

Technical University of Košice
Faculty of Mining, Ecology, Process Control
and Geotechnologies
Student Scientific Conference

Section S2A Control and Logistics

Automatický tvorca predikčných modelov
Automatic prediction model builder

Name::	Bc. Aleš Jandera
Level of study:	II.
Year of study:	2.
Study Programme:	Process control of raw materials and material extraction and processing
Supervisor:	doc. Ing. Tomáš Škovránek, PhD.

Abstract in English

Neural network data classification has been successfully applied to a wide range of data classification problems. This paper presents a Neural Network Data Classification model builder system in the form of an application with a user-friendly user interface. The application is based on a combination of machine learning algorithms with a statistical approaches such as Monte Carlo and Markov chains. The classification of the data is carried out using a machine learning algorithm, which provides the optimal solution for the creation of the prediction model. Application is created in Matlab.

Keywords in English

Mathematic modeling, forecasting, linear prediction, neural network, prediction model builder

Abstract in Slovak

Klasifikácia údajov neurónovej siete bola úspešne aplikovaná na širokú škálu problémov klasifikácie údajov. Táto práca predstavuje systém na tvorbu predikčných modelov vo forme aplikácie s užívateľsky prívetivým užívateľským rozhraním. Aplikácia je založená na kombinácii algoritmov strojového učenia so statistickými metódami ako sú Monte Carlo a Markovove reťazce. Klasifikácia údajov sa vykonáva pomocou algoritmu strojového učenia, ktorý poskytuje optimálne riešenie problému klasifikácie v aplikácii Matlab.

Keywords in Slovak

Matematické modelovanie, predpoved, lineárna predikcia, neurónová sieť

Contents

1	Analysis	1
1.1	Mathematical models for data prediction	1
1.1.1	Regression models	2
1.1.2	Time-series models	2
1.2	Neural networks	3
1.2.1	Classification	7
1.2.2	Activation functions	8
2	Implementation	10
2.1	Mathematical models	10
2.2	Application	10
2.2.1	Dataset import	11
2.2.2	Settings	11
2.2.3	Results	14
	Bibliography	16

List of Figures

1.1	Perceptron preview. [3]	4
1.2	Typical feed-forward neural network composed of three layers. [4]	5
1.3	Illustration of (a) Convolution, (b) Tiled Convolution, (c) Dilated Convolution, and (d) Deconvolution. [5]	5
1.4	Typical recurrent network. [6]	6
1.5	Long short-term memory network. [7]	6
1.6	An autoencoder neural network. [8]	7
1.7	The conditional GAN schema. [9]	7
1.8	Neural network activation functions.	9
2.1	Dataset warning	11
2.2	Manual settings	12
2.3	Automatic settings	13
2.4	Results	14

1 Analysis

1.1 Mathematical models for data prediction

Mathematical prediction models are tools used to forecast the behaviour of a system or process. They are typically built using mathematical equations or algorithms that are designed to describe the relationship between the input and output variables of the system. There are several types of mathematical prediction models, including linear regression, time series analysis, and machine learning algorithms such as neural networks and decision trees. Each type of model has its strengths and weaknesses, and the choice of model depends on the specific problem being addressed.

Linear regression models are used to describe the relationship between two or more variables by fitting a straight line to the data. Time series analysis is used to predict future values of a variable based on its past values, and can be used to forecast trends, seasonal patterns, and other patterns in time series data. Machine learning algorithms are increasingly being used for prediction modelling, as they can learn complex relationships between input and output variables and adapt to changing data patterns. Neural networks, for example, are designed to simulate the structure and function of the human brain and can be used for tasks such as image recognition, natural language processing, and predicting the outcome of events.

Mathematical prediction models are used in a wide range of fields, including finance, economics, engineering, and the natural sciences. They can be used to forecast stock prices, predict the spread of disease, optimise industrial processes, and much more.

