa of the connection points.

To perform optimization for the investigated option of the origin data, the next technique can be used. In this case, the hypothesis is accepted that the true value of the optimal connection point is within a certain interval from which several (for example, five) discrete values are selected. If the optimum abscissa is out of the selected interval, its range must be expanded. For the selected five values of the switching points, the corresponding approximating functions can be computed using the ordinary least squares method.

For initial data of Table 1 the following mathematical models were obtained:

$$\psi(\theta) = 34.554 - 614.629\theta + 3390\theta^2 - 3068(\theta - 0.08)^2 H(\theta - 0.08).$$

$$\psi(\theta) = 29.653 - 432.501\theta + 1897\theta^2 - 1600(\theta - 0.1)^2 H(\theta - 0.1).$$

$$\psi(\theta) = 27.347 - 354.488\theta + 1338\theta^2 - 1074(\theta - 0.12)^2 H(\theta - 0.12).$$

$$\psi(\theta) = 25.769 - 306.487\theta + 1039\theta^2 - 806.268(\theta - 0.14)^2 H(\theta - 0.14).$$

$$\psi(\theta) = 24.673 - 275.853\theta + 866.475\theta^2 - 673.248(\theta - 0.16)^2 H(\theta - 0.16).$$

A visual view of the initial data and their approximation using obtained options of regression are presented in Fig. 3.

For each approximation, standard deviations are calculated. The computation results for the given empirical data are given in Table 4.

The second order parabola approximated the data from the Table 4 in order to find the best value of connection point [31]. The resulting parabola is:

$$\sigma(\theta_{sw}) = 1.350 - 18.069\theta_{sw} + 91.577\theta_{sw}^2.$$

The optimum of calculated parabola corresponds to the best value of abscissa of the switching point $\theta_{sw \text{ opt}} = 0.0991$.

Table 4
Standard Deviations for Different Abscissas of Switching Points

Abscissas of Switching Points	Standard Deviations
0.08	0.501
0.1	0.438
0.12	0.494
0.14	0.644
0.16	0.789

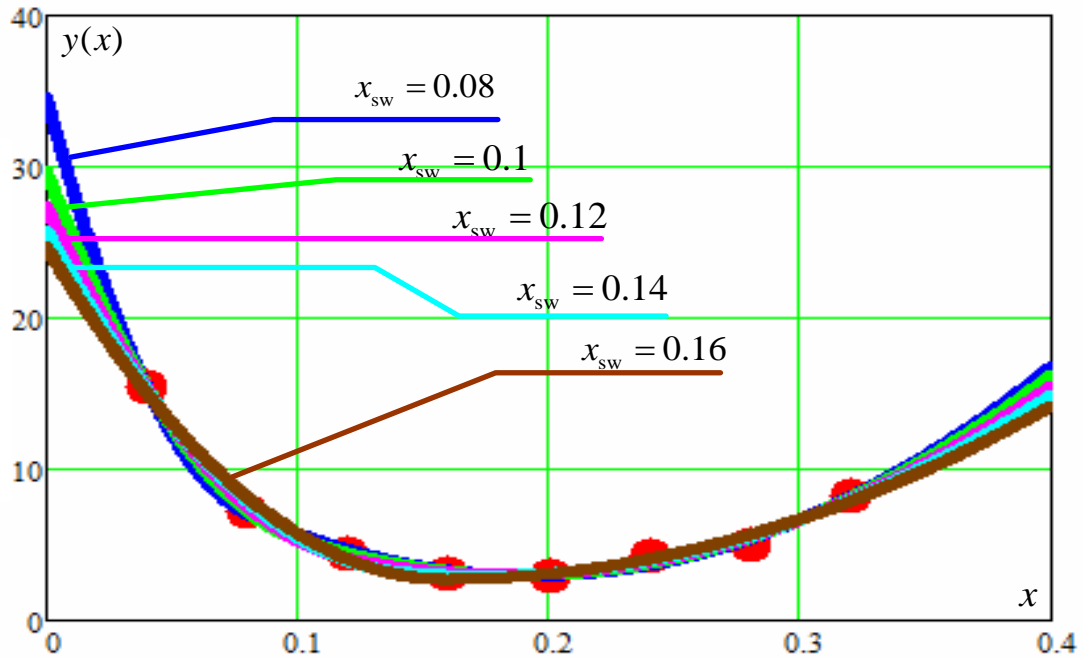


Figure 3: Approximation of empirical data by two-segmented parabolic regression

Then the final formula for optimal two-segmented parabolic regression can be obtained:

