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Original Research

Artificial Neural Networks for Surface Ozone Prediction: Models and Analysis

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Abstract

Ozone is one of the most important constituents of the Earth's atmosphere. Ozone is vital because it maintains the thermal structure of the atmosphere. However, exposure to high concentrations of Ozone can cause serious problems to human health, vegetation, and damage to surfaces. The complexity of the relationship between the main attributes that severely affect surface ozone levels have made the problem of predicting its concentration very challenging. Innovative mathematical modeling techniques are urgently needed to get a better understanding of the dynamics of these attributes. In this paper, prediction of the surface ozone layer problem is investigated. A comparison between two types of artificial neural networks (ANN) (multilayer perceptron trained with backpropagation and radial basis functions (RBF) networks) for short prediction of surface ozone is conclusively demonstrated. Two models that predict the expected values of the surface ozone based on three variables (i.e. nitrogen-di-oxide, temperature, and relative humidity) are developed and compared.

Keywords: air pollution, surface ozone, multilayer perceptron neural network, radial basis function (RBF) neural network, modeling

Introduction

Ozone (O_3) is a constituent and the most important photochemical oxidant of the troposphere (the lowest portion of Earth's atmosphere). It is also an important constituent of the stratosphere which is the second major layer of Earth's atmosphere (just above the troposphere and 10 to 50 km altitude above the surface). The stratosphere is known as the ozone layer. Ozone is vital because it maintains the thermal structure of the atmosphere [1]. Surface ozone is a secondary photochemical pollutant formed by a set of complex chemical interactions of nitrogen oxides NOx and volatile organic compounds (VOC) (also known as non-methane hydrocarbons) in the presence of ultraviolet radiation (UV) [2]. These primary pollutants are generated from urban and industrial sources such as transportation emissions, mobile sources, burning of fuel, and petrochemical processes. Ozone formulation can be expressed in the following formulas:

$$NO_2 + UV \rightarrow NO + O$$
$$O + O_2 + M \rightarrow O_3 + M$$

...where M is a third body molecule that doesn't change in the reaction. Ozone has a complex relationship with its precursors such as NOx, because the meteorological and chemical reactions vary from slow to fast rates. In order to estimate ozone concentrations, determining the emission rates of these pollutants and meteorological factors is essential. Many previous studies applied different techniques based on these rates to predict ozone levels. Such studies include statistical regression, fuzzy theory, and heuristic approaches. Some of these techniques are more preferable over others for empirical implementation, if they proved the capability of giving insight into the relationships between these primary pollutants.

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Health and Environmental Problems

Several studies and reports pointed out that ozone is one of the most crucial pollutants regarding air quality and climate change. For instance, ozone is an effective anti- greenhouse gas and has a direct effect on oxidizing photo- chemical smog [3, 4]. However, the World Health Organization (WHO) has reported that the health effects of ozone have been investigated less than other pollutants like particulate matter (PM), therefore more research is required [5]. Recent epidemiological research studies have shown that ozone can cause many hazard health problems depending on short and long-term exposure. Some of these effects include the following:

- Long-term exposure can cause lung damage and inflammatory responses.
- Respiratory irritation reduces lung functions, causing difficulty in breathing, coughing, throat irritation and aggravate asthma problems, and chronic lung diseases.
- With high concentrations of ozone, people with asthma are likely to have more attacks.
- Short-term exposure with high concentrations affects mortality and respiratory morbidity and causes eye irritation and may affect the respiratory tract.
- Ozone can significantly increase the risk of death (between 0.2% and 0.6% per each increase in 10 g/m^3 or 5 ppb) [5]. In general, exposure to ozone increased hospital admissions for cardiovascular and death counts.

In addition to its potential human and animal health hazards, ozone affects vegetation, causing noticeable foliage damage; reduces photosynthesis, growth, and other plant functions; and it could be toxic to certain crops. It was reported that tropospheric ozone could be the cause of over 90% of vegetation damage [6]. Moreover, ozone can cause damage to surfaces, fabrics, and rubber materials.

It is important to note that ozone has seasonal patterns different than other pollutants. Ozone concentrations have strong correlation with the season in a peak at summer. Therefore, a control of seasonal patterns should be applied in order to develop effective ozone prediction models. In this research, only one season (three months from May 2009 to July 2009) was selected for the case study of this research as mentioned and detailed in section II.