1.1.1 Regression models

Regression models are statistical models used to examine the relationship between a dependent variable and one or more independent variables [1]. The goal of regression analysis is to model the relationship between these variables and make predictions about the dependent variable based on the values of the independent variables. Regression models are widely used in many fields, including economics, finance, marketing, and social sciences, to make predictions and understand the relationship between variables. There are several types of regression models, including:

- Linear regression, that uses a linear equation to describe the relation between independent and dependent variables,
- Logistic regression, where the dependent variable is binary, being either 0 or 1,
- Multiple regression is used, when there are multiple independent variables,
- Polynomial regression is used when the relationship between the dependent and independent variables is non-linear.

The choice of regression model depends on the nature of the data and the research question being asked.

1.1.2 Time-series models

Time-series models are mathematical models used to analyse and forecast data that are collected over time [2]. These models are used to study and make predictions about the trends, patterns, and behaviour of the data over time, taking into account historical values and their relationship with the present. Time-series models are widely used in areas such as economics, finance, and weather forecasting, among others. The models are based on various statistical techniques, including ARIMA (AutoRegressive Integrated Moving Average), SARIMA (Seasonal ARIMA), and exponential smoothing, among others. The goal of time-series modelling is to build a mathematical representation of the underlying process that generates the time-series data, allowing for accurate prediction of future values. Time-series models are statistical models used to analyse and make predictions about time-dependent data. They are widely used in various fields, including finance, economics, engineering, and social sciences.

Time-series models make use of past values of a variable to predict future values. They assume that there is a pattern or trend in the data that can be used to forecast future behaviour. Some commonly used time-series models include:

- Autoregressive Integrated Moving Average (ARIMA) is used to analyse and forecast stationary time-series data. It consists of three components: autoregression, differencing, and moving average.
- Seasonal Autoregressive Integrated Moving Average (SARIMA) is an extension of ARIMA that takes into account seasonal patterns in the data.
- Exponential Smoothing (ETS) is used to forecast time-series data that have a trend and/or seasonality. It uses a smoothing parameter to assign more or less weights to past observations based on their recency.
- Vector Autoregression (VAR) is used when there are multiple time-series variables that influence each other. It can be used to analyse the relationships between these variables and to make predictions about their future behaviour.

All these models are valuable tools for analysing and predicting time-series data, but they require careful consideration of the specific characteristics of the data being analysed and the appropriate model to use.

1.2 Neural networks

A neural network is a type of machine learning algorithm inspired by the structure and function of biological neuron in the human brain. It is composed of interconnected nodes, called neurons, that are organised into layers. The input layer receives raw data, such as images or text, and passes it on to the hidden layers, which perform calculations and apply weights to the input data to create a prediction. Finally, the output layer produces the final prediction or classification.

As we can see on image 1.1 each input X_n should be properly weighted by a certain weight W_n before all the signals enter the summation stage. Afterwards, the weighted summation is forwarded into the activation unit producing the neuron's output signal.

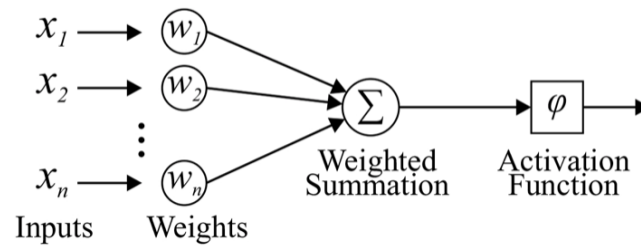


Figure 1.1: Perceptron preview. [3]

Neural networks are trained on large datasets using a process called back-propagation, which adjusts the weights and biases of the neurons to minimise the error between the predicted output and the actual output. Once a neural network has been trained, it can be used to make predictions on new data.

A neuron is a basic building block of a neural network, also known as an artificial neuron or a perceptron. It is modelled based on the biological neuron in the human brain, which receives input signals from other neurons, processes them, and sends output signals to other neurons.

