Using neural networks for prediction of air pollution index in industrial city

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Abstract. This scientific paper is dedicated to the use of artificial neural networks for the ecological prediction of state of the atmospheric air of an industrial city for capability of the operative environmental decisions. In the paper, there is also the described development of two types of prediction models for determining of the air pollution index on the basis of neural networks: a temporal (short-term forecast of the pollutants content in the air for the nearest days) and a spatial (forecast of atmospheric pollution index in any point of city). The stages of development of the neural network models are briefly overviewed and description of their parameters is also given. The assessment of the adequacy of the prediction models, based on the calculation of the correlation coefficient between the output and reference data, is also provided. Moreover, due to the complexity of perception of the «neural network code» of the offered models by the ordinary users, the software implementations allowing practical usage of neural network models are also offered. It is established that the obtained neural network models provide sufficient reliable forecast, which means that they are an effective tool for analyzing and predicting the behavior of dynamics of the air pollution in an industrial city. Thus, this scientific work successfully develops the urgent matter of forecasting of the atmospheric air pollution index in industrial cities based on the use of neural network models.

1. Introduction
At present, the air pollution is observed almost in all cities and industrial centers of chemistry and petrochemistry. In separate periods, the meteorological conditions unfavorable for the dispersion of the emissions affect the most part of cities and they contribute to the accumulation of anthropogenic emissions in the air basin of cities. To avoid the raising of the air pollution under such conditions, it is necessary to predict the content of pollutants in air taking into account these conditions.

However, the well-known prediction methods, based on the exponential smoothing, time-series analysis, regression analysis etc, do not give proper and adequate prediction results, since a set of the non-formalizable and poorly researched factors, which are difficult to take into account in the prediction models, affects the air pollution process. Moreover, the monitoring data of the industrial city air pollution are characterized by the multidimensional and multivariate properties of the ecological data and the pollution process is characterized by non-linearity and uncertainty, and these aspects make the ecological prediction significantly difficult.

In the last several years, the artificial neural networks, which are capable to work in conditions of fuzzy initial information and take into account the hidden dependencies, are often used to improve the efficiency and accuracy of the ecology management decisions.
The artificial neural networks [1, 2] are the specialized mathematical models and their hardware and software implementation, which are designed in accordance with the principle of the organization and functioning of the biological neural networks, i.e. the networks of nerve cells of the living creatures. The models, based on the artificial neural networks, were arisen within the study of processes occurring in the human brain during thinking and the attempts to simulate these processes. Subsequently, these models were used for practical purposes and prediction tasks, in particular. The neural networks are not programmed in the usual sense of the word, they are trained. Trainability is one of the most important advantages of the neural networks in comparison with the traditional models and algorithms. Technically, the purpose of the training is to find the connections between the neurons. During the training process, the neural network is capable to reveal complex dependencies between input and output data. After training completion the neural network is capable to predict the future values of some given sequence on the basis of given previous values and existing factors.

Within the scope of the scientific research, the authors have observed the existing results in the field of the neural network models for air pollution prediction [3, 4] and analyzed the possibility of usage of the neural networks in prediction of the air pollution on example of the industrial city of Sterlitamak (Russian Federation). The choice of this city was caused by the fact that it is one of the largest industrial centers of chemistry and petrochemistry in the Russian Federation. In the 2009, 2010 and 2013, it was on the list of Russian cities with very high level of air pollution. The specificity of its pollution and environmental conditions is typical for a number of urban ecosystems in the east of the European part of the Russia. In such cities, the monitoring of the environment is provided for many years; however, generalization of monitoring data for the development of the environmental mathematical models and short-term prediction of pollution in future with the aim of the operative environment protection decisions has not been made yet.

The first step in this direction was the development of the neural network models for temporal and spatial prediction of the air pollution index for the industrial city of Sterlitamak with using of the previously obtained results within the authors scientific research in the field of air pollution for this city [5, 6]. The temporal prediction is based on the capability to provide the short-term forecast of air pollution for the next 24 hours. The spatial forecast is based on the determination of the air pollution index at any point of the industrial city, taking into account its orographic features.