Previous Work

Recently, soft computing models were widely applied to environmental problems. Soft computing is a term that covers artificial intelligence approaches that resemble biological processes in solving complex and nonlinear problems. Predicting ozone levels is one of these problems that has been extensively examined. Among these approaches, artificial neural networks (ANN) is the most applied in the domain. ANN can be briefly described as an information-processing system that consists of a pool of simple processing units (called "neurons") that communicate by sending signals to each other over a large number of weighted connections. ANN is distinguished by certain performance characteristics such as its architecture, its training algorithm, and the activation function.

In several previous works, ANN-based models proved it better to obtain ozone prediction results rather than other statistical based approaches like autoregressive moving average (ARMA) models and linear regression models [7-9]. A wide variation of ANN-based models were implemented as empirical predicting tools for ozone surface. These models are varied according to ANN structure and their learning algorithms. Some implementations include the commonly used multilayer perceptron (MLP) with backpropagation training algorithms [4, 10, 11]. Hybrid ANN based approaches also were investigated in [3, 12-14].

Some other studies investigated other approaches. For example, authors in [15] developed support vector machine (SVM) models that showed promising results for ozone pollution forecasting. Fuzzy based models are another example. In [16] authors used fuzzy rule generation methodology for a grid located in Upper Austria in order to forecast ozone levels. Fuzzy models expressed the relationships between precursor emissions of NOx, VOC, and ozone concentrations.

Since ANNs showed their ability to model non-linear functions in a wide range of applications, two ANN-based models have been developed in this work for short-term surface ozone concentrations. The first approach is a multilayer perceptron neural network (MLP) trained with backpropagation algorithm, while the second approach is a radial basis functions (RBF) neural network. The proposed models can predict the mean surface ozone based on three attributes that can be easily measured with low cost measuring tools and sensors. These attributes include: nitrogen-di-oxide, temperature, and relative humidity. Both developed models will be evaluated using different performance criteria and a comparison study is conducted. Moreover, the presented work will perform sensitivity analysis on the selected attributes to study which of these parameters has a higher impact on the ozone concentration level.

Area of Study and Data Description

The study area is Chenbagaramanputhur (8º15'1"N, 77º29'19"E) (Fig. 1), a countryside in Kanyaku- maridistrict which is about 12 kms from Nagercoil town. The operating temperature range is from 5ºC to 50ºC, and relative humidity limits are 5% and 95%. On the other hand, nitrogen dioxide NO_2 was measured using a gas-sensitive semiconductor (GSS)[1]. The sampling was carried out for three months from May 2009 to July 2009. For ozone, seven readings were taken per day starting from 530 h to 2,330 h with three-hour intervals. For NO_2, only two readings were taken: one in daytime and the other at night. Furthermore, the data set used in this work was carried out for three months from May 2009 to July 2009. For the ozone, seven readings were taken per three-hour interval. For the NO_2, only two readings were taken each day: one in daytime and the other at night. The model inputs and output are given in

[1]Description available in www.aeroqual.com

Table 1. Inputs and output for the surface ozone model.

Inputs	Nitrogen dioxide concentration	x1
	Mean temperature	x2
	Prevailing % relative humidity	x3
Output	Mean surface ozone concentration	y

Table 1. The forecasting horizon of the model is three hours ahead. Fig. 2 shows the values of the variables used to develop the model as measured and collected by R. Samuel Selvaraj et al. in [17].

Artificial Neural Network

The human brain has the ability to perform multi-tasking. These tasks include controlling human body temperature, controlling blood pressure, heart rate, breathing, and other tasks that enable human beings to see, hear, smell, and so on. The brain can perform these tasks at a rate that is far faster than the rate at which a conventional computer can perform the same tasks [18]. The cerebral cortex of the human brain contains over 20 billion neurons with each neuron linked with up to 10,000 synaptic connections [18]. These neurons are responsible for transmitting nerve signals to and from the brain. Very little is known about how

