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The prediction of atmospheric concentrations of toluene using artificial neural network methods in Tehran

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Abstract. In recent years, raising air pollutants has become as a big concern, especially in metropolitan cities such as Tehran. Therefore, forecasting the level of pollutants plays a significant role in air quality management. One of the forecasting tools that can be used is an artificial neural network which is able to model the complicated process of air pollution. In this study, we applied two different methods of artificial neural networks, the Multilayer Perceptron (MLP) and Radial Basis Function (RBF), to predict the hourly air concentrations of toluene in Tehran. Hourly temperature, wind speed, humidity and NO_x were selected as inputs. Both methods had acceptable results; however, the RBF neural network produced better results. The coefficient of determination (R^2) between the observed and predicted data was 0.9642 and 0.99 for MLP and RBF neural networks, respectively. The results of the mean bias errors (MBE) were 0.00 and -0.014 for RBF and MLP, respectively which indicate the adequacy of the models. The index of agreement (IA) between the observed and predicted data was 0.999 and 0.994 in the RBF and the MLP, respectively which indicates the efficiency of the models. Finally, sensitivity analysis related to the MLP neural network determined that temperature was the most significant factor in air concentration of toluene in Tehran which may be due to the volatile nature of toluene.

Keywords: air quality; MLP neural network; RBF neural network; toluene; prediction

1. Introduction

Nowadays, predicting air quality is one of the most important and useful issues in atmospheric and environmental sciences because it has a direct effect on human health. Toluene (methyl benzene) is a bright, colorless, volatile and flammable liquid, without corrosion characteristic and has an odor like benzene (Bloemen and Burn 1993). Its formula is $C_6H_5CH_3$. About 99% of toluene released into the environment is caused by the production, transport, use and disposal of gasoline. Chronic hygienic exposure to toluene includes headache, dizziness and memory reduction. Short-term exposure to 100 ppm of toluene causes psychiatric disorders, movement disorders and cognitive disorders, which are symptoms of central neural system disorders (US.EPA 1993). Therefore, having an efficient model to predict air pollution is needed, and plays a significant role in air pollution management. An artificial neural network (ANN) is a branch of artificial intelligence which can discover new connections, functions or algorithms between

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parameters and predict data.

Many researches have studied predicting air pollution by using neural networks.

Ruiz-Suarez *et al*. (1995) predicted ozone concentration in five stations in Mexico City by applying a multilayer perceptron (MLP) neural network and a nonlinear regression. They reported suitable results for MLP. Yi and Prybutok (1996) applied an artificial neural network to predict daily maximum ozone level. Their results indicated that an artificial neural network model is superior to the regression and the Box-Jenkins model. Gardner and Dorling (1999) studied hourly NO_x and NO_2 concentrations in central London using MLP. Their results indicated MLP neural network performed well compared with the regression based models. Kolehmainen *et al*. (2001) applied MLP neural network and a combination of the periodic regression method and neural algorithms to hourly time series of NO_2 and basic meteorological variables collected in the city of Stockholm in 1994-1998. Their results presented that a combination of periodic regression method and neural network did not have any benefit over an MLP neural network. Viotti *et al*. (2002) used an artificial neural network to predict short, middle and long term concentrations of some air pollutants in the city of Perugia in Italy. They predicted air quality 24-48 hours in advance, requiring only the meteorological conditions and the traffic level. Tasadduq *et al*. (2002) tested the MLP efficiency to predict the average hourly temperature in Jeddah, Saudi Arabia, which confirmed the suitability of back propagation learning algorithm. Ozcan *et al*. (2006) applied MLP neural network to predict methane gas concentrations in the Istanbul Landfill and used CO and CO_2 as inputs and achieved the coefficient of determination equal to 0.983. Grivas and Chaloulakou (2006) employed an artificial neural network and a regression model to predict PM_{10} in the air of the Greater Athena’s Area. They concluded that the artificial neural network had a higher coefficient of determination and index of agreement than the regression model. Owega *et al*. (2006) identified the patterns of dust transmission in Toronto, Canada use an artificial neural network. They mentioned that the back propagation is a powerful learning algorithm. Moustris *et al*. (2010) forecasted the maximum daily value of the European Regional Pollution index as well as the number of consecutive hours using an artificial neural network. Three days-ahead forecasting of the Regional Pollution Index for the Pollutants NO_2, CO, SO_2, and O_3 using a neural Networks in Athens, Greece was predicted their results were in a very good agreement with the real-monitored data. Voukantsis *et al*. (2011) applied principal component analysis and artificial neural networks to compare air quality and meteorological data, and to predict the concentration levels of air pollutants. They used data of the urban areas of Thessaloniki and Helsinki in Greece and Finland, respectively, and forecasted the daily mean concentrations of PM_{10} and $PM_{2.5}$ for the next day. Chattopadhay and Chattopadhay (2012) used MLP neural network to predict monthly ozone concentrations. They found that cloud cover and rainfall can act as good predictors for monthly total ozone. Mysteries *et al*. (2013) applied ANN to predict 24h ahead daily concentration of PM_{10} in five different stations a Mediterranean City. They concluded that ANN can able to predict 1 day ahead PM_{10} concentration Haiming and Xiaoxiao (2013) applied ANN using PM_{10}, SO_2, NO_2, temperature, pressure, humidity, wind direction parameters and wind speed were selected as the influence factor. They predicted $PM_{2.5}$ with reasonable accuracy. Asadollahfardi *et al*. (2015) developed an MLP and a RBF neural network in the Southwest of Tehran to predict benzene. Their results indicated that RBF achieved a better accuracy. The study area is located in the southeast of Tehran, the capital city of Iran. The geographic coordinates are between 51° 2' to 51° 36' E and 35° 50' N latitude and its elevation is 2000 meters from the highest points in the north, 1200 meters in the middle and 1050 meters in the south. Tehran is between the Alborz Mountain in the north and desert in the south.The Alborz Mountains and Atlantic winds that blow

