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An improved ANN-based sequential global-local approximation for small medical data analysis

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Abstract

INTRODUCTION: The task of approximation of complex nonlinear dependencies, especially in the case of short datasets, is important in various applied fields of medicine. Global approximation methods describe the generalized behavior of the model, while local methods explain the behavior of the model at specific data points. Global-local approximation combines both approaches, which makes such methods a powerful tool for processing short sets of medical data that can have both broad trends and local variations.
OBJECTIVES: This paper aims to improve the method of sequential obtaining global and local components of the response surface to increase the accuracy of prediction in the case of short sets of medical data.
METHODS: In this paper, the authors presented the method that combined two ANNs: a non-iterative SGTM neural-like structure for obtaining the global component and GRNN as a powerful tool of local approximation in the case of short datasets.
RESULTS: The authors have improved the method of global-local approximation due to the use of a General Regression Neural Network instead of RBF ANN for obtaining the local component, which ensured an increase in the accuracy of the body fat prediction task. The authors optimized the operation of the method and investigated the efficiency of the sequential obtaining global and local components of the response surface in comparison with the efficiency using a number of existing methods.
CONCLUSION: The conducted experimental studies for solving the body fat prediction task showed the high efficiency of using the improved method in comparison with a number of existing methods, including ensemble methods.

Keywords: small data approach, non-iterative training, global-local approximation, GRNN, machine learning, body fat prediction task

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1. Introduction

The task of approximating tabular datasets in medicine remains one of the important tasks during the diagnosis or treatment of a patient, especially in conditions for their partial automation [1,2]. Today, there are many approaches to prediction based on tabular datasets, in particular, using machine learning methods that provide a certain level of accuracy when analyzing such data [3]. However, each of them has several limitations and disadvantages [4]. In particular, linear methods of regression analysis do not

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always provide high prediction accuracy, especially in the case of complex nonlinear relationships inside medical datasets [5,6]. In the vast majority, they include only the global component of the response surface without taking into account the importance of its local component [7,8]. The task of approximation by more complex machine learning methods can take into account the local components of the response surface, but it can be significantly complicated by the available short amount of data for the implementation of training procedures [9]. These circumstances reduce the accuracy, and in some cases make it impossible to perform effective intellectual analysis of such datasets [10]. In addition, in the case of the analysis of short datasets, the existing methods do not provide a high ability to generalize, and their application may be accompanied by overfitting [11].

The combination of a global-local approach can significantly reduce the manifestations of these shortcomings, especially in the case of the analysis of short datasets. Such methods can provide a very accurate approximation of the response surface, especially in the case of high-dimensional functions. This happens due to taking into account the local structure of the response surface. In addition, such methods can be fully automated, which allows to significantly reduce the time and effort required to build the model. In addition, they allow the use of different machine learning algorithms for training local models, which allows for getting better results.

Despite the above-mentioned advantages, several significant disadvantages characterize the existing global-local methods. First, training local models requires a large amount of data, which can be problematic in the case of a limited dataset. Second, in the vast majority, methods of global-local approximation of the response surface based on machine learning have many parameters that need to be adjusted to achieve better prediction accuracy. Third, such approximation methods can be sensitive to random errors in the data that may appear because of noise or measurement errors, as well as overfitting. This can lead to inaccurate results, which requires the selection of machine learning models with the highest generalization properties.

That is why this work aims to improve the method of sequential obtaining of global and local components of the response surface to eliminate the above-mentioned shortcomings in the case of analysis of short sets of medical data.

The main contribution of this paper is as follows:

(i) we improved the global-local approximation method by using a General Regression Neural Network (GRNN) instead of the RBF ANN to extract the local component, which ensured an increase in both the accuracy of the analysis of short datasets and the generalization properties of the method as a whole;
(ii) we optimized the method of sequential obtaining of the global and local components of the response surface and evaluate the accuracy of its work using various performance indicators;
(iii) due to comparison with state-of-the-art methods, the highest accuracy of the proposed method was established.