In a neural network, a neuron receives input from other neurons or directly from the input data, applies a mathematical function to the input, and produces an output that is sent to other neurons in the network. The input to a neuron is usually a vector of numbers, and each input is multiplied by a corresponding weight. The neuron then sums up the weighted inputs, adds a bias term, and applies an activation function to the result.

The purpose of the activation function is to introduce nonlinearity into the neuron, which allows the neural network to learn complex patterns and relationships in the data. There are several different types of activation functions that can be used, such as the sigmoid function, ReLU (Rectified Linear Unit) function, and tanh (hyperbolic tangent) function.

The output of a neuron is typically fed into other neurons in the next layer of the neural network. The weights and biases of the neurons are adjusted during the training process using a technique called backpropagation, which involves computing the gradient of the error with respect to the weights and updating them using an optimization algorithm such as stochastic gradient descent.

Feedforward Neural Networks

These are the most basic types of neural networks, where the information flows only in one direction, from input to output. These networks can have one or more

hidden layers and are often used for classification or regression tasks. The schema of a basic feedforward NN is on Fig. 1.2.

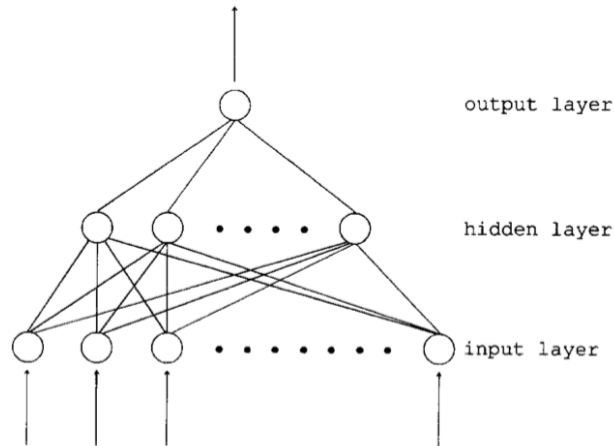


Figure 1.2: Typical feed-forward neural network composed of three layers. [4]

Convolutional Neural Networks (CNNs)

These networks are specialised for processing images and are commonly used in computer vision tasks. They use convolutional layers to extract features from images and can learn to recognise patterns and objects in images see in Fig. 1.3.

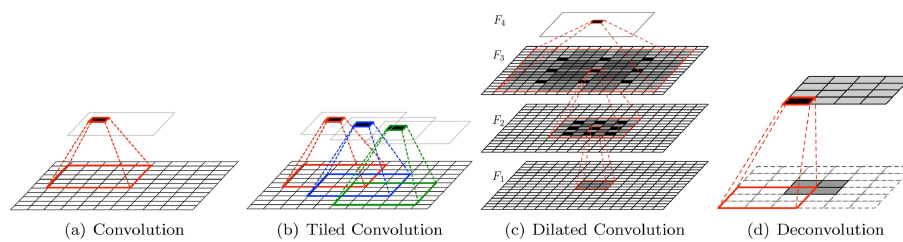


Figure 1.3: Illustration of (a) Convolution, (b) Tiled Convolution, (c) Dilated Convolution, and (d) Deconvolution. [5]

Recurrent Neural Networks (RNNs)

These networks are designed to work with sequential data, such as time-series or natural language data. They have loops that allow information to be passed from one time-step to the next, enabling them to capture temporal dependencies in the data, described on Fig. 1.4.

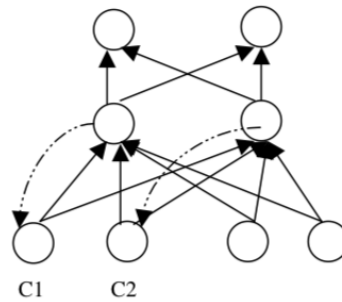


Figure 1.4: Typical recurrent network. [6]

Long Short-Term Memory Networks (LSTMs)

These are a type of RNN that are designed to address the problem of vanishing gradients in traditional RNNs. They use memory cells and gates to selectively retain or forget information over time, making them well-suited for learning from long sequences. As you can see on Fig. 1.5 colour indicates degree of memory activation.