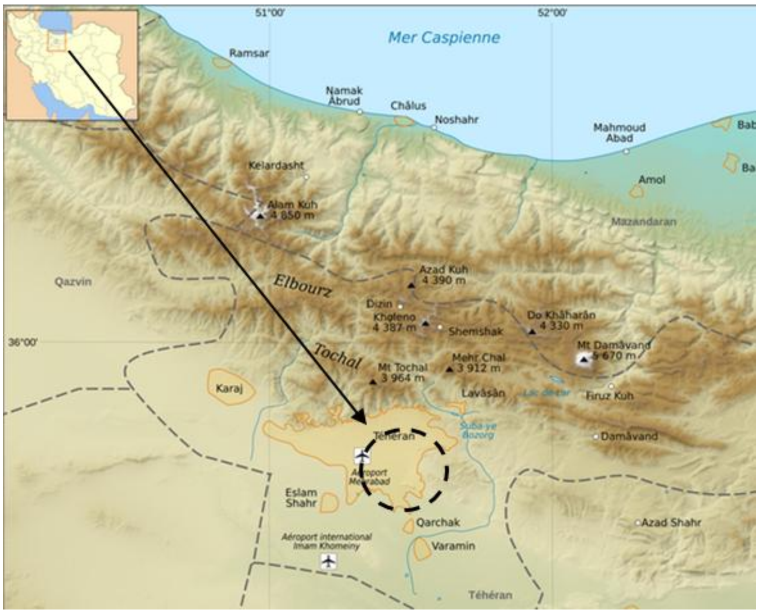

Fig. 1 The location of study area

from the West act as a barrier to prevent the penetration of air masses (Asadollahfardi *et al*. 2015). Tehran is also located in an arid and semiarid region. The temperature variations are between 40 Celsius in summer and -5 Celsius in winter. The annual rainfall is about 250 millimeters (Asadollahfardi *et al*. 2015). Fig. 1 presents the study area.

The first objective of the study was to predict toluene concentrations in the south of Tehran using both an MLP and a RBF neural networks. A second aim was to determine which of the input data including temperature, NO_X, humidity and wind speed are significant to generate toluene concentrations by using sensitivity analysis.

2. Material and method

Artificial neural networks are regarded as a capable, universal method to approximate any arbitrary, nonlinear system without any prior assumptions (Lu *et al*. 2004). The ability of neural network depends on the accuracy and sufficiency of the primary data; therefore, the availability or the preparation of input data is one of the most important issues in the training process to cause the network to extend or predict the desired outputs. To select data, we applied parameters based on the significance of input parameter and independence as Wu *et al*. (2014) mentioned in their protocol for developing ANN models. Therefore, hourly air temperature, wind velocity and humidity data were selected as input data. The data were monitored by the Air Quality Control Company (AQCC) of the municipality of Tehran. The AQQC collected data during late July through late September 2010.