2. State-of-the-arts

Global-local approximation methods based on machine learning are used to model complex response surfaces, which consist of several local functions, which in turn can have different properties. Similar methods are quite often used to solve various tasks.

Especially the paper [8] solve the missing data recovery task. They introduce the concept of local and global components. A polynomial algorithm determines the global approximation here. However, the local approximation demonstrates more accurate results compared to the global one. Despite the high accuracy of the approximation, the whole approach proposed by the authors for finding both global and local components is quite difficult to implement.

In [12], and [13] the authors demonstrated approaches of the combined use of global-local approximation to increase the prediction accuracy in engineering fields. The authors show that the global approximation takes into account the general behavior of the system, while the local approximation provides a very good approximation at its specific points. The combination of both of these approaches demonstrates a significant increase in the prediction accuracy for a variety of tasks.

The authors of [14] applied the global-local approximation approach to solving tasks in the field of mathematical analysis. They solve the system of discrete nonlinear equations using the proposed iterative procedure. It is based on the selection of global and local components. The authors show that a local approach can lead to ill-posed problems, and only in its combined use with a global approach can provide a reliable algorithm that can be effectively used in practice.

The authors of [15] investigated the possibility of performing local and global approximation using Artificial Neural Networks (ANNs). Based on the results of such studies, they developed a hierarchical method of global-local approximation. According to the method, the global component is synthesized at the root of the tree, while the local component is synthesized at its lower levels. The construction of the tree took place using self-organizing maps. This is precisely the drawback of the method, where the efficiency of the clustering algorithm significantly affects the overall efficiency of the global-local approximation method.

In [16] the authors proposed a neural network approach to global-local approximation. The authors developed a hybrid RBF-sigmoid ANN capable of capturing both global and local components of the response surface. The new training algorithm of this ANN is three-stage. It is based on the evaluation of the global component before adding local components to it. Experimental studies on five different (artificial and real-world) datasets demonstrated a

significant increase in the accuracy of the proposed ANN. Despite this, the selection of optimal parameters for the operation of this hybrid architecture requires a lot of effort.

The paper [17] described the method of sequential obtaining the global and local components of the response surface to improve classification accuracy in case of analysis of large volumes of data. It is based on the sequential use of 1) SGTM neural-like structure and 2) RBF-based SGTM neural-like structure. The first ANN in the auto-associative mode is used to obtain the global component of the output signal due to the possibility of fast synthesis of values very close to the principal components. In turn, the RBF-based SGTM neural-like structure, as a non-linear non-iterative ANN, is used to obtain the local components of the response surface. Their results are summed up, which ensures a significant increase in classification accuracy in the case of analysis of large volumes of data.

The main drawback of the above method is the use of RBF ANN for the synthesis of the local component of the response surface. In particular, the author of [18] investigated the performance of the RBF neural network as a good local approximator. He established that the synthesis of local components occurs through the use of RBF functions, while the global component is formed as a linear combination of all output signals. The main problem of the RBF neural network, in this case, is that during its optimization, the global component comes first, while the local components are leveled off. This causes a deterioration in the prediction accuracy in the case of using neural networks of this type for the synthesis of the local component in hybrid algorithms, such as the previous one. In addition, among the disadvantages of RBF ANN, it should be noted the random nature of the selection of RBF centers, which is accompanied by a new prediction result at each new run [19]. Also, the performance of this neural network type depends significantly on how many RBF centers are used, and choosing the optimal number of such centers is a difficult task [20,21].

This paper proposes the use of GRNN instead of RBF to extract the local component of the response surface to eliminate the shortcomings of previous methods. This neural network type, which doesn't require the training procedure, provides the highest generalization properties among existing ANNs and is also capable of increasing accuracy when analyzing small and extremely-small datasets.

3. An improved ANN-based approach for the global-local approximation

In this section, the proposed approach is described in detail, and all steps of the non-iterative procedure of its learning and application are presented. Since the method consists of two components, which are intended for the synthesis of global and local signal components, respectively, we will consider them in more detail.

