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Prediction of Maximum Ground Ozone Levels using Neural Network

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Abstract: Ozone is one of the most effective pollutants in lower atmosphere. Concentration of ozone in atmosphere reveals its impact on plants, human and on other organic materials. Many techniques had been used in past to calculate the concentration of ozone with the help of other environmental factors like wind, humidity, temperature and etc. Prediction models like Artificial Neural Network (ANN) have gained much reputation in calculating accurate results with learning data. This paper shows a study of integration of predicted ozone concentration by two ANN proposed models. The study initiated with data collection from the study area. The collected data is then fed to the proposed ANN models as training data to get the concentrations of ozone with many input variables temperature, humidity, wind speed, incoming solar radiation, sulfur dioxide, nitrogen dioxide, and previous ozone data as predictor. The study shows the great dependence of ozone concentration upon environmental factors. The two proposed Back Propagation (BP) models clearly gave good results according to statistical indicators. In terms of the gradient, mean error and the standard deviation values, the proposed two BP models perform well for both data sets.

Keywords: Air Quality; air pollution problem; Artificial Neural Network; Back propagation.

1. INTRODUCTION

Ground-level ozone (O3) has recently become a serious air pollution problem in many urban areas around the world. Numerous studies indicate that exposure to an elevated concentration of tropospheric ozone is a potential human health hazard [1],[2],[3] and affects vegetation adversely. The negative effects may relate to visible foliar injury, to physiological impairment and consequently to significant yield and growth reduction in agricultural crops and forests [4],[5],[6],[7]. Prediction and controlling ozone concentrations can therefore minimize effects of tropospheric ozone on human health and ecosystems.

Ozone prediction models as any other air pollution model can be either relied on the statistical models or on deterministic models. Deterministic models are based on a fundamental mathematical description of atmospheric physical and chemical processes in which effects are generated by causes [8],[9],[10]. These models, which numerically solve the complete set of time dependent equations incorporating complex photochemical reaction mechanisms, have been used to study pollution of photochemical smog in urban areas, regional scale dispersion of chemical species, long range transport, etc.

However, the deterministic models are highly sophisticated because they require a high level of human resources and powerful computer as well as detailed emission data and meteorological inputs for the region of interest. Some input data are not easily acquired by environmental protection agencies or local industries. This means that if these inputs are unknown, then the application of the deterministic models is problematic.

Statistical models are based on semi-empirical statistical relations among available data and measurements. They do not necessarily establish deterministic cause-effect relationships. They attempt to determine the underlying relationship between sets of input data (predictors) and targets (predicted). Many different statistical techniques have been proposed to predict ozone peaks. These include multiple linear regression [11],[12],[13], generalized additive models [14], classification and regression tree analysis [15], and application of principal component analysis and clustering technique [16],[17].

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However, the ozone formation process involving precursor emissions, atmospheric transport and mixing, and a complex system of photochemical reactions, is extremely nonlinear and non-stationary. None of the traditional statistic models were sufficiently dynamic to capture the rapid fluctuations in the ozone time series. Therefore, all the models appeared to have some difficultly forecasting high ozone events.

Other statistical approaches frequently used include several artificial neural network implementations. At present, the use of Artificial Neural Networks (ANNs) which can be trained to approximate virtually any smooth, measurable function, have become popular in atmospheric science and produced promising results. Particularly, the use of the neural networks in air quality modeling has been shown to give acceptable results for atmospheric pollution forecasting of pollutants such as ozone [18],[19], SO2 [20], PM10 [21],[22] and PM2.5 [23].

Many large urban areas experience elevated concentrations of ground-level ozone pollution during the dry season. This study investigates the potential for using a proposed neural network technique to predict daily and monthly maximum ozone levels models over Shobra Al Kheima urban area, Egypt during the summer dry season. Back Propagation (BP) neural network was used. The models were trained and validated using ambient air quality monitoring data and observed meteorological data during four ozone season (January to December) over Shobra urban area for year 2010.