2.1 Neural network structure

The artificial neuron is made of three exclusive principal components: weight (w), bias (b) and

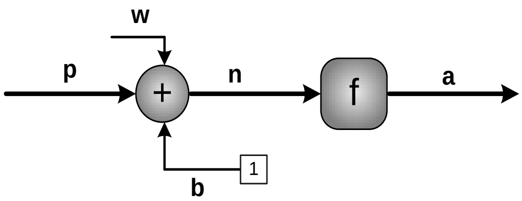

Fig. 2 An artificial neuron schematic (Asadollahfardi 2015)

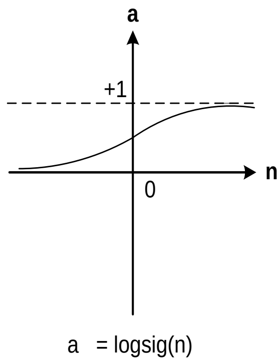

Fig. 3 Log sigmoid transfer function

transfer function (f). Fig. 2 presents a schematic of an artificial neuron. In this figure, *p* and *a*, *n* are inputs and outputs of neurons. Weight and bias are indicated with *w* and *b*, respectively. *F* is transfer function (Menhaj 1998). Eq. (1) indicates the relation between the mentioned parameters.

$$a = f(n) = f(wp + b) \tag{1}$$

Several transfers' functions are available. In this study, we applied a log sigmoid transfer function, which creates an output in the range of 0 to 1 and introduces nonlinearity into the network. Eq. (2) describes the function.

$$a = f(n) = \frac{1}{1+e^{-cn}}, c > 0 \tag{2}$$

Where *a* is the input and the *c* determine the linear domain of the function. Fig. 3 indicating that *c* equal *1* (Menhaj 1998).

2.2 MLP neural network

The multi-layer perceptron (MLP) neural network provides a flexible and non-linear tool for tackling regression problems in air quality modelling (Niska *et al*. 2004). Several hidden layers can be selected, although one to three hidden layer model are more common. The number of neural neurons in the hidden layers for each model can be computed by trial and error. Fig. 4 illustrates the schematic figure of Multilayer neural network, which contains *R* inputs and *S* outputs.

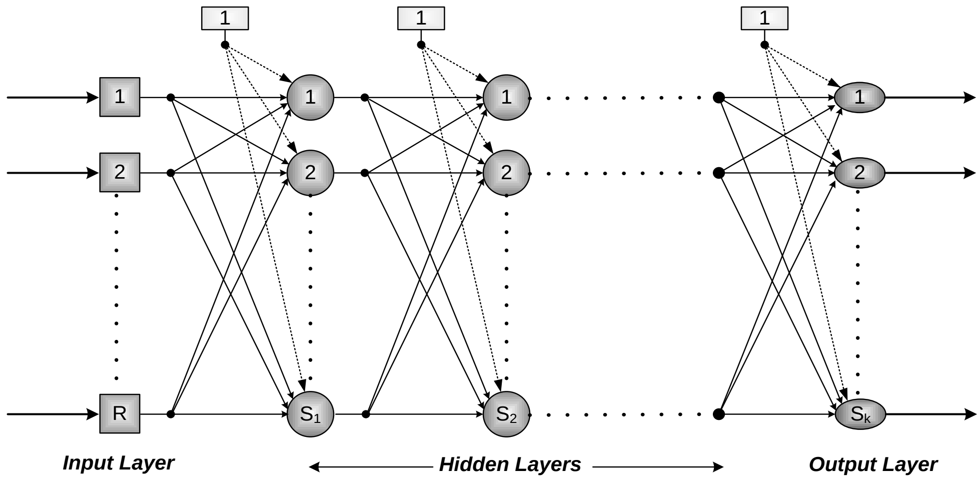

Fig. 4 Schematic figure of multi-layer neural network (Asadollahfardi *et al*. 2012)

2.3 Learning neural networks

Learning is a process in which a neural network adjusts its parameters including weights and biases. Neural networks have the ability to use their old experiences and improve accuracy in each step. In back propagation algorithms the learning rate is one of the important process which specifies the velocity of convergence. The performance of the steepest descent gradient algorithm is enhanced if the learning rate is allowed to change during the training processes (Asadollahfardi *et al*. 2015). An adaptive learning rate attempts to cause the learning step as big as possible to keep the learning stable and needs some changes in the training process (Asadollahfardi *et al*. 2015).