3.1. SGTM neural-like structure

SGTM neural-like structure was developed by Prof. Roman Tkachenko. In [22] he proposed a new greedy algorithm with non-iterative training to improve the performance of feedforward neural networks when solving various data mining tasks. Its feature is the consideration of lateral connections between neurons of the hidden layer. The basic operating mode of the SGTM neural-like structure is the unsupervised mode (Fig.1)

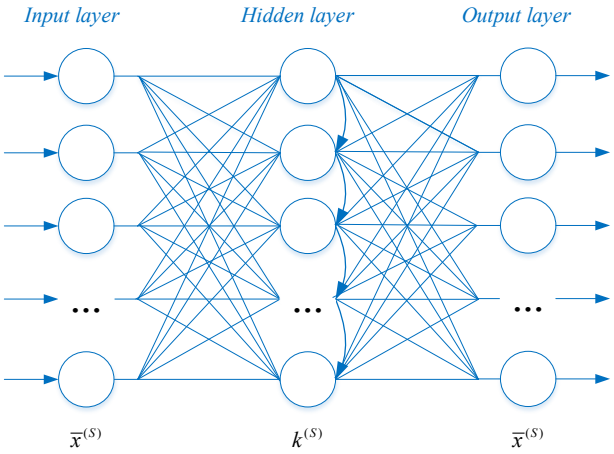

Figure 1. Topology of the unsupervised SGTM neural-like structure

It is characterized by the fact that the same signals are applied to the input and output, and the neuro-like structure forms values in the hidden layer that are very close to the principal components [22]. This process is significantly faster than using classical PCA. However, the main advantage of this approach is the ability to perform an exact inverse transformation of the principal components into vectors of the initial set [17]. In particular, the methodological error using this approach is zero. Details of the algorithmic implementation of the proposed PCA method are given in [22].

In the supervised mode, the non-iterative training algorithm also generates values close to the principal components in the hidden layer of the topology from Fig. 2. However, in this case, we have input and output signals that are fed to the corresponding layers of the topology of the neuro-like structure. Therefore, the exact values of the principal components can only be found for observations from the training sample. For the test sample, they are sought as an approximate value of the function, which is given tabularly from the principal components of the training sample [22].

Details for both training and application algorithms of the supervised SGTM neural-like structure can be found in [17], [22].

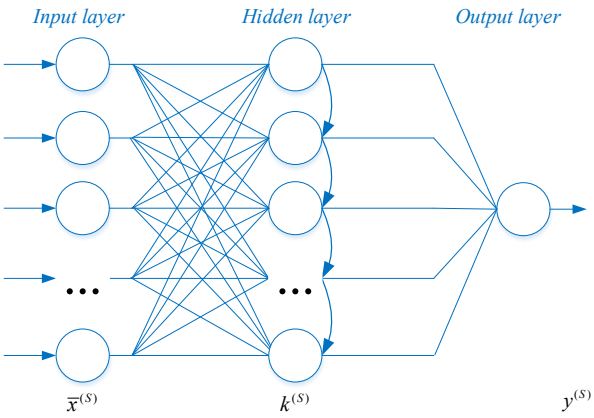

Figure 2. Topology of the supervised SGTM neural-like structure

According to [22], if the output signal is included as an additional variable in the topology from Fig. 1 or 2, and also if we reduce the number of neurons of the hidden layer by 1, then we can get the global component of the signal for the training sample. In a geometric interpretation, it can be explained as follows. Applying to the input and output topology from Fig. 1 given set of data, or at the input of the topology from Fig. 2 - all the input features plus 1, which is the output of each particular data vector - we get the exact predicted value. Assuming that we have only three features at the input of the topology from Fig. 2 that can correspond to the length, width, and height of the response surface, we will get an exact copy of it. However, if we reduce the number of hidden layer neurons by 1, i.e. remove the last principal component, we deform the response surface in such a way that it reproduces only the length and width – i.e. the global component. The height of the response surface will be the local component that should be found.