The inputs to the neural network were the concentration of primary pollutants (sulpher dioxide and nitrogen dioxide) and meteorological conditions (wind speed, relative humidity, temperature and solar radiation).
While many studies related to the use of ANNs in air quality modeling are being done in other countries, no similar study has been done for Shobra Al Kheima urban area, where the highest ozone level was recorded in the period from June to August (summer dry season). Such studies are necessary in order to provide the alternative modeling tools for air pollution control in Shobra.
The rest of the paper is organized as follows. Section II describes, the Methology includes the area of study and data, the model building. Section III, represents the proposed two prediction Back Propagation Network models. Section IV represents the comparative analysis of the proposed two proposed models and evaluating their performance. Finally, the conclusions are drawn in Section V.

2. METHOLOGY

A. Area of Study and Data Ease

The dataset comprises daily average concentrations of ground level ozone concentration, sulpher dioxide, and nitrogen dioxide over Shobra Al Kheima area; it is located in a densely populated residential area. The most direct influence of the elevated level of ozone at that area is believed to be generated from the adjacent electric power plant.

B. The Model Buildings

In this study we selected the feed-forward back-propagation for proposed ANN model to predict daily and monthly maximum ozone concentration over Shobra.
Seven variables were selected as inputs and the output for the back propagation model is the value of maximum ozone levels. In this study, the learning algorithm used was Levenberg-Marquardt [24]. The activation function selected for the layers were logistic sigmoid for hidden layer and linear for the output layer. The number of hidden layers and hidden neurons (nodes) were tried and increased systematically, checking each time if the prepared neural network obtained the stable performance error in its.

The best Back Propagation (BP) network was the optimum found by the iterative process. The trained proposed BP network model was used to test the model’s performance with testing dataset of 200 and 100 patterns, respectively. The resulting predictions were then compared with observed data, and performance statistical indicators were calculated.

3. THE PROPOSED PREDICTION BACK PROPAGATION NETWORK MODELS

The highest maximum (1-hour) hourly ozone levels and frequency of ozone exceeding the Egyptian air quality standard (200μg/m^3, 1 h average). The results of the analysis also indicated that high ozone pollution over Shobra occur mainly in summer and lowest during winter season. Examination of diurnal distribution frequency of maximum hourly ozone levels over all the study area showed the highest ozone concentrations over Shobra occur in the period from June to August, so that we interested to predict ozone concentrations over Shobra in July.

The prediction of atmospheric ozone concentrations using our proposed two models based on the thermodynamic equilibrium of chemical components present in air. The proposed predication algorithm has user window interface for selecting the type of predicted model for ozone prediction daily or monthly as shown in the Figure (1). The proposed models can be learned and predicted ozone for any day or month in any year just by press on tab chosen in the program, then the program ask for name of the input file and output file.

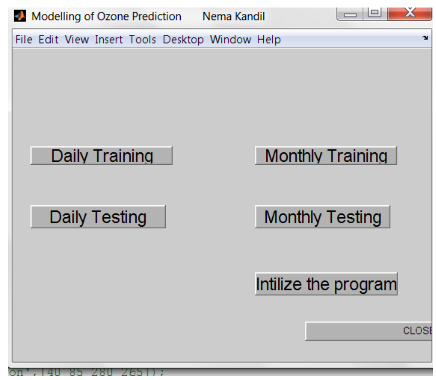


Figure (1): Screen shot of the proposed ozone prediction algorithm.

- Selection of Input and Output Variables

The goal of neural networks is to generalize a relationship of the form

$$Y^m = f(X^n) \qquad (1)$$

where X^n is an n-dimensional input vector consisting of variables $x_1,\ldots\ldots x_i,\ldots\ldots x_n$; and Y^m is an m dimensional output vector consisting of resulting variable of interest y_i.

The selection of an appropriate input vector that will allow neural net-works to successfully map to the desired output vector is not a trivial task. Unlike physically based models, the set of variables that influence the system are not known a priori. A neural network should not be considered mere a black box, a firm understanding of the system under consideration is an important aspect.

In our proposed Back Propagation model, the value of input data x_i in equation (1) causal variables metrological data. The values of y_i is ambient concentration of ozone, the following parameters were used as input data in the proposed two models:

1) Relative Humidity
2) Wind Speed.
3) Temperature.
4) Incoming Solar Radiation.
5) Sulfur Dioxide Data.
6) Nitrogen Dioxide Data.
7) Previous Ozone Data as Predictor.