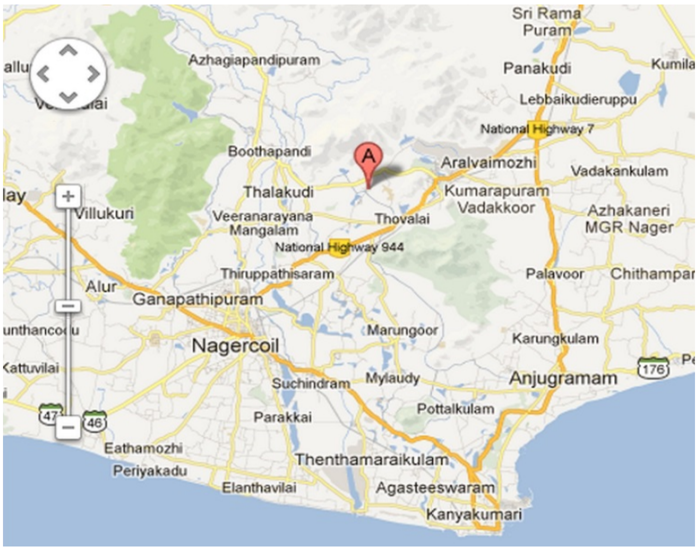

Fig. 1. Location of the study area.

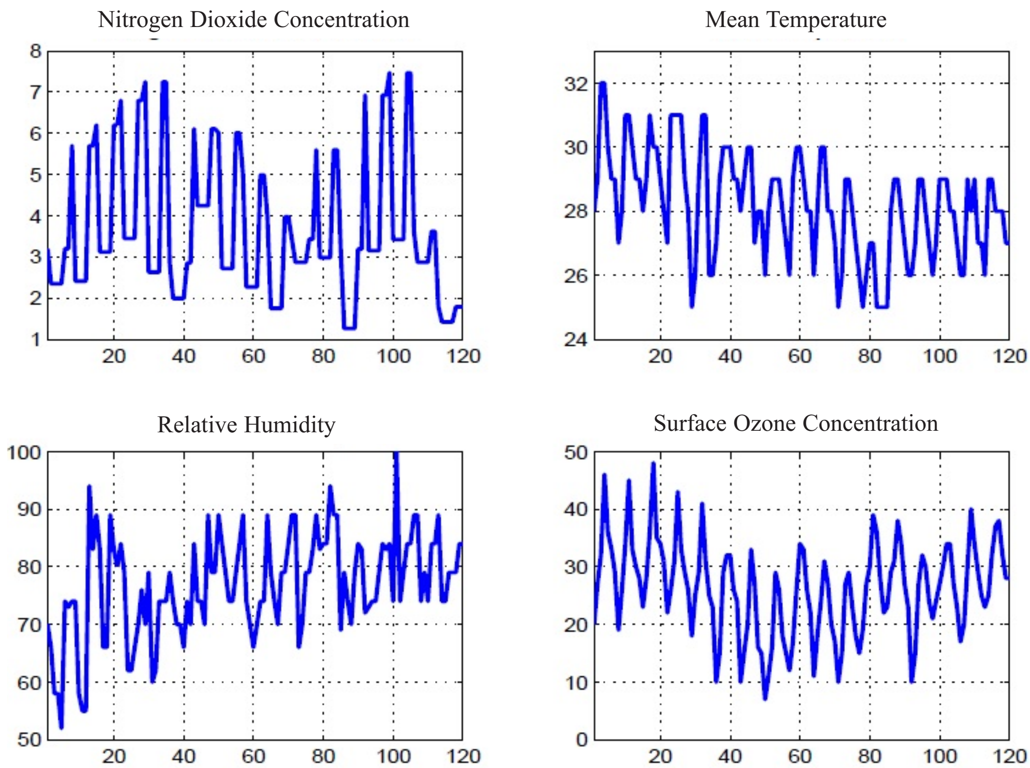

Fig. 2. Training and testing data set [17].

the brain actually works, but there are computer models that try to simulate the same task that the brain carries out. These computer models are called *Artificial Neural Networks*, and the method by which the neural network is performed is called a *Learning Algorithm*, which has the duty of training the network and modifying weights in order to obtain a desired response.

Each neuron has a number of inputs and a single output. Each input has an assigned factor or parameter called weight. The way a neuron works is as follows: input signal to each neuron is multiplied by the corresponding weight, then the result from the multiplication is summed and passes through a transfer function, most likely to be a sigmoid function. There are two main features making neural networks a very useful tool in solving prediction and modeling problems. Those features include the ability to learn and generalize. The learning process depends on providing a set of training data that is used to adjust network weights using a described learning algorithm. After the training process the network will be able to recognize a certain output when new data is presented to its input layer. This is what we mean by generalization. Finding the network weights, such that the difference between the network output and the desired output, is the main job of the ANN learning algorithm. One of the most well-known neural network architectures is the feedforward neural network (FFNN).