3.2. GRNN

The General Regression Neural Network (GRNN) is currently one of the best ANNs for working with short tabular datasets. This is explained primarily by the highest generalization properties of this neural network type compared to all other existing architectures [23]. In addition, due to the lack of a training algorithm, as well as the ease of implementation of this ANN, it is often used to solve various applied tasks [24].

The GRNN topology consists of 4 layers, which are shown in Fig. 3.

The method is based on the following basic steps [25]:

- searching of Euclidean distances from the current vector $x_{k,j}$ to each vector from the support sample $x_{i,j}$:

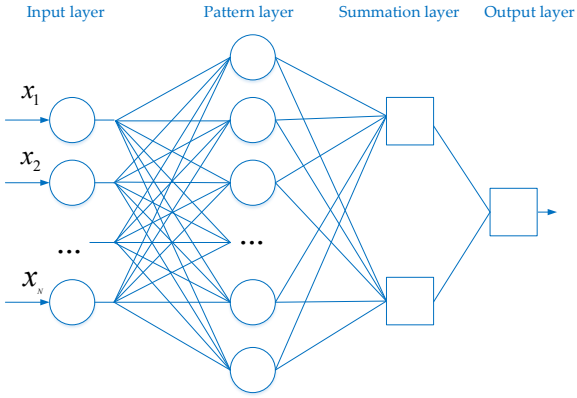

Figure 3. GRNN topology

$$E_{k,i} = \sqrt{\sum_{j=1}^{n} (x_{k,j} - x_{i,j})^2}, \quad (1)$$

- searching for Gaussian functions from the Euclidean distances obtained in the first step:

$$G_{k,i} = \exp\left(-\frac{(E_{k,i})^2}{\sigma^2}\right), \quad (2)$$

- searching for the predicted value according to the GRNN formula:

$$y_k^{pred} = \frac{\sum_{i=1}^{N} y_i G_{k,i}}{\sum_{i=1}^{N} G_{k,i}}. \quad (3)$$

In our case, to predict the local component of the signal, the choice of GRNN, in addition to all the above, is also based on the next its advantages:

- Flexibility. GRNNs can model complex dependencies between input and output data, which allows them to flexibly adapt to different applications [26];
- High accuracy in case of analysis of short datasets. GRNNs can account for complex dependencies between input and output data that may not be easy to detect using traditional regression methods or existing machine learning techniques [27].

3.3. Proposed approach

The method improved in this paper for sequential obtaining global and local components of the response surface includes the use of two ANNs: SGTM neural-like structure and GRNN. The first is used to predict the global component, while the second is used to predict the local component of the response surface.

However, their sequential application is preceded by the PCA mode, which is implemented using the topology from Fig. 1 and is necessary for further synthesis of the global

component of the response surface. So, let's consider the main operation modes for the improved method of global-local approximation.

PCA mode

The algorithmic implementation of this mode involves the following steps:

- we divide the sample into training and testing. In this mode, we work only with the training sample for which the output values (dependent variable) are known;
- we add the output value (dependent variable) as an additional feature to the existing training sample with n features $x_{i1},..,x_{in1} \to y_i$, resulting in a new dataset with an increased number of independent variables by 1:

$$x_{i1},..,x_{in1}, y_i \to y_i . \quad (4)$$

- we use the SGTM neural-like structure topology from Fig. 1, setting the number of neurons of the hidden layer to 1 less than the number of input features (the number of neurons of the input and output layers).

The main result of this mode is the synthesis of the value of the global component y_g_i, which will be used in the next operation mode of the method.

Application mode

The algorithmic implementation of the application mode involves the following steps:

- we train a supervised SGTM neural-like structure from Fig. 2 based on the features of the initial dataset and the output signal of the PCA mode: $x_{i1},..,x_{in1} \to y\_g_i$ (it should be noted that in this case the number of neurons of the input and hidden layers is the same).