2.4 Back Propagation error algorithm (BP)

Least Mean Square (LMS) algorithm is a great method of learning, neural networks; however, its usage domain is limited and restricted to ADALINE networks and just the problems which are linearly separable. Determining this restrict, a tendency to use multilayer networks increases; however, the lack of a reliable, useful algorithm in learning multilayer networks is a great obstacle. Innovating Back Propagation (BP) error method with greater backup in various basis of science made artificial neural networks introduce themselves again. As mentioned previously, the bases of this method are “maximum descent gradient” and its purpose is to minimize the network output errors squares summation (Menhaj 1998).

2.5 RBF neural network, nonlinear separation

One of the nonlinear separating methods is the RBF neural network. In recent years, the RBF networks have been popular due to their simple structure and efficient learning methods.

An RBF neural network consists of an input layer, a single hidden layer and an output layer, which at each output node, makes available a linear combination of the outputs of the hidden-layer nodes. By using Eq. (3), we can compute the output of the hidden network.

$$hj = \frac{[\varphi\ (X - Cj)]}{\sigma j} \tag{3}$$

Where h_j is the J^{th} neuron and φ is a function of RBF nonlinear operation. X is an input vector. Cj is the center of the neuron and σ_j is the amount of the neuron’s center span. Nonlinear characteristic of an RBF neural network is due to the operation of function φ. Neurons have a linear operating function in the layer. In fact, outputs of an RBF neural network are equal to the weighted summation of the hidden layer of neuron's output attached to the output layer.

An RBF neural network is capable of estimating nonlinearly. Therefore, an RBF neural network can be used for interpolation problems. A Gauss RBF is a normalized form of Gauss distribution function and nonlinear. It has good properties from increasing learning and also well-known mathematical characteristic. Gauss neural networks which are used for complex problems are used for learning, recognition, simulation and dynamic nonlinear system control (Dayhoff 1990). Training an RBF includes two steps. First, the basic functions are computed using an algorithm to cluster data in the training set. Secondly, the weights linking the hidden and the output layer are computed directly applying the simple matrix inversion and multiplication. The direct calculation of weights in an RBF makes it faster in training in comparison with an equivalent MLP (Asadollahfardi *et al*. 2015).

2.6 Preparing data

One of the important points in neural networks is preparing input data. According to the form of log sigmoid transfer function which was mentioned before, all of the data is used, including input and output changes 0 to 1 range using Eq. (4). We applied the neural Network Toolbox, MATLAB version 2012 for analyzing the data. At the end, the predicted amounts returned to the real scale with the same formula.

$$As(scaled) = \left[\frac{A_i - A}{B - A}\right] \times 2 - 1 \tag{4}$$

Where A_i, i^{th} observed value and A_s scaled amount of component A. A and B is the lowest and highest values of temperature, wind speed, relative humidity and toluene concentrations.

2.7 Error estimation functions

To assess the applicability of the models, we used Root Mean Squared Error (RMSE) and Mean Bias Error (MBE) which are indicated in Eqs. (5) and (6). (Kennedy and Neville 1964).

$$\text{RMSE} = \sqrt{\frac{1}{n}\sum_{t=1}^{n}(A_t - F_t)^2} \tag{5}$$

$$\text{MBE} = \frac{1}{n}\sum_{t=1}^{n}\left|\frac{F_t - A_t}{A_t}\right| \tag{6}$$

Where n is the number of data. A_t is the observed toluene concentrations and F_t is the predicted toluene concentration.

2.7 Model efficiency

The coefficient of determination, R^2, was applied to determine the model efficiency (Eq. (7))

$$R = \frac{\sum(A_t - \bar{A})(F_t - \bar{F})}{\sqrt{\sum(A_t - \bar{A})^2 - \sum(F_t - \bar{F})^2}} \tag{7}$$

Where $\bar{A}$ and $\bar{F}$ are the average of A and F (Kennedy and Neville 1964). The reliability and accuracy of the model also assess using the Index of Agreement (IA) (Eq. (8)) which is a dimensionless measure limited to the range of 0–1 and thus, allows the comparison of different models (Niska *et al*. 2004).

$$I = 1 - \frac{\sum_{t=1}^{N}(A_t - F_t)^2}{\sum_{t=1}^{N}(|F_t - \bar{A}| + |A_t - \bar{A}|)^2} \tag{8}$$