MLP-ANN

The most common and well-known feedforward neural network (FFNN) model is called multi-layer perceptron (MLP). MLP has been successfully applied in a number of applications, including regression problems, classification problems, or time series prediction using simple autoregressive models. The structure of a simple MLP network (with single hidden layer) is shown in Fig. 3. Moreover, MLP allows the data flow to travel in one direction, only from input to output. There is no feedback; it tends to be straight-forward networks that associate inputs with outputs.

Any MLP network can be distinguished by a number of performance characteristics, which can be summarized into three points [19, 20]:

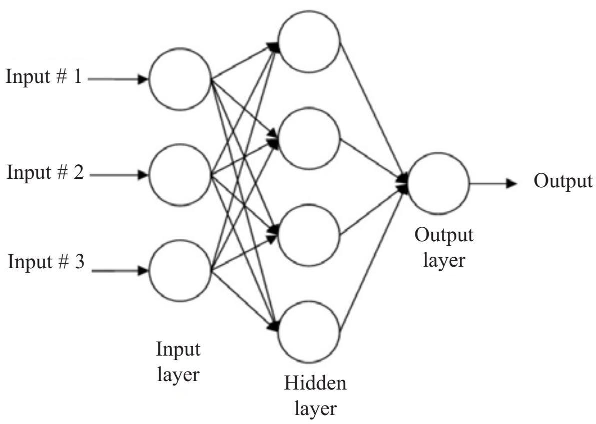

Fig. 3. MLP structure.

Table 2. Examples of some common transfer functions.

Transfer function	Definition
Linear	$f(x) = x$
Sigmoid	$f(x) = \dfrac{1}{1+e^{-x}}$
Hyperbolic	$f(x) = \dfrac{e^{x}+e^{-x}}{1+e^{-x}}$
Hard limit	$f(x) = f(x) = \begin{cases} 0, & x < 0 \\ 1, & x \geq 0 \end{cases}$
Hard limit	$f(x) = f(x) = \begin{cases} -1, & x < 0 \\ 1, & x \geq 0 \end{cases}$

- Neural network architecture: In general, MLP architecture can be defined as the pattern of connections between the neurons in different layers. MLP architecture consist of three layers: input layer, hidden layers, and output layer. Two nodes of each end-to-end layer are connected. MLP is always fully connected. Each link has a weight that is defined based on the training algorithm. More complex architectures have more layers.
- Training algorithm: The method of selecting one model from the set of models allowed, which determines the weights of the connections.
- Transfer function: Transfer function is applied by each neuron to its net input (sum of weight input signals) to determine its output signal. This function is usually nonlinear. Sigmoid function (S-shaped curve) is one of the most commonly used transfer functions. The sigmoid function and other common transfer functions are listed in Table 2.

In order to understand the algorithm of the learning process, suppose that a given MLP has N neurons in the input layer and m neurons in the hidden layers, and one output neuron. The learning process can be divided into a number of stages as described below:

1 Hidden layer stage: Given a number of inputs ψ_i and a set of corresponding weights between the input and hidden neurons w_{ij}, the outputs of all neurons in the hidden layer are calculated by the following equations:

$$O_i = \sum_{i=0}^{N} w_{ij}\psi_i \qquad (1)$$

$$y_i = z(O_j) \qquad (2)$$

...where $i = 1, 2, ..., N$ and $j = 1, 2, ..., m$. z and y_j are the activation function and output of the j^{th} node in the hidden layer, respectively. z is usually a sigmoid function given by Eq. (3).

$$z(x) = \frac{1}{1+e^{-x}} \qquad (3)$$

2 Output stage: The outputs of all neurons in the output layer are given by Eq. (4). l is defined as the number of neurons in the output layer. For simplicity, l is one.

$$\hat{Y} = f\left(\sum_{j=0}^{m} W_{jl} y_j^H\right) \quad (4)$$

...where f is the activation function of the output layer, which is usually a linear function. $\hat{Y}$ is the neural network output from the single neuron in the output layer as in our case study.