As a result of performing this step, we obtain the desired value of the global component of the response surface for both training $y\_g_i^{pred}$ and test $y\_g_u^{pred}$ samples (by applying them to the previously trained supervised SGTM neural-like structure).

- we calculate the difference between the real value of the output and the global component obtained in the previous step for each *i-th* vector of the training sample, $y\_l_i = y_i - y\_g_i$;
- we form a support sample from n independent features of the initial training sample $x_{i1},..,x_{in1}$ and a dependent output y_l_i found in the previous method's step: $x_{i1},..,x_{in1} \to y\_l_i$;
- we obtain the predicted value of the local component of the response surface $y\_l_u^{pred}$ for the u-th input vector of the test sample $x_{u1},..,x_{un1}$, applying GRNN according to (1)-(3) based on the reference sample from the previous step;
- the desired predicted result for each u-th vector of the test sample is calculated as the sum of the global and local components:

$$y_u^{pred} = y\_g_u^{pred} + y\_l_u^{pred} \quad (5)$$

A detailed flowchart for both modes of the proposed global-local approximation method is presented in Fig. 4.

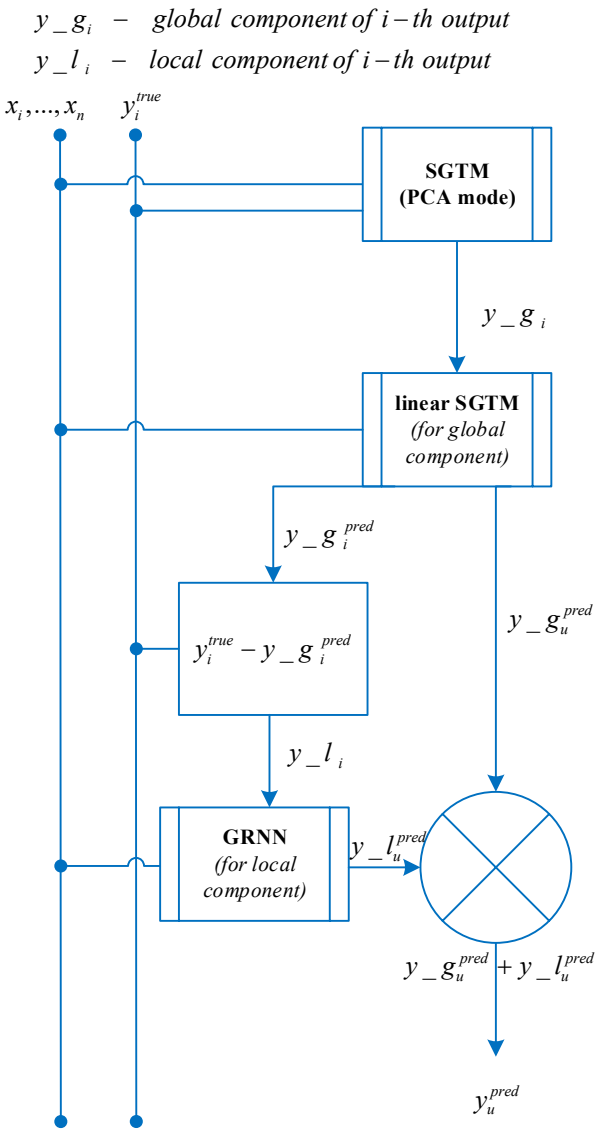

Figure 4. An improved sequential global-local approximation

The main advantages of the proposed approach are the following:

- increasing the accuracy of analysis of short sets of medical data;
- non-iterativeness of the training algorithm for the improved method and the simplicity of its implementation;

- high speed in application mode.

4. Modeling and results

In this section, we describe the simulation of the improved method using the real-world dataset for solving body fat prediction tasks. The selection of its optimal parameters was carried out. A comparison of its efficiency with the efficiency of several existing methods that were used to solve the body fat prediction task was also conducted.