2. The short-term prediction model on basis of the feedforward neural network

At the first stage of scientific research, the authors developed a neural network model for short-term prediction of content of air pollutants, specific for the city with developed chemical and petrochemical industry, such as: dust, ammonia, hydrogen sulfide, phenol, vinyl chloride, nitrogen dioxide. The offered model provides forecast with an advance up to several days depending on the meteorological characteristics of the following days.

An important issue of the development was the selection of input data for the neural network model: concentration of the air pollutants in previous time periods, concentration of the air pollutants at the moment of application of the model and the meteorological parameters for the next day: direction and speed of wind, air temperature, atmosphere pressure, unfavorable meteorological conditions mode, which is due to the high closeness of connection between them.

Within the scope of the scientific work, the different kinds of the neural networks were probed by the authors. As a result, the multilayer feedforward neural network [7, 8] showed the best adequacy of prediction. In addition, a research for determination of the optimal number of the neurons in the hidden layers was carried out by the authors. However, the variation of the number of the neurons in the hidden layers did not lead to a significant change in the quality of the neural network model.

Figure 1 shows the topology of the feedforward neural network finally offered by the authors. As for activation functions of the neurons, there are used hyperbolic tangent in the neurons of the first layer and linear function in the neurons of the second layer.
Figure 1. Topology of the offered feedforward neural network for the short-term prediction model.

Here,

- $C$ – current value of the pollutant concentration;
- $T$ – air temperature; $W$ – wind direction;
- $U$ – wind speed; $P$ – atmosphere pressure;
- $M$ – unfavorable meteorological conditions mode;
- $C_p$ – forecasted value of the pollutant concentration.

Within the scientific research, the different learning algorithms for the feedforward neural network with the further assessment of adequacy of the trained neural network model for the different air pollutants were probed by the authors.

For each learning algorithm, the authors assessed the adequacy of the neural network model by the way of entering input values $[x_{1(q)},\ldots,x_{6(q)}]$ into the trained neural network and comparing the obtained value $y_{(q)}$ on output of the neural network with the given reference value $d_{(q)}$ in the control set $\{[x_{1(q)},\ldots,x_{6(q)}],d_{(q)}\}_{q=1}^Q$ with further calculation of the correlation $r$ between the two sets of values:

$$r = \frac{\sum_{q=1}^{Q} (d_{(q)} - \bar{d})(y_{(q)} - \bar{y})}{\sqrt{\sum_{q=1}^{Q} (d_{(q)} - \bar{d})^2} \sqrt{\sum_{q=1}^{Q} (y_{(q)} - \bar{y})^2}}.$$  \hspace{1cm} (1)

Here, $\bar{d}$ is average value of the all reference values; $d_{(q)}$ is the control set; $\bar{y}$ is average value of all output values $y_{(q)}$, obtained for the input values in the control set; and $Q$ is the size of the control set.

Table 1 shows the results of training of the feedforward neural network by the different learning algorithms in particular for ammonia.

It is quite obvious that for ammonia the best adequacy of the short-term prediction model is the one achieved in the feedforward neural network with the learning algorithm based on Conjugate Gradient Back-propagation with Powell-Beale restarts.
Table 1. Results of application of different learning algorithms for the feedforward neural network and assessment of adequacy of the neural network model (on example of ammonia).

| Learning algorithm                                | Adequacy of the NN-model |
|---------------------------------------------------|--------------------------|
| Broyden-Fletcher-Goldfarb-Shanno algorithm         | 72%                      |
| Conjugate Gradient Back-propagation algorithm with Powell-Beale restarts | 73%                      |
| Gradient descent algorithm                        | 2%                       |
| Gradient descent algorithm with adaptive learning rate | 67%                      |
| Levenberg-Marquardt algorithm                      | 43%                      |
| Resilient back-propagation algorithm               | 70%                      |

In order to use the offered neural network model in the practical calculations of air pollution, the authors also developed a software implementation by using the MatLab software with the built-in Neural Networks Toolbox package. The mathematical core of the developed software tool is the trained feedforward neural network, exported from the MatLab, which is used as a key unit for processing the input values and calculating the air pollution.

Using the developed software in the city of Sterlitamak shows that it is quite effective prediction tool. The accuracy of the forecasts is more than 70%.