The MLP network is attempted to minimize the *Error* via the Backpropagation (BP) training algorithm with momentum term. BP learning starts with all weights initialized randomly, then weights are then modified as the algorithm progress until a steady state values are reached. The use of momentum causes a portion of previous weight change to be reapplied during the current weight update, which keeps the weight change in the same direction. Moreover, the role of momentum term is to keep the ball rolling through small local minima to avoid the descent, and to improve learning speed by gradually increasing the step size of the search in regions where the gradient is unchanged [19].

3 Error validation stage: ANN continues the learning process until the error minimization criteria is reached. Assuming that the desired output is Y and the produced ANN output is $\hat{Y}$. The learning process should stop with the error difference given in Eq. (5) is minimum. T is the total number of observations used to build the ANN model during training. Another set of data must be used to validate the developed ANN model performance.

$$Error = \frac{1}{T}\sum_{i=1}^{T}(Y_i - \hat{Y}_j)^2 \quad (5)$$

In MLP all the network weights and bias values are assigned with random values initially, and the goal of the training is to find the set of network weights that cause the output of the network to match the teacher values as closely as possible.

RBF-ANN

Radial basis functions (RBF) is another type of FFNN. The basic idea of RBF Network is to fit a curve of the data into a high dimensional space. RBF network typically has three layers in its basic form: an input layer, a hidden layer with a non-linear RBF activation function, and an output layer with linear activation functions as shown in Fig. 4. The input layer is connected to the hidden layer. The hidden layer transforms the input to a high dimensional space where each neuron in the hidden layer is implementing a radial function. The output layer is the last layer of the network, where all the hidden neurons are connected to the output neuron by adjusting output weights. The output neuron calculates the sum of the linear combination of the radial basis function of the hidden neuron parameter.

Let RBF with D input units, N internal (hidden) units, and L output units, the activation function of the i^{th} neuron with a fixed kernel is given as follows:

$$\phi_i(x) = \exp\left[-(x-\mu_i)^T \sum_i^{-1}(x-\mu_i)\right] \quad (6)$$

...where x is the input feature vector, u_i and Σ_i are the mean and covariance matrix of the i^{th} Gaussian function.

RBF networks are different on emphasizing the training part as it retrains as much as possible. This emphasizing gives the network very simple mathematics as it is basically linear algebra, and hence the computations will be very light and also fast. Moreover, RBF is used mainly for regression and for performing complex pattern classification tasks.

In the offline (batch) training mode of RBF network, the output unit weights are computed using any linear regression model, we used Ridge Regression given by the following equation:

$$W_{out} = (G + \lambda I)^{-1} y \quad (7)$$

...where I is the identity matrix and $\lambda > 0$ is a regularization factor, and G is an interpolation square matrix containing the activation functions of all neurons for all training samples. We used Gaussian kernels in our RBF model.

Model Evaluation

In order to check the performance of the developed FFNN models (MLP and RBF), the output weights of these models can be trained by minimizing a given loss function. In most cases we evaluate the model performance via the root mean squares error (RMSE) and the mean absolute error (MAE).

These performance criteria are assessed to measure how close the measured values to the values developed using the FFNN approaches. RMSE and MAE are computed as:

1) Root Mean Squares Error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y - \hat{y})^2} \quad (8)$$

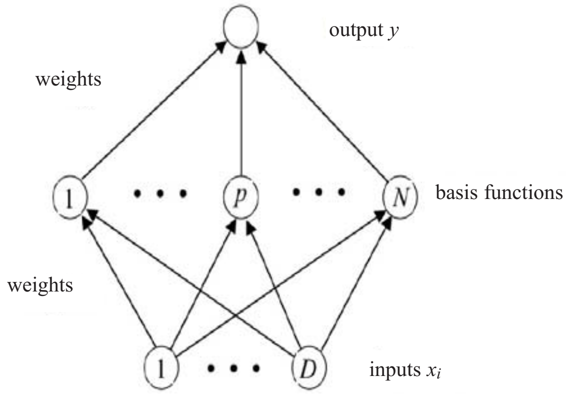

Fig. 4. RBF network structure.

Table 3. Prediction performances of the MLP models using different learning parameters.

