

Identification of the Best Architecture of a Multilayer Perceptron in Modeling Daily Total Ozone Concentration over Kolkata, India

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Abstract

Autoregressive neural network (AR-NN) models of various orders have been generated in this work for the daily total ozone (TO) time series over Kolkata (22.56°N, 88.5°E). Artificial neural network in the form of multilayer perceptron (MLP) is implemented in order to generate the AR-NN models of orders varying from 1 to 13. An extensive variable selection method through multiple linear regression (MLR) is implemented while developing the AR-NNs. The MLPs are characterized by sigmoid non-linearity. The optimum size of the hidden layer is identified in each model and prediction are produced by validating it over the test cases using the coefficient of determination (R^2) and Willmott's index (WI). It is observed that AR-NN model of order 7 having 6 nodes in the hidden layer has maximum prediction capacity. It is further observed that any increase in the orders of AR-NN leads to less accurate prediction.

Key words: autoregressive neural network, daily total ozone, multilayer perceptron, coefficient of determination, Willmott's index.

1. INTRODUCTION

During the last few decades, the study of ozone dynamics has gained immense importance for the communities of climatologists and meteorologists. Tropospheric ozone, which amounts to approximately 10% of the total ozone (TO) content, is a significant greenhouse gas. Kondratyev and Varotsos (2001a) gave a detailed account of the dynamics of the tropospheric ozone, and discussed the complexity of the dynamics through the consideration of a great number of relevant substances, like nitrogen compounds, volatile organic compounds, peroxyacetyl nitrate, hydroxyl radical, carbon monoxide, and alkyl nitrates. A review of the numerical modeling of ozone dynamics was made in Kondratyev and Varotsos (2001b) for the variability of the ozone concentration in the troposphere. The major motivation behind the research on ozone dynamics was the discovery of springtime ozone hole over Antarctica in the mid-1980s. Many attempts have been made to understand the ozone dynamics by performing different mathematical and statistical approaches (*e.g.*, Claude *et al.* 2004, Kondratyev and Varotsos 2000, Varotsos 2005). Thompson *et al.* (2001) discussed the increase in the tropospheric ozone over tropics as an impact of huge biomass burning over Indonesia and consequential responses to the El Niño and Indian Ocean Dipole. Jacob (2000) discussed the heterogeneous chemistry involving reactions in aerosol particles and cloud droplets that affect the tropospheric ozone. Eskes *et al.* (2005) identified the importance of ozone in numerical weather forecast modeling as:

- Ozone has a strong influence on the temperature and dynamics in the atmosphere on the time scale of weeks to months;
- Accurate knowledge on the ozone may improve satellite retrievals, especially the radiation modeling for the TOVS instruments;
- The assimilation of ozone observations in a modern 4D-Var or Kalman filter approach will have a direct impact on the wind field.

Ozone is formed from complex and non-linear photochemical reactions (Comrie 1997, Wolff 1998) and exists at different heights surrounding the Earth in different proportions based on the physical situation of its formation (Rubin 2001). It is mainly formed by the interaction of solar UV radiation with some organic and inorganic species within the upper atmosphere. In suitable ambient meteorological conditions (*e.g.*, warm, sunny/clear day) ultraviolet radiation (UV) causes the precursors to interact photochemically in a set of reactions that result in the formation of ozone (Comrie 1997, Corani 2005). Since the atmospheric processes are governed by non-linear physical laws and the ozone formation is governed by a number of atmospheric processes, application of different mathematical tools like Fourier spectral analysis, wavelet analysis, fractal analysis, detrended fluctuation

analysis have been accentuated by several authors (Varotsos 2005 and references therein). In tropospheric lower level, ozone is formed primarily from reactions between two major classes of air pollutants, *e.g.*, Volatile Organic Compounds (VOCs) and Nitrogen Oxides (NO_x) (Seinfeld and Pandis 1998). These reactions depend on the presence of heat and sunlight. There are many other combinations of reactions that yield ozone. The influence of meteorological events on the formation of tropospheric ozone has been discussed in several papers. Role of lightning on NO_x in the formation of tropospheric ozone was discussed by Hauglustaine *et al.* (2001). Complexity in modeling the tropospheric ozone is discussed by Pastor-Bárceñas *et al.* (2005), Sousa *et al.* (2006), and Demir *et al.* (2008).

The total ozone (TO) is a measure of the number of ozone molecules between the ground and the top of the atmosphere which is the integral of the ozone concentration with respect to height and measured in Dobson units (DU). The TO includes both tropospheric and stratospheric ozone. Since the stratospheric ozone varies on different time scales, the influence on the related tropospheric ozone chemistry acts on different time scales too. Thus, the total ozone time series is characterized by huge non-linearity attributed to meteorological variables, tropospheric ozone, and stratospheric ozone.

The TO concentrations are very difficult to model because of the different interactions between the pollutants and meteorological variables. Plethora of literature are available where statistical methodologies have been executed to look into different features of tropospheric and stratospheric ozone and their relationship with various meteorological parameters (*e.g.*, Cartalis and Varotsos 1994, Allen and Reck 1997, Varotsos *et al.* 2001, Varotsos 2005, Varotsos and Krik-Davidoff 2006, Hansen and Svenøe 2005, Aksoy *et al.* 2009). In these studies, the statistical methodologies are centered on multiple regression technique, which requires different meteorological variables as the predictors. In recent decades, research on non-linear deterministic dynamics has created new insights in the problems associated with complex phenomena (Sivakumar *et al.* 2004). Deterministic chaos within the total ozone is discussed in some literatures (Bandyopadhyay and Chattopadhyay 2008, Koçak *et al.* 2000). In recent times, the competence of artificial neural network (ANN) (Rojas 1996) in forecasting chaotic time series has been established by several authors (*e.g.*, Principe *et al.* 1992, Oliveira *et al.* 2000, Silverman and Dracup 2000). Earlier workers established that ANN is better than multiple regression models for weather-based ozone forecasting (Prybutok *et al.* 2000, Viotti *et al.* 2002, Corani 2005). Wang *et al.* (2003) combined statistical approaches with ANN in forecasting maximum daily ozone level. In this work, the relevance of different input parameters for developing the ANN model in the prediction of tropospheric ozone concentration has

been analyzed. Monge Sanz and Medrano Marques (2003) attempted ANN in studying total ozone time series over some urban areas of Europe.