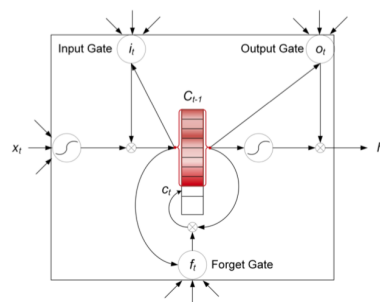


Figure 1.5: Long short-term memory network. [7]

Autoencoder Neural Networks

These networks are used for unsupervised learning and are designed to learn a compressed representation of the input data. As we can see on Fig. 1.6 they consist of an encoder that maps the input data to a compressed representation, and a decoder that maps the compressed representation back to the original data.

Generative Adversarial Networks (GANs)

These networks consist of two networks, a generator and a discriminator (see on Fig. 1.7), that are trained together in a game-theoretic framework. The generator is trained to generate realistic data samples, while the discriminator is trained to distinguish between real and generated data samples.

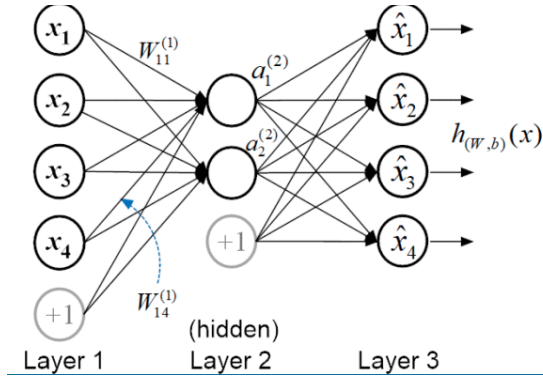


Figure 1.6: An autoencoder neural network. [8]

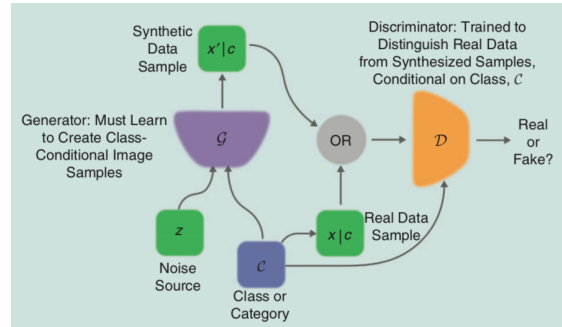


Figure 1.7: The conditional GAN schema. [9]

1.2.1 Classification

Neural network data classification is a technique for categorising data into different classes or categories based on patterns and features present in the data. a neural network is a type of machine learning algorithm that is modelled after the structure and function of the human brain. It is composed of interconnected nodes or neurons that are organised into layers.

In a classification task, the neural network is trained on a dataset that is labeled with the correct class for each example. During training, the network learns to recognize patterns and features in the input data that are associated with each class. The process of training involves adjusting the weights and biases of the neurons in the network to minimise the error between the predicted class and the actual class of each example in the training set.

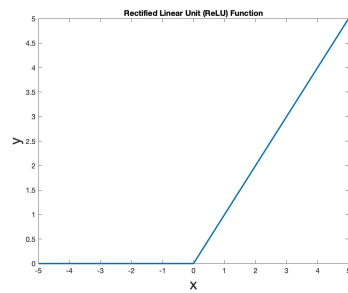
Neural network data classification has been successfully applied to a wide range of tasks, including image classification, speech recognition, natural language processing, and fraud detection, among others [10].