Data	Epochs	Hidden neurons	Alpha	Momentum	Training		Testing	
					RMSE	MAE	RMSE	MAE
Not	650	2	0.1	0.2	6.915	5.468	5.671	4.45
Norm					0.072	0.057	0.0582	0.047
Not	1,850	4	0.1	0.1	6.438	4.983	6.477	5.229
Norm					0.0671	0.052	0.0726	0.0586
Not	850	6	0.1	0.3	6.572	5.217	6.698	5.608
Norm					0.0685	0.0543	0.0686	0.0529
Not	950	8	0.3	0.6	**6.222**	**4.848**	**5.367**	**4.073**
Norm					**0.0618**	**0.0505**	**0.0568**	**0.0448**
Not	1,100	10	0.2	0.3	6.255	4.919	7.232	6.084
Norm					0.0652	0.0512	0.0862	0.07

Bold means best results obtained

Table 4. Prediction performances of the RBF models using different numbers of hidden neurons.

Data	Hidden neurons	Training		Testing	
		RMSE	MAE	RMSE	MAE
Not	2	7.536	5.981	5.484	4.545
Norm		0.0785	0.0623	0.0854	0.0714
Not	4	7.636	6.022	5.311	**4.354**
Norm		0.0795	0.0627	0.0867	0.0728
Not	6	**6.485**	5.545	**5.282**	4.681
Norm		**0.0626**	0.0568	**0.0741**	**0.0612**
Not	8	6.596	5.466	6.725	5.481
Norm		0.0697	0.0569	0.0767	0.0657
Not	10	6.669	**5.438**	6.263	4.86
Norm		0.0705	**0.0566**	0.0921	0.0741

Bold means best results obtained

2) MEAN Absolute Error (MAE):

$$MAE = \frac{1}{n}\sum_{i=1}^{n} |y - \hat{y}|^2 \tag{9}$$

...where y and $\hat{y}$ are the actual and the estimated ozone measurements based on proposed models and n is the number of measurements used in the experiments.

Experimental Results

The definitive objective of our experiments in this work is to find the values of the surface ozone layer produced by each model of a function of nitrogen-di-oxide, temperature, and relative humidity. Therefore, our goal is to build two models structures (MLP and RBF), each of which has multiple inputs and a single output as given in Table 1.

The data set was divided into two parts. The first 75% of the data set was used for training while the rest (25%) was used for testing. For MLP we optimize the number of epochs by a step of 50, the learning rate α and *Momentum* in the range [0, 1] (step size 0.1). For RBF we optimized the regularization factor λ in the range [0, 1] (step size 0.1). For the two models (MLP and RBF) we varied the number of hidden nodes from 2 to 10 (step 2).

RMSE and MAE performance were used to measure the prediction results against the observed values as they verified in the previous section to see the most stable and suitable model for the ozone layer. Finally, the actual values are compared with the results (predictions) obtained by each model, where we present the errors (NMSE, MAE) for the original ozone data set (Not) and a normalized (Norm) version so that the dataset have zero mean and unity standard deviation.

The results in the training and testing stages for both MLP and RBF are given in Tables 3 and 4, respectively.

It can be seen clearly that the performance of the prediction capability of MLP-ANN outperformed the RBF-ANN.

The difference between the actual and estimated ozone results for both training and testing are given in Fig. 5, Fig. 6 for MLP, and Figs. 7 and 8 for RBF.

Sensitivity Analysis Using Change of MSE (COM) Method

This method ranks input variables in a given dataset according to the change of mean square error (MSE) when each input is deleted from the dataset in the training phase. Suppose we have *K* input variables. In order to measure the importance of each variable using COM technique, the dataset is trained *K* times with *K-1* variables, excluding a different variable each time. Therefore, variables which make the largest change in the MSE are considered the most important. One drawback of this method is that when there is noise and redundancy in the training set, there will be degradation in its reliability [21]. In our case, sensitivity analysis with the MSE method is applied on the best MLP and RBF models obtained earlier. Results of both cases are listed in Tables 5 and 6. It can be noticed that training and testing the ANN models without the temperature or the relative humidity makes a remarkable increase in the error values. While excluding the nitrogen-di-oxide values is less significant in predicting ozone concentrations.

Table 5. Sensitivity analysis for best MLP model.