A survey on the univariate modeling of ozone may now be introduced. The multivariate modeling of tropospheric ozone using meteorological variables as predictors has been attempted in several papers (*e.g.*, Massart and Kvalheim 1998, Soukharev and Hood 2006). However, the purpose of the present paper is to generate univariate models for TO time series. Yi and Pybutok (1996) pointed out that the development of forecasting models for ozone is difficult because the meteorological variables and photochemical reactions involved in ozone formation are complex. It is obvious that incorporating various meteorological variables in the input set leads to a cumulative effect of the complexities in the ongoing model and model output. Univariate time series consists of observations recorded sequentially over equal time increments. The advantage of a univariate model is that it depends only upon the values of the variable itself, observed at equidistant time points. In the limited data environment, a univariate model can enlighten various intrinsic features of the time series and can estimate the future values without taking the values of other related variables into account. A survey of the available works reveals some significant publications on the modeling of tropospheric ozone in a univariate environment (*e.g.*, Yi and Pybutok 1996, Chen *et al.* 1998, Graf-Jacottet and Jaunin 1998, Nunnari *et al.* 1998, Koçak *et al.* 2000, Gilleland and Nychka 2005, Abdollahian *et al.* 2006).

The univariate approach to the tropospheric ozone is not limited to the conventional statistical approaches. The ANN, in various forms, has been implemented by several authors to model the tropospheric ozone using the past values of the same variable. Yi and Pybutok (1996) justified with Box-Jenkins autoregressive integrated moving average (ARIMA) and ANN to forecast daily maximum ozone concentration in an industrialized urban area and revealed the supremacy of ANN over ARIMA for the said job. Prybutok *et al.* (2000) revealed the dominance of ANN over regression in modeling surface ozone with univariate approach in an urban atmosphere. In a recent work, Hrust *et al.* (2009) used univariate regression approach to select input variables for a multivariate ANN model for forecasting hourly concentration of ozone and some other pollutants. Ozone chemistry in the stratosphere is described by two parametrizations. One consists of a linearization of the gas-phase chemistry with respect to production and loss, the ozone amount, temperature and UV radiation, and the second parametrization scheme accounts for a heterogeneous ozone loss. Lahoz *et al.* (2007) reviewed univariate modeling of stratospheric ozone along with other stratospheric constituents. Other works on the univariate modeling of stratospheric ozone include Errera and Fonteyn (2001), and Struthers *et al.* (2002). However, none of the works include modeling stratospheric ozone in univariate man-

ner using ANN. The available ANN applications to the stratospheric ozone are multivariate in nature (Muller *et al.* 2003).

This work presents a new approach to the prediction of daily TO concentrations over Kolkata using an autoregressive neural network (AR-NN) in the form of a multilayer perceptrons (MLP). The proposed approach differs from the previous ones in the following aspects:

- Here, the daily TO is modeled in univariate manner over Kolkata which is a highly polluted urban area within the Gangetic West Bengal, characterized by severe pre-monsoon thunderstorms and heavy rainfall during the summer monsoon. No such study is available for this zone.

- In the available works mentioned above, univariate approaches are adopted for either tropospheric or stratospheric ozone. However, in the present paper, TO that comprises both stratospheric and tropospheric ozone is modeled.

- Autoregressive neural network (AR-NN) has been adopted instead of implementing ANN in multivariate manner.

2. METHODOLOGY

Description of data

In the present work, the data are derived from the measurements made by the Earth Probe Total Ozone Mapping Spectrometer (EP/TOMS). The EP/TOMS was the only instrument on board. The EP satellite was launched by a Pegasus XL rocket on 2 July 1996. The satellite reached its initial orbit of 500 km at an inclination of 98° and a local equator crossing time of 11:16 AM some 12 days later, and regular ozone measurements began on 25 July. The EP/TOMS experiment provides measurements of the Earth's TO by measuring the backscattered Earth radiance in the six 1 nm bands (NASA 1998). Here, the daily TO data over Kolkata for the period 2003-2005 are used to generate the neuro-computing based autoregressive model. The data are collected from the website <ftp://jwocky.gsfc.nasa.gov/pub/eptoms/data/overpass/OVP075epc.txt>. The implementation procedure and assessment of ANN models are discussed in the subsequent section.

A brief overview of multilayer perceptron (MLP)

An ANN can be viewed as a computing system that is made up of several simple and highly interconnected processing elements, which process information by their dynamic state response to inputs. It provides a powerful tool for problems difficult to solve by traditional approaches, and frequently many of them have been addressed with neural networks (Benvenuto and Marani 2000). Advent of the feed forward ANN or multilayer perceptron

(MLP) with backpropagation learning, an adaptation of the steepest descent method, opened up new avenues for the application of ANN for problems of practical interest (Kamarthi and Pittner 1999, Widrow and Lehr 1990). In MLP, the input and output