3. The spatial prediction model on the basis of the Elman recurrent neural network

The second stage of scientific research of the authors was dedicated to the development of a neural network model describing the air pollution index in any given point of the city, taking into account its local orographic characteristics.

The following parameters were used as the input data for the neural network: the relief mark at the given point of city and the toxicity indices of the samples obtained with the use of watercress and daphnia magna. The air pollution index at the given point has been assumed as the output data.

Within the scope of the scientific research, the different kinds of the neural networks was probed by the authors. As a result the Elman neural network [9, 10] showed the best adequacy of air pollution index prediction. In addition, a research for determination of the optimal number of the neurons in the hidden layer was carried out by the authors. However, variation of the number of the neurons in the hidden layer did not lead to a significant change in the quality of the neural network model.

Figure 2 shows the topology of the Elman neural network, finally offered by the authors.

Within the scientific research, the different learning algorithms for the Elman neural network with the assessment of adequacy of the trained neural network model were also probed by the authors.

For the each learning algorithm the adequacy of the neural network model was assessed by the way of entering the input values \([x_1(t), x_2(t), x_3(t)]\) into the trained neural network and comparing the obtained value \(y(t)\) on the output of neural network with the given reference value \(O(t)\) in the control set \(\{[x_1(t), x_2(t), x_3(t)], O(t)\}_{t=1}^{Q}\) with calculation of the correlation \(r\) between the two sets of values:

\[
r = \frac{\sum_{t=1}^{Q} (O(t) - \bar{O})(y(t) - \bar{y})}{\sqrt{\sum_{t=1}^{Q} (O(t) - \bar{O})^2} \sqrt{\sum_{t=1}^{Q} (y(t) - \bar{y})^2}}.
\]
Where, $\overline{O}$ is the average value of all reference values $O(t)$ in the control set, \( \overline{Y} \) is the average value of all output values $y(t)$, obtained for the input values in the control set and $Q$ is the size of the control set.

The results of training of the Elman neural network by the different learning algorithms are shown in Table 2.

![Figure 2. Topology of the offered Elman neural network for the spatial prediction model.](image)

Here,

$L$ – Relief mark at the given point of the city;

$D$ – Toxicity index of samples obtained with the use of watercress;

$H$ – Toxicity index of samples obtained with the use of daphnia magna;

$API$ – Air pollution index;

Delay – delay unit for one time interval used in the feedback loop in the Elman neural network.

**Table 2.** Results of application of the different learning algorithms for the Elman neural network and assessment of adequacy of the neural network model.

| Learning algorithm                                      | Adequacy of the NN-model |
|---------------------------------------------------------|--------------------------|
| Gradient descent algorithm                              | 66.1%                    |
| Gradient descent with adaptive learning                 | 76.2%                    |
| Gradient descent with momentum                          | 21.3%                    |
| Gradient descent with momentum and adaptive learning    | **86.7%**                |
| Bayesian regularization                                 | 33.6%                    |

It is quite obvious that the best adequacy of the spatial prediction model is achieved in the Elman recurrent neural network with the learning algorithm based on gradient descent with momentum and adaptive learning.
In order to use the offered neural network model in the practical calculations of the air pollution index, the authors also developed a software implementation using the MatLab software with the built-in Neural Networks Toolbox package. The mathematical core of the developed software tool is the trained Elman neural network, exported from the MatLab, which is used as a key unit for processing the input values and calculating the air pollution index.

Using of the developed software in the Sterlitamak city shows that it is quite effective prediction tool. The accuracy of the forecasts is more than 83%.

4. Conclusion
The neural network models for the forecasting of the air pollution level, obtained by the authors, are sufficiently effective. The daily summary of new data on the air pollution proves the adequacy of the offered models. It should also be noted that there is a possibility of the periodic additional training of the obtained neural networks on the basis of the additional daily experimental data.

The adoption of the neural networks models in the air basin monitoring system of the industrial city will undoubtedly improve the quality of work of the both municipal authorities and the environmental safety departments of the industrial enterprises in the city.

However, despite the obvious advantages of the neural network models, they should not be considered as a panacea. The best way to achieve the adequate environmental results is to use the neural network models in conjunction with a competent strategy of the environmental management.

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