3. Results and discussion

3.1 The MLP neural network results

Table 1 presents the statistical summary of the data.
From the 195 available data, we used the 15% for testing, 15% for validating and the rest of 70% data for training the network. Fig. 5 presents the results of training, validation and testing errors for the MLP neural network with different iteration numbers (Epoch). As illustrated in Fig. 5, the

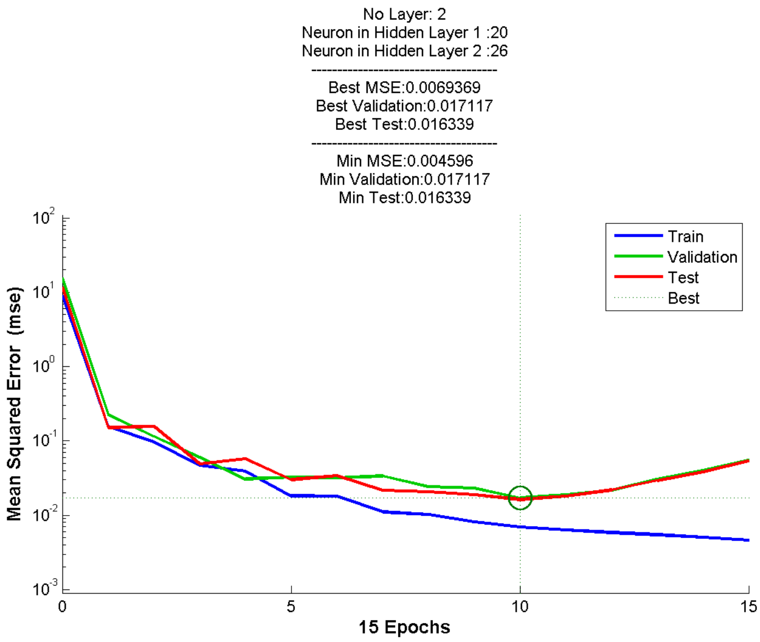

Fig. 5 Training, validation and testing errors of the MLP neural network

Table 1 Statistical summary of data

Statistical parameters	Moisture (%)	Wind speed (m/s)	Temperature (℃)	NOX (ppb)	Toluene $\frac{\mu g}{m^3}$
Average	23	2.42	31	30.79	68
Peak	29	9.8	36	97.71	100
Minimum	12	0.3	23	3.93	25
Number	195	195	195	195	195

Table 2 The testing error values for the MLP network with two hidden layers and different neurons

Neuron number	MBE	RMSE
5-7	0.113	0.156
5-21	0.105	0.138
10-10	-0.098	0.124
10-45	-0.087	0.100
15-10	0.031	0.075
20-12	0.025	0.061
20-26	**-0.014**	**0.056**
22-30	0.043	0.100
25-28	0.030	0.071
30-30	-0.061	0.141
35-35	0.111	0.252

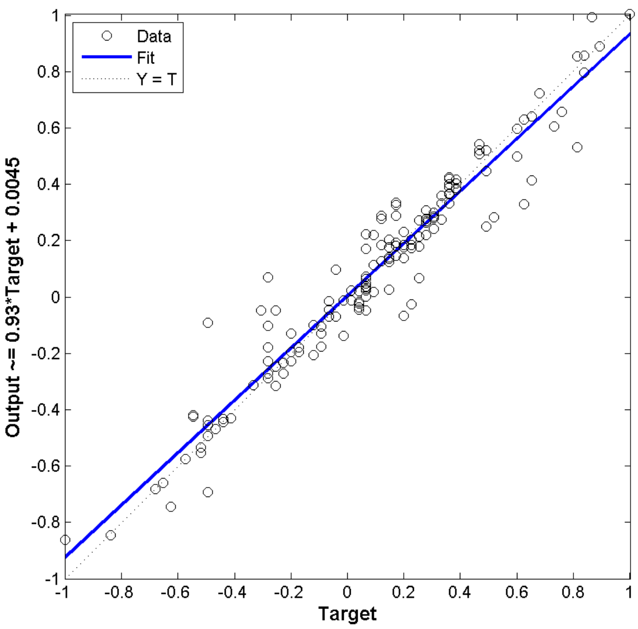

Fig. 6 The normal plot between observed and predicted toluene concentrations on the MLP network