A. The Proposed Prediction BP Model Daily Prediction

In the neural network development, different scenarios on the number of hidden layers, the number of neurons in each layer, and the type of transfer function for each neuron were analyzed, all with a learning rate of 1.0 and training goal of 10^{-6}. Then the trained networks were tested using the testing data sets and the minimum Mean Squared Error (MSE) method by modifying the network weights. It has been noticed that networks with two hidden layers of neurons may tend to remember the training data instead of generalizing it into patterns. The experience obtained by these exercises is consistent with the above conclusion. After unsuccessful attempts of the two hidden layer network architectures, two hidden layer networks were tried. By increasing the amount of neurons in the input layer, the training objective was achieved successfully.

Based on the results of iterative process in training stage, it was found that the architecture of the best proposed Back Propagation (BP) network contains two hidden layers with 7 input layer neurons, 10 hidden neurons for the first hidden layer, 14 hidden neurons for the second hidden layer and one output layer neuron (architecture 7-10-14-1). The proposed daily BP network was found to give good predictions for both the training and testing data set.

The different arrangements of input and output variables were carried out. The average daily values were used from the measured area in July for year 2010. Each of the three data sets consisted of about 200 to 100 input-output pairs. Each data set was divided into two subsets: for the fitting step (learning set) and for the model validation (test set). In order to avoid extrapolations at the validation step, the test set variables were kept within the range of the learning set variables.

This training stopped when the validation error increased for six iterations, which occurred at iteration of 42. The training performance for Gradient- descent algorithm reached to the goal with Mean Square Error (MSE) for the training dataset were $7.8X10^{-7}$ μg/m^3 after 42 epochs. Performance in the training window, a plot of the training errors, validation errors, and test errors appears, as shown in the following Figure (2). The results are reasonable because of the following considerations:

• The final mean-square error is small.
• The test set error and the validation set error have similar characteristics.
• No significant over fitting has occurred by iteration 42(where the best validation performance occurs).

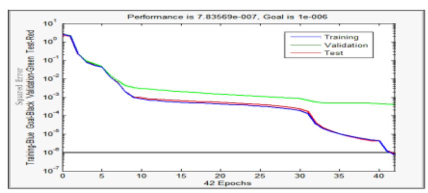
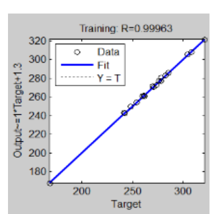
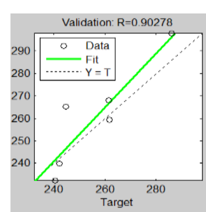


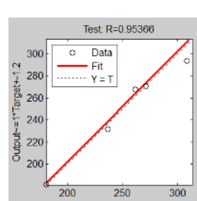
Figure (2): The best model training for the proposed daily BP model.

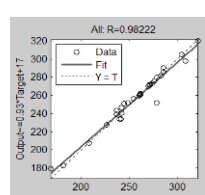
After the network had been trained, we used it to compute the network outputs. The following code calculates the network outputs, errors and overall performance. Figure (2) represents the scatter plots of observed data versus predicted ozone levels of the proposed daily Back Propagation model (a) Training dataset; (b) Validation dataset; (c) Testing dataset; and (d) all dataset.





(a) Training dataset (b) Validation dataset





(c) Testing dataset (d) All dataset

Figure (3 a-d): Scatter plots of observed versus predicted ozone levels (μg/m^3) for July of regression model.

The above figures a, b, c and d are regression plots display the network outputs with respect to targets for training, validation and test sets. For a perfect fit, the data should fall along a 45 degree line, where the network outputs are equal to the targets. For this problem, the fit is reasonably good for all data sets, with R(regression) values in each case of 0.9000 or above.

The proposed monthly Back Propagation (BP) model gives good predictions and the results produced are satisfactory. The correlation between observed and predicted ozone concentrations is found to be r = 0.99 (R^2= 0.9922), the R^2 value can be interpreted as the proportion of the variance in the simulated values attributable to the variance in the actual values.

To further check the accuracy of the proposed daily Back Propagation model, a plot of predicted versus observed ozone concentrations was shown in Figure (4). The predicted values are in good agreement with the recorded ozone concentrations, indicating that the maximum ozone levels are captured fairly well by the proposed daily BP model.