1.2.2 Activation functions

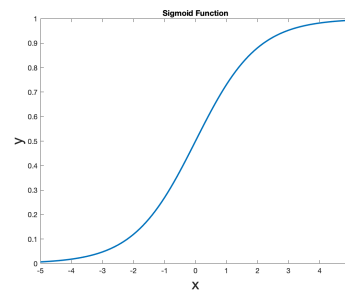
There are several types of activation functions [11] used in neural networks, as we can see on Fig. 1.8 including:

- **Sigmoid Function:** the sigmoid function is a commonly used activation function that maps any input value to a value between 0 and 1. It is typically used in binary classification problems and in the output layer of neural networks that produce probability estimates 1.8b.
- **ReLU (Rectified Linear Unit):** the ReLU function is another popular activation function that maps any input value less than 0 to 0, and any input value greater than or equal to 0 to the input value itself. It is computationally efficient and has been shown to work well in deep neural networks 1.8a.
- **Tanh Function:** the tanh (hyperbolic tangent) function is similar to the sigmoid function, but it maps input values to a range between -1 and 1. It is commonly used in the hidden layers of neural networks 1.8c.
- **Softmax Function:** the softmax function is often used in the output layer of neural networks that produce multi-class classification predictions. It maps the outputs to a probability distribution over the possible classes 1.8d.
- **Leaky ReLU:** the Leaky ReLU function is similar to the ReLU function, but it allows a small, non-zero gradient when the input value is negative. This can help to prevent the "dying ReLU" problem, where some ReLU units become inactive and stop contributing to the network's output 1.8e.
- **ELU (Exponential Linear Unit):** the ELU function is similar to the ReLU function, but it allows negative values to have non-zero outputs. This can help to prevent the "dying ReLU" problem and can improve the performance of deep neural networks 1.8f.

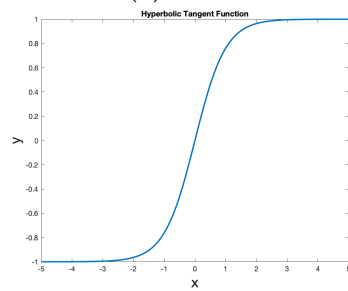
These are some of the most commonly used activation functions in neural networks, but there are many other types of activation functions that have been developed for specific tasks or to address certain problems.



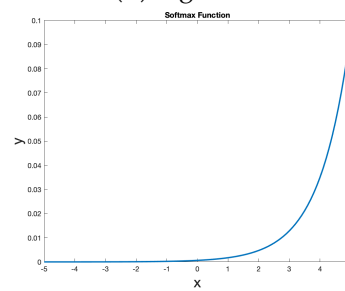
(a) ReLU



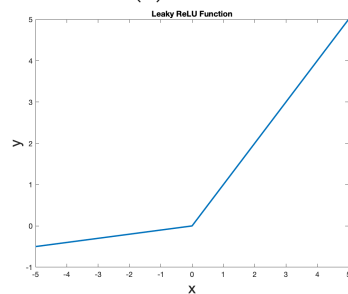
(b) Sigmoid



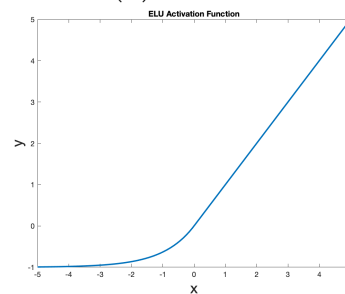
(c) Tanh



(d) Softmax



(e) Leaky ReLU



(f) ELU

Figure 1.8: Neural network activation functions.

2 Implementation

The proposed project is focused on the design and development of the *Automatic prediction model builder system* in the form of an application with an user-friendly interface, implemented in the cloud environment, and that uses all the principles described in 1. As the development environment Matlab ecosystem was used.