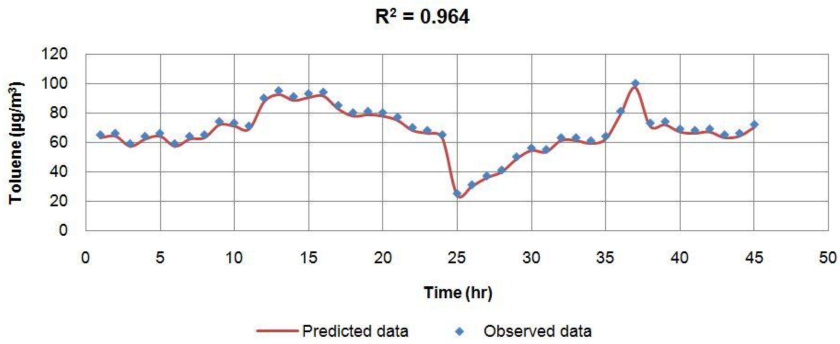

Fig. 7 Comparison between observed and predicted toluene concentrations using the MLP neural network

Mean Squared error was relatively unchanged after 15 iteration numbers. Therefore, we stopped the train of the network at 15th Epoch.

Table 2 indicates some of the neuron results together with their errors in two hidden layers. The results indicate that the MLP neural network with 20 neurons in the first layer and 26 neurons in the second layer, had minimum errors. The Mean Bias Error (MBE) and MSE in this case were -0.0142 and 0.0069 (Fig. 5), respectively, which proved the accuracy of the network. The negative amount of MBE presents the simulated values are underestimated.

As indicated in Fig. 6, in the MLP neural network the coefficient of determination between predicted and observed data was 0.9642 in the two hidden layer neural networks with 20 and 26 neurons in first and second layer, respectively, which indicated a good performance of the model. In Fig. 6, the observed and predicted data are illustrated in horizontal and vertical axis, respectively.

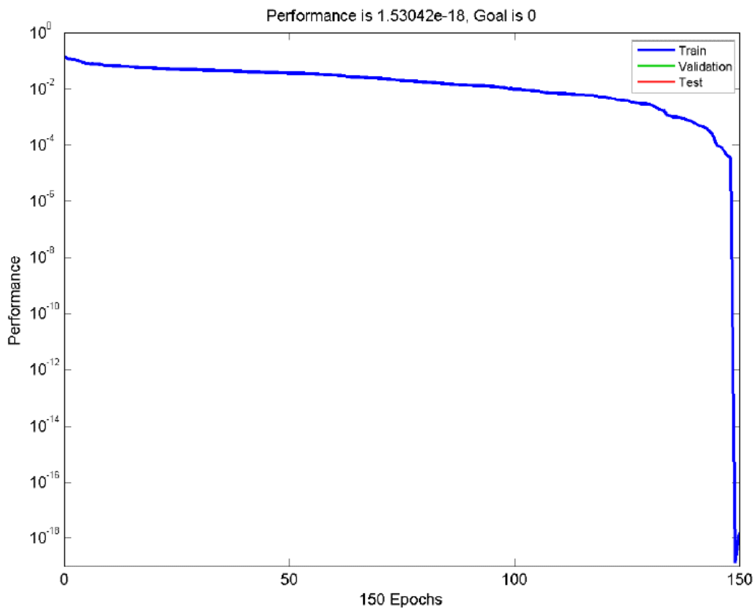

Fig. 8 Training, validation and testing errors of the RBF neural network

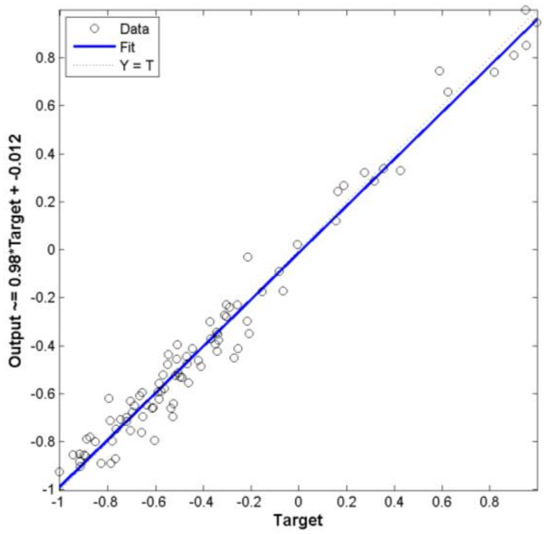

Fig. 9 The normal plot between observed and predicted toluene concentrations of the RBF neural network in testing