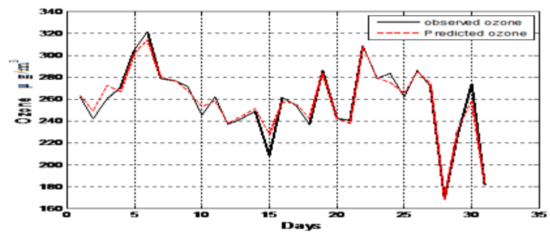


Figure (5): Comparison of observed and predicted ozone levels (µg/m^3) for the daily training dataset of the proposed daily Back Propagation model.

E. The Proposed Prediction BP Model for Monthly Prediction

The different arrangements of input and output variables were carried out. Monthly averaged values of the variables from the measured area for the year 2010 were used. Each of the three data sets consisted of about 200 to 100 input-output pairs. Each data set was divided into two subsets: for the fitting step (learning set) and for the model validation (test set). In order to avoid extrapolations at the validation step, the test set variables were kept within the range of the learning set variables.

Based on the results of iterative process in training stage, it was found that the architecture of the best proposed Back Propagation network contains two hidden layers with 7 input layer neurons, 12 hidden neurons for the first hidden layer, 20 hidden neurons for the second hidden layer and one output layer neuron (architecture 7-12-20-1). The proposed monthly BP model was found to give good predictions for both the training and testing data set.

As shown in Figure (5) the training stopped when the validation error increased for six iterations, which occurred at iteration 60. Performance in the training window, a plot of the training errors, validation errors and test errors appears. The results are reasonable because of the following considerations:

- The final mean-square error is small.
- The test set error and the validation set error have similar characteristics.
- No significant over fitting has occurred by iteration 60 (where the best validation performance occurs).

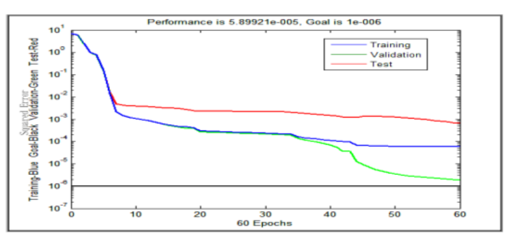
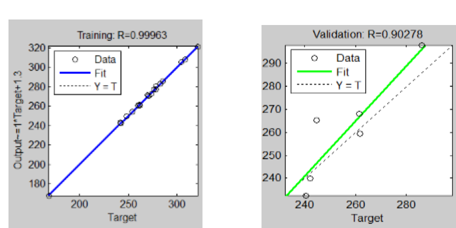
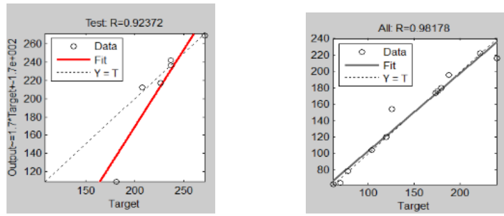


Figure (6): The best model training for the proposed monthly BP model

Figure (6) shows the Mean Square Error (MSE) for the training dataset was 5.9X10^{-5} µ g/m^3. After the network has been trained, you can use it to compute the network outputs. The following code calculates the network outputs, errors and overall performance. Figure (7 a-d) represented the scatter plots of observed versus predicted ozone for year levels of the model. (a) Training dataset; (b) Validation dataset; (c) Testing dataset; and (d) all dataset.



(a) Training dataset (b) Validation dataset



c) Testing dataset (d) All dataset

Figure (7a-d): Scatter plots of observed versus predicted ozone levels (μ g/m^3) year 2010 of the proposed monthly Back Propagation model.

The figures a, b, c and d are regression plots display the network outputs with respect to targets for training, validation and test sets. For a perfect fit, the data should fall along a 45 degree line, where the network outputs are equal to the targets. For this problem, the fit is reasonably good for all data sets, with R(regression) values in each case of 0.9000 or above.

The proposed monthly BP model gives good predictions and the results produced are satisfactory. The correlation between observed and predicted ozone concentrations is found to be r = 0.89 (R^2= 0.98178). The R^2 value can be interpreted as the proportion of the variance in the simulated values attributable to the variance in the actual values.