$$\psi(\theta) = 24.673 - 275.853\theta + 866.475\theta^2 - 673.248(\theta - 0.0991)^2H(\theta - 0.0991).$$

A visual view of the initial data and their approximation using obtained optimal two-segmented parabolic regression are given in Fig. 4.

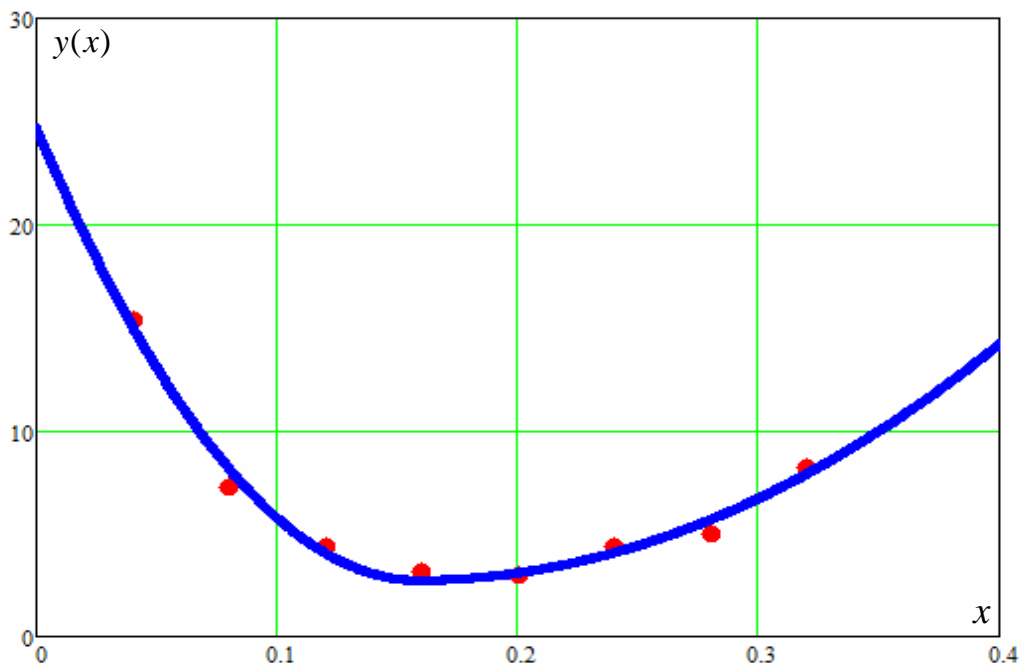


Figure 4: Approximation of empirical data by optimal two-segmented parabolic regression

Let us analyze the deviations and variances for this approximation option. The deviation values are given in Table 5.

Table 5

Deviations of the Approximated Value from the Empirical

The Percentage θ of Silicon in Steel	Deviations
0.04	-0.00926
0.08	0.092
0.12	-0.077
0.16	-0.108
0.2	-0.109
0.24	0.562
0.28	-0.467
0.32	0.116

The variance is 0.195. The criterion for choosing the best approximation is the minimum total variance and the minimum maximum deviation.

As can be seen from the analysis of both the total variances and the maximum deviations, the proposed two-segment parabolic regression increases the accuracy of approximation according to the selected criteria by several times.

4. Conclusion

The paper discusses the tasks of building mathematical models for statistical data using the mathematical apparatus of segmented regression analysis and OLS method. A comparative analysis of three approximation options was performed: using the quadratic and cubic polynomials and the two-segmented parabolic regression.

The analysis showed that the accuracy of approximation using segmented regression increased in three times compared with cubic regression. At the same time, the predictable properties have also improved.

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