Data	Inputs	Training	Testing
		MSE	MSE
Not	Nitro + Temp	48.525	34.246
Norm		0.00527	0.00349
Not	Nitro + RH	47.748	55.816
Norm		0.00518	0.01346
Not	Temp + RH	42.445	28.228
Norm		0.00461	0.00343

Conclusion and Future Work

In this paper, two neural network models were developed for short-term predictions of surface ozone in order to have an early and accurate alert. The first approach is a multilayer perceptron (MLP) neural network trained with a

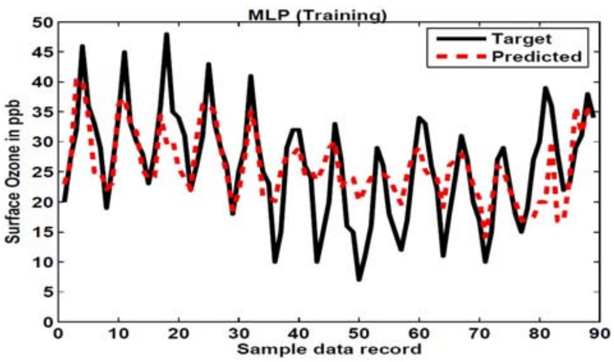

Fig. 5. Actual and estimated surface ozone measurements using best.

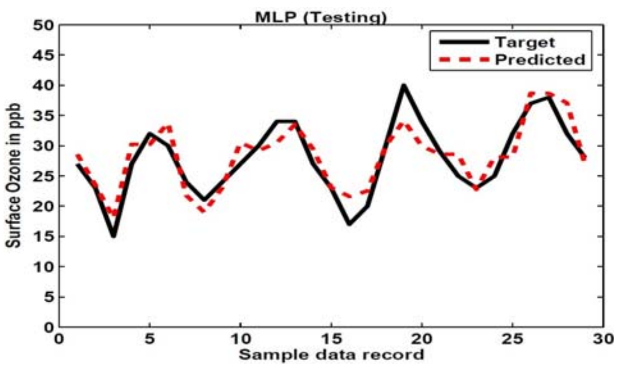

Fig. 6. Actual and estimated surface ozone measurements using best.

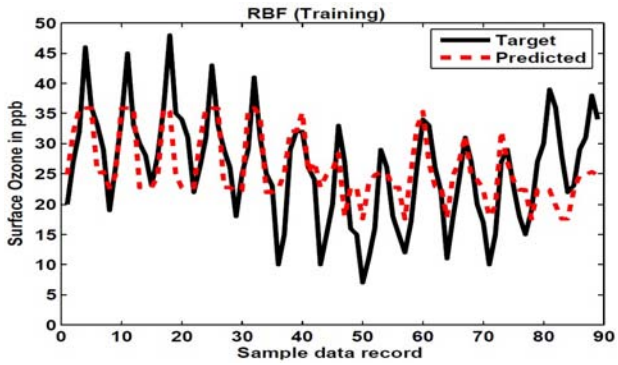

Fig. 7. Actual and estimated surface ozone measurements using best RBF.

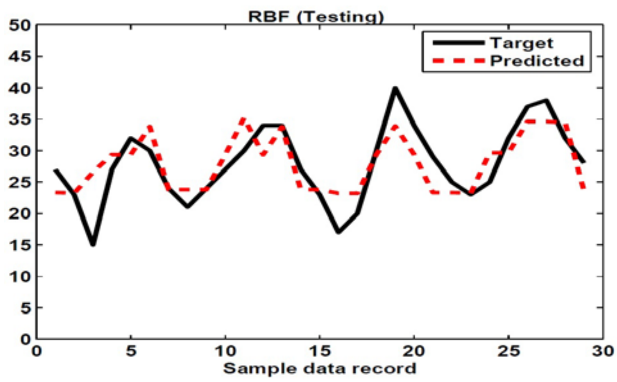

Fig. 8. Actual and estimated surface ozone measurements using best RBF.

Table 6. Sensitivity analysis for best RBF model.

Data	Inputs	Training	Testing
		MSE	MSE
Not	Nitro + Temp	49.224	41.719
Norm		0.00534	0.00419
Not	Nitro + RH	49.533	45.441
Norm		0.00537	0.01143
Not	Temp + RH	43.257	55.517
Norm		0.00469	0.00397

backpropagation algorithm, while the second approach is a radial basis functions (RBF) neural network. We have empirically demonstrated that the MLP neural network can lead to performance improvements over the RBF model, where the developed MLP network provided good estimation and prediction capabilities in training and testing cases as has been shown in the results section. Moreover, sensitivity analysis was conducted using the latter techniques in order to show which of the measured attributes has more influence on the ozone concentration level.

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