To further check the accuracy of the proposed monthly BP model, a plot of predicted versus observed ozone concentrations was shown in Figure (8). The predicted values are in good agreement with the recorded ozone concentrations, indicating that the maximum ozone levels are captured fairly well by the proposed Back Propagation (BP) model.

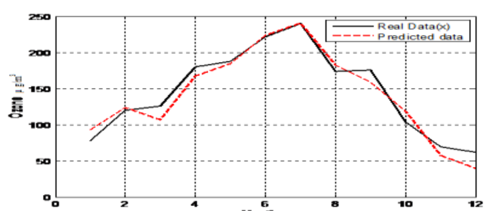


Figure (8): Comparison of observed and predicted ozone levels for the monthly training dataset of the proposed BP monthly model.

4. COMPARATIVE ANALYSIS COMARATIVE ANALYSIS OF THE PROPOSED TWO MODELS AND EVALUTING PERFORMANCE

Many model performance statistics are available in order to assess the accuracy of the estimates. For this particular work, the model performance and predicting results were compared by a set of three statistics (Gradient, MSE and Standard Deviation) .

The performance of the developed models was evaluated using statistical indicators comparisons. The relative effectiveness of the proposed two models in predicting ozone levels using the training data set is shown in Table (1). In addition, we examined the relative effectiveness of the proposed two models in predicting ozone levels using the testing data set is shown in Table (2).

TABLE I. PERFORMANCE STATISTICAL NDICATORS FOR TRAINING THE PROPOSED MODEL

Predication	Gradient	Mean square Error μg/m^3	Standard Deviation
Daily	1.81758e-04	$7.8X10^{-7}$	5.0766e-04
Monthly	2.1465e-01	$5.9X10^{-5}$	7.786e-02

TABLE II. PERFORMANCE STATISTICAL NDICATORS FOR tESTING THE PROPOSED MODEL

Predication	Gradient	Mean square Error μg/m^3	Standard Deviation
Daily	3.81758e-03	7.81268e-06	2.7643e-04
Monthly	1.1465e-02	5.82231e-05	3.2186e-02

From Tables (1) and (2), it can be noticed that the two proposed BP models clearly gave good results according to statistical indicators. In terms of the Gradient, Mean Error and the Standard Deviation values, the proposed two BP models perform good for both datasets.

The two BP models were proposed for Shobra urban area but they are not considered specific to only this area. Since, they can be extended to predict other sites, the methodology is probably generalizable. Another concern with our specific model is that the data chosen in this study was restricted from January to December for 2010. The period is of interest because it represents the worst case for ozone pollution in the Shobra Al Kheima area.

The proposed two prediction models in this study employed the independent variables measured in the morning on the prediction month. The use of the prediction day's values does not seriously limit the usefulness of the models for predicting ozone level in advance because the model can be modified using more surrogate variables.

5. CONCLUSION

This paper presents the development and use of ANN model for predicting the daily maximum ozone levels in Shobra. This study shows that the ANNs can be used in air pollution modeling. These ANNs can be a simple alternative model to provide reliable estimates of pollution by using only limit information.

The two proposed BP models clearly gave good results according to statistical indicators. In terms of the Gradient, Mean Error and the Standard Deviation values, the proposed two BP models perform good for both data sets.

The results shown here are indications that the two proposed neural predicted models techniques can be useful tool in the hands of practitioners of air quality management and prediction. The two models studied in this study are easily implemented and they can deliver prediction in real time, unlike other modeling techniques. The models can very well easily deal with in-put noise and uncertainty.

Forecasting the level secondary pollutant surface ozone forming over Shobra Al Kheima city in order to improve the knowledge and understanding troposphere processes.

The work will be helpful in future fort calculation of ozone in atmosphere and for drawing spatial interpolation of O_3. Moreover study high lights the areas of high concentration to control it before it increase above alarming levels.

The two BP models were proposed for Shobra urban area but they are not considered specific to only this area. Since, they can be extended to predict other sites, the methodology is probably generalizable. Another concern with our specific model is that the data chosen in this study was restricted from January to December for year 2010. The period is of interest because it represents the worst case for ozone pollution over Shobra Al Kheima area.

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