4.1. Dataset description

Modeling of the proposed method was done using a real-world dataset. It is taken from an open source [28]. The dataset contains 13 different anthropometric measurements for 252 men. Twelve of the features are independent attributes and one is dependent. The task is to predict body fat percentage (it is a dependent feature). A detailed description of each variable is given in [28]. Statistical analysis of this dataset was carried out in [29].

4.2. Hyperparameters selection

The method proposed in this work is based on the use of two neural networks: SGTM neural-like structure and GRNN. Classical SGTM neural-like structure does not require additional configuration and ensures repeatability of the solution at each run, other things being equal. However, GRNN requires the selection of one parameter for its work, smooth factor (σ). Accordingly, the developed method also requires the selection of the optimal value of this parameter [30]

In this paper, we used the brute-force method to select the value of σ . Such procedure was carried out on the interval specified in Table 1 with a given step. The optimal performance parameters of the proposed method according to the results of the optimization are given in Table 1. In addition, Table 1 shows the optimal value of the smooth factor (σ) for the classical GRNN.

Table 1. Optimal parameters for the proposed method

Method	Brute force	Optimal parameters
Proposed method	Sigma range = [0.01, 10], step = 0.01	σ = 0.09
GRNN	Sigma range = [0.01, 10], step = 0.01	σ = 0.05

The difference in the values of the smooth factor (σ) for the classic GRNN and the proposed method indicates the need to optimize the selection of this parameter for the method proposed in this paper. That is the optimal value of σ found for the GRNN is not suitable for the developed method.

It is the parameters specified in Table 1 were used to perform all subsequent studies

4.3. Results

All experiments in this section were performed based on the use of K-fold cross-validation with N repetitions of the experiment to ensure the reliability of the prediction results obtained using the proposed method. It should be noted that this approach was also applied to all methods used for comparison.

In the experiments carried out for each of the methods, K = 5 and N = 20. That is, the experiments were repeated 20 times and each experiment was evaluated based on 5-fold cross-validation. The final result is the average of 20 iterations.

All performance indicators for the method proposed in this paper after performing the above procedures are summarized in Table 2. In addition, Table 2 shows the errors of the training mode for evaluating the generalization properties of the method and the overfitting probability.

Table 2. Performance indicators for the proposed method

Performance indicators	Values of the performance indicators	
	Training mode	Application mode
MAE	2.79	3.31
MAPE	0.31	0.35
MSE	12.42	17.17
MaxE	9.14	9.56
MedianAE	2.46	3.06
RMSE	3.52	4.14
R^2	0.81	0.78

To visualize the results from Table 2, Fig. 5 shows the values of RMSE and MAE errors in the training and application modes of the proposed method.

Figure 6 clearly shows that the developed method does not cause overfitting, which is very typical when working with short datasets. In particular, the values of both training errors are lower than the values of application errors (RMSE and MAE). In addition, as can be seen from the results of Table 2 and Fig. 5, the developed method provides high generalization properties. The difference between training and application errors is not large. This is explained by the high generalization properties of GRNN, which is a component of the developed method for synthesizing the local component of the response surface.

In addition, in order to evaluate the effectiveness of using the proposed method, we compared it with the effectiveness of existing methods.

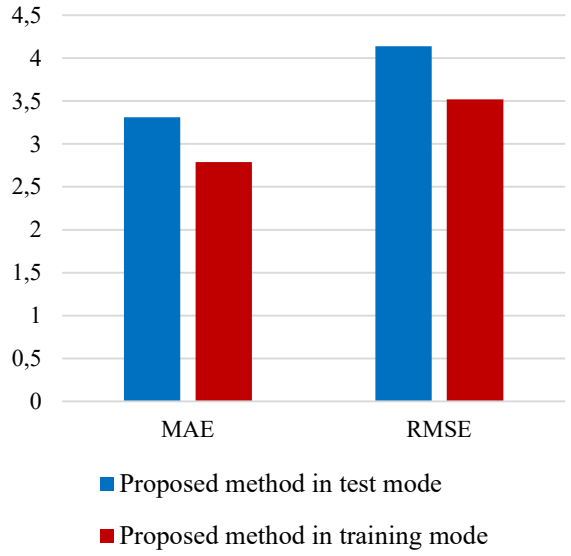

Figure 5. RMSE and MAE values for the proposed method in training and test modes

5. Comparison and discussion

The proposed method was compared with several existing methods. In particular, two ANNs were used, which are the basis of the proposed method; the basic RBF-based global-local approximation method which we improved, and four existing methods that were used by other researchers to solve the stated task, namely:

- SGTM neural-like structure [22];
- General Regression Neural Network (GRNN) [25];
- Basic RBF-based global-local approximation method [17];
- Multilayer perceptron (MLP) [1];
- Support Vector Regression with RBF kernel (SVR) [1];
- Random Forest [1];
- XGBoost [1].

The comparison was based on the use of RMSE, MAE, and application time. The optimal operating parameters of all four methods are taken from [1] and are the same as those of the authors of that paper.

The performance results of all studied methods based on RMSE and MAE are shown in Fig. 6 and Fig.7 respectively.

As can be seen from Fig. 6 and Fig. 7, the lowest prediction accuracy is provided by the multilayer perceptron. Then there are two neural networks, which became the basis of the method of local-global approximation of the response surface proposed in this paper.

The methods investigated in [1] to solve the body fat prediction task showed slightly better results than the previous three methods. In addition, the basic RBF-based global-local approximation method [17], which was improved in this paper also shows a good result. Despite this, the accuracy of the proposed method significantly outperforms all the investigated methods in terms of both performance indicators.

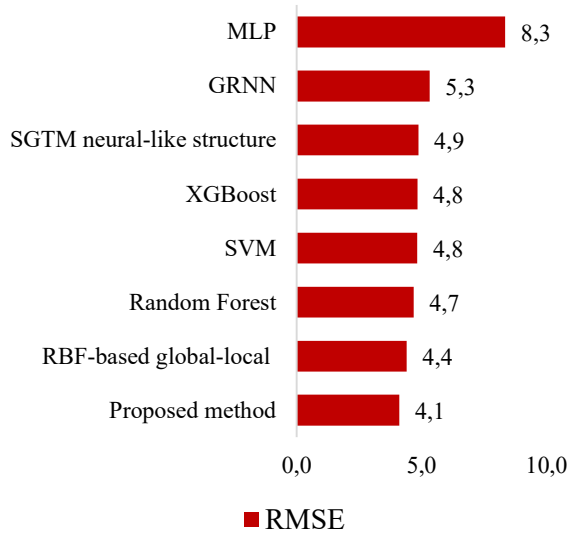

Figure 6. RMSE for all investigated methods

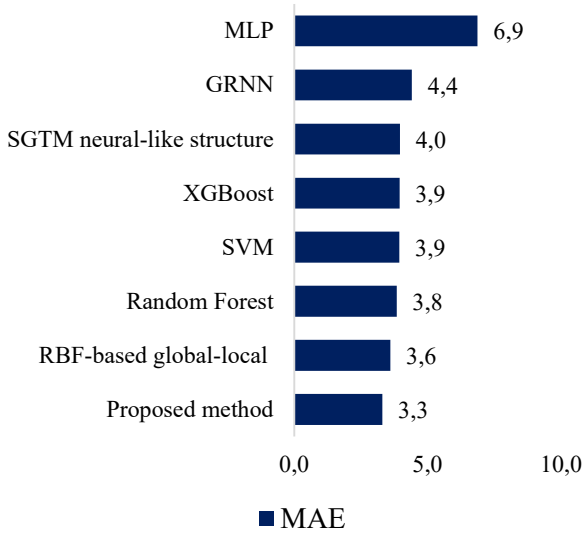

Figure 7. MAE for all investigated methods

In general, the method presented in this work is focused on the analysis of short datasets, but the time of its application still plays an important role. That is why, Fig. 8 shows the time of application of all investigated methods in the paper.