2.1 Mathematical models

The implemented prediction models are based mainly on the principle of linear prediction (LP) and its modifications, such as non-integer linear prediction (fractional-order linear prediction - FLP), LP extended by parameters capable of capturing short-term and long-term trendiness in data (extended linear prediction - ELP), etc., that were developed by the author and his supervisor. These approaches are extended by further statistical methods such as Monte Carlo, Markov chains, etc.

For the identification of the appropriate structure of economic and behavioural models and the identification of the parameters of the selected models, machine learning algorithms are used, which provide the optimal solution for the selected data and thus the use-case.

2.2 Application

The developed application makes it possible to easily and accurately predict various socioeconomic macro and micro indicators, such as gross/net domestic/national product, economic wealth, unemployment, inflation, average/minimum wage, purchasing power of the population but also the behaviour of customers (customers can also be perceived as households), intended for sectors such as public or state administration, public planning (but also private) finance, banking.

From the point of view of commercial use, a possible application would be

predicting the number of customers and the number of orders, the company's income, the success of marketing strategies, or based on the prediction, the planning of the warehouse stocks.

2.2.1 Dataset import

To import the dataset to be processed, one has to use the button in the left bottom corner (Fig. 2.2). Application is able to process datasets in *.csv or *.xlsx format. The dataset is firstly checked, if it is of correct format, and in the case of error a warning is shown (Fig. 2.1) with the tips how to format the uploaded dataset.

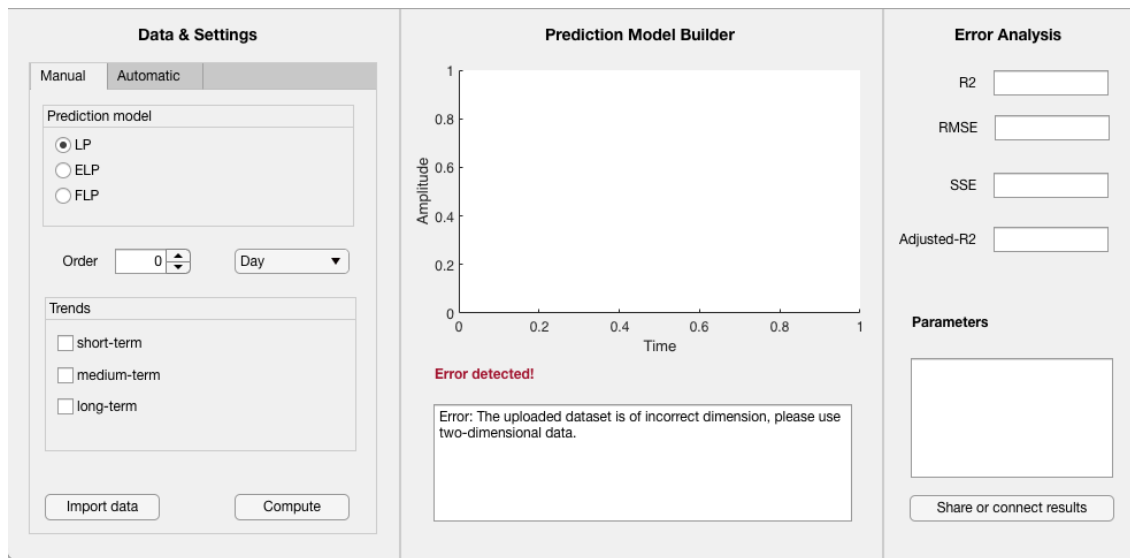


Figure 2.1: Dataset warning

2.2.2 Settings

The developed application has two main possibilities of settings, one can decide to choose a mathematical model and set other related parameters manually (Fig. 2.2), or to choose automatic settings (Fig. 2.3) of application to detect the best prediction model based on uploaded dataset.

Manual settings

In the *Manual settings* environment one is allowed to choose a prediction model (one among three) based on the type of linear prediction and to set two other settings:

- **Prediction models**

One can choose one of three types of linear prediction, *Standard linear predic-*

Figure 2.2: Manual settings

tion 2.1, *Extended linear prediction* 2.2, and *Fractional-order linear prediction* 2.3.

The Standard linear prediction can be defined as:

$$\hat{x}(n) = \sum_{i=1}^p a_i x(n-i), \quad (2.1)$$

where $\hat{x}(n)$ is the predicted value of $x(n)$, p is the order of the predictor, and a_i are the predictor coefficients. The predictor coefficients can be found by minimizing the prediction error.

The Extended linear prediction can be defined as:

$$\hat{x}(n) = \left(\sum_{i=1}^p a_i x(n-i) + \sum_{i=1}^q b_i x(n-S-i) \right) * \gamma(n), \quad (2.2)$$

where $\hat{x}(n)$ is the predicted value of the order at time n , $x(n-i)$ is the past short-term prediction part p samples of the dataset, $x(n-S-i)$ is the past long-term prediction part with seasonal shift S , and a_i and b_i are the predictors coefficients. The order of the predictor is p for short-term and q for the long-term linear prediction. The seasonal weights are represented by $\gamma(n)$.

The Fractional-order linear prediction can be defined as:

$$\hat{x}(n) = \frac{a}{h^\alpha} (x(n-1) - \alpha x(n-2)), \quad (2.3)$$

that uses two-samples memory, is dependent on one parameter a and the order of fractional derivative α CITE T. Skovranek, V. Despotovic and Z.

Peric, "Optimal Fractional Linear Prediction With Restricted Memory," in IEEE Signal Processing Letters, vol. 26, no. 5, pp. 760-764, May 2019, doi: 10.1109/LSP.2019.2908278. .

- **Prediction order**

In this step we are able to set up the order of linear prediction and the period of predicted values.

- **Trends detection**

In this setting you are able to choose the length of the period to identify the prediction model parameters and trends.

Automatic settings

The *Automatic settings* can be used to set up the parameters of neural network, which is used to estimate optimal parameters for prediction. For the set up of

Figure 2.3: Automatic settings

automation part of application we are able to use these parameters:

- **Machine learning cycles**

Number of observations used to find optimal parameters of the model.

- **Machine learning sensitivity**

Sensitivity is a measure of how well a machine learning model can detect positive instances. It is also known as the true positive rate (TPR) or recall.

- **Machine learning algorithms**

In this section we are able to choose the neural network or hidden Markov model to run in background. HMM is statistical approach and in specific dataset can provide better results.

- **Identification criteria**

In this part we can choose the maximisation or minimisation as the criterion to find optimal parameters.

2.2.3 Results

For the test purpose, we used the automatic settings of the application and run the application with the uploaded dataset. Figure 2.4 shows the results of the developed application. Application successfully detects the model equation, identifies

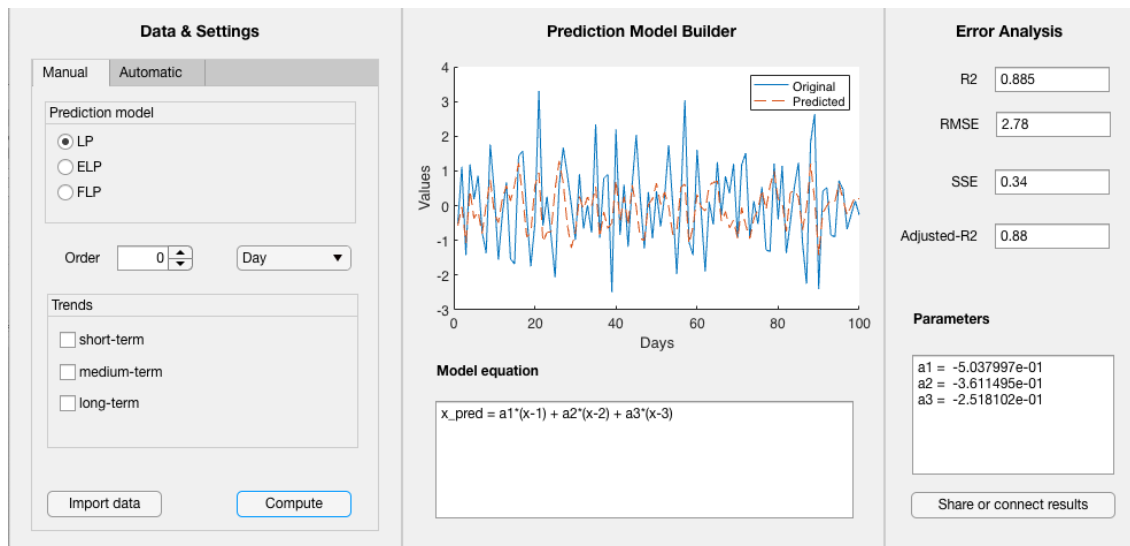


Figure 2.4: Results

optimal parameters and calculates the fitting criteria. Model builder creates the model with $R^2 = 0.885$. The application displays the results in these four sections:

Plot of results

Figure 2.4 shows the main window of the application, where in the middle of the screen the uploaded dataset as well as the modeled fitting-curve are plotted.

Model equation

Under the main section with plotted results, one can find the model equation section, where the mathematical model proposed by the application is shown.

Parameters

In the right bottom corner one can see the parameters of the identified model. When the Model equation and Parameters section are combined, we are able to use the created model in other applications and approaches if necessary.

Error Analysis

The last part of the application is Error Analysis, where we can find the results of the created model. Application provides R^2 , adjusted R^2 , Root Mean Square Error and Sum Squared Error.

Bibliography

1. FAHRMEIR, Ludwig; KNEIB, Thomas; LANG, Stefan; MARX, Brian D. Regression models. In: *Regression: Models, methods and applications*. Springer, 2022, pp. 23–84.
2. CRYER, Jonathan D. *Time series analysis*. Duxbury Press Boston, 1986.
3. MOURGIAS-ALEXANDRIS, G.; TSAKYRIDIS, A.; PASSALIS, N.; TEFAS, A.; VYRSOKINOS, K.; PLEROS, N. An all-optical neuron with sigmoid activation function. *Opt. Express*. 2019, vol. 27, no. 7, pp. 9620–9630. Available from DOI: 10.1364/OE.27.009620.
4. SVOZIL, Karl. Quantum logic. 1997.
5. GU, Jiuxiang et al. Recent advances in convolutional neural networks. *Pattern Recognition*. 2018, vol. 77, pp. 354–377. ISSN 0031-3203. Available from DOI: <https://doi.org/10.1016/j.patcog.2017.10.013>.
6. MEDSKER, Larry R; JAIN, LC. Recurrent neural networks. *Design and Applications*. 2001, vol. 5, pp. 64–67.
7. CHENG, Jianpeng; DONG, Li; LAPATA, Mirella. Long short-term memory-networks for machine reading. *arXiv preprint arXiv:1601.06733*. 2016.
8. LUO, Tie; NAGARAJAN, Sai G. Distributed anomaly detection using autoencoder neural networks in WSN for IoT. In: *2018 IEEE International Conference on Communications (ICC)*. 2018, pp. 1–6.
9. CRESWELL, Antonia; WHITE, Tom; DUMOULIN, Vincent; ARULKUMARAN, Kai; SENGUPTA, Biswa; BHARATH, Anil A. Generative adversarial networks: An overview. *IEEE signal processing magazine*. 2018, vol. 35, no. 1, pp. 53–65.
10. FÉRAUD, Raphael; CLÉROT, Fabrice. A methodology to explain neural network classification. *Neural networks*. 2002, vol. 15, no. 2, pp. 237–246.
11. GÉRON, Aurélien. *Hands-on machine learning with Scikit-Learn, Keras, and TensorFlow*. " O'Reilly Media, Inc.", 2022.