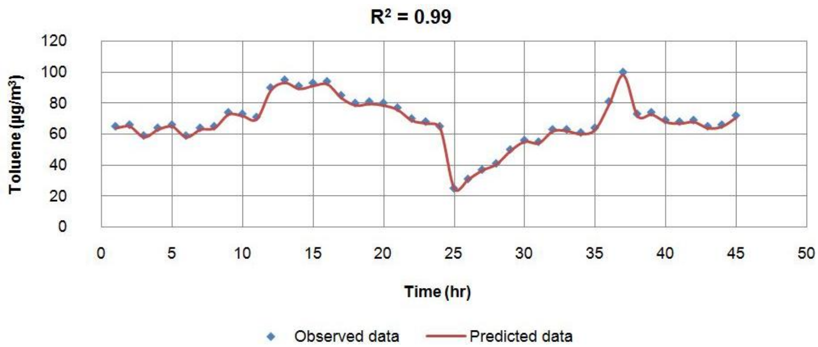

Fig. 10 Comparison between observed and predicted toluene concentrations using the RBF neural network

Fig. 7 indicates the observed data and the predicted data. As illustrated in this figure, the results of observed and predicted data are in good agreement. The coefficient of determination between the predicted and the observed data was 0.964, which means that the prediction for toluene concentrations was reliable. The efficiency (E) and index of agreement (IA) were 0.979 and 0.994, respectively, which may prove the workability and efficiency of the model.

3.2 The RBF neural network results

To train the model in the RBF neural network, 195 neurons in the single hidden layer were selected. In Fig. 8, in the training process of the RBF network, the errors of the network decrease while iteration numbers (epoch) increase. We stopped training the neural network when increasing the amount of the epoch did not change the amount of error significantly. As illustrated in Fig. 8, the amount of MSE error was about 0.01. Decreasing the number of errors, improves the performance of the model. The MBE was 0.00, which means the model is adequate.

Table 3 The results of sensitivity analysis

Parameters	R^2		
	Changing data		Not changing data
	+ 20%	– 20%	
Temperature	0.912	0.894	0.964
Wind speed	0.954	0.944	0.964
NO_x	0.961	0.962	0.964
Relative Humidity	0.955	0.959	0.964

As indicated in Fig. 9, because of the nonlinear separation nature in RBF neural artificial network, the coefficient of determination between the predicted and the observed data were 0.999 which is higher than the MLP neural network. The index of agreement (IA) and the efficiency (E) were 0.999 and 0.991, respectively, which describes the accuracy and workability of the model. In Fig. 9, the horizontal axis are observed data and the vertical axis indicates predicted data.

Fig. 10 presents the predicted and observed toluene concentrations. The coefficient of determination is 0.999 which may indicate the accuracy of the model.

3.3 Sensitivity analysis

Sensitivity analysis is a method to assess the importance of each input parameter on the value of the output. We decreased and increased each of the input parameters 20%, when the other input parameter data was kept unchanged. After that, the impact of each parameter in prediction of the toluene concentrations was identified.

Table 3 presents the results of sensitivity analysis. As indicated in Table 3, temperature had the greatest impact (about 72%) on the toluene concentration prediction. After that, wind speed, relative humidity and NO_x were effective, respectively. The high effect of temperature on toluene concentration may be caused by volatile nature of this component.

4. Conclusions

The results of the application of the MLP and the RBF neural networks to predict toluene concentrations in the southeast of Tehran can be summarized as follows:

- In both the MLP and RBF model, we obtained the high coefficient of determination which were 0.964 and 0.99, respectively.
- In the MLP model, a network with two hidden layers with 20 neurons in the first and 26 neurons in the second layer had a minimum of errors in testing. The RMSE and MBE were 0.056 and -0.014, respectively.
- In the RBF neural network, with a hidden layer, we obtained the minimum error in comparison with the MLP network. In the RBF network the MBE was 0.00 while in the MLP the MBE was -0.014 which indicated that the adequacy of the RBF model is higher than the MLP neural network.
- The results of sensitivity analysis indicated that temperature has the greatest impact on the prediction of toluene concentrations. After that, wind speed, humidity and NO_x were in the

second, third and fourth positions, respectively.

- Considering the results of forecasted data and the amount of E and IA, the RBF in comparison with MLP, has a higher efficiency and more workability in predicting air pollutants with acceptable accuracy.

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