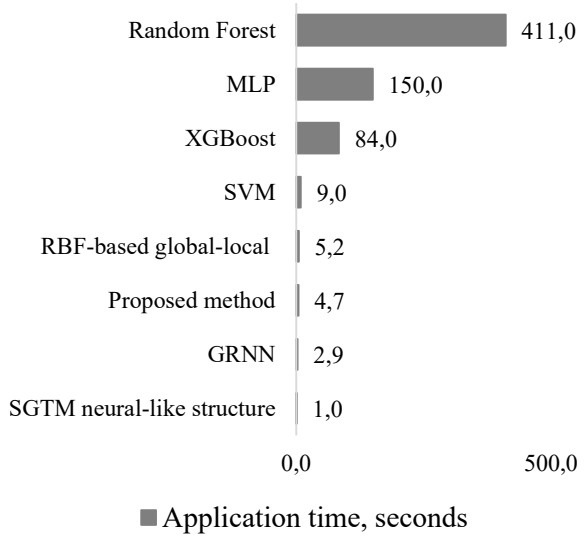

Figure 8. Application time for all investigated methods

In particular, as can be seen from Fig. 8, the longest application time is demonstrated by the Random Forest algorithm. A somewhat shorter time is shown by a multi-layer perceptron. The shortest application time among the methods from [1] is demonstrated by SVR. Linear SGTM neural-like structure, as expected, demonstrates the shortest application time among all the methods considered in the paper. A slightly higher application time is demonstrated by GRNN. Having said that, both of the latter methods show low prediction accuracy.

The method proposed in this work, as expected, shows a longer application time compared to the methods that form it. In particular, it works 5 times slower than SGTM neural-like structure and almost two times slower than GRNN. However, it provides the highest prediction accuracy when solving the body fat prediction task, and considering the size of the datasets for which it is intended, this drawback can be leveled

6. Conclusion

The task of approximating tabular datasets in medicine is crucial for accurate di-agnosis and treatment of patients, particularly in cases small dataset of available for implementation training procedures. While various machine learning methods have been employed for prediction based on tabular datasets, each approach has limitations and disadvantages. Linear regression analysis methods often lack accuracy, especially when dealing with complex nonlinear relationships in medical datasets. On the other hand, more complex machine learning methods can consider the local components of the response surface but face challenges due to limited data availability, leading to re-duced accuracy and ineffective analysis.

To address these shortcomings, a combination of a global-local approach can be employed, which significantly reduces these limitations, particularly when analysing short datasets. Such methods offer accurate approximation of the response surface by considering both global and local components, especially for high-dimensional func-tions. Moreover, these methods can be fully automated, reducing time and effort re-quired for model building, and allow the use of different machine learning algorithms for training local models, leading to improved results. However, existing global-local methods have their own disadvantages. They often require a large amount of data for training local models, which can be problematic for limited datasets. Additionally, these methods involve numerous parameters that need to be adjusted to achieve better prediction accuracy. Furthermore, they can be sensitive to random errors in the data and prone to overfitting, necessitating the selection of machine learning models with high generalization properties.

The improved approach presented in this paper consists of two ANNs: the SGTM neural-like structure for predicting the global component and the GRNN for predicting the local component. Prior to their sequential application, a PCA mode is utilized to obtain the global component. The proposed method offers increased accuracy and generalization properties, especially for analysing short tabular medical datasets.

In summary, the improved ANN-based approach for global-local approximation presented in this paper addresses the limitations of existing methods. By using a combination of the SGTM neural-like structure and GRNN, the proposed approach achieves accurate approximation of the response surface, considering both global and local components. Comparisons with state-of-the-art methods demonstrate the highest accuracy achieved by the proposed approach (7% according to RMSE in comparison with existing method). Further research and experimentation can be conducted to explore the applicability of this approach in other domains [31–33] as well as a development of new method for independently obtaining global and local components using two non-linear SGTM neural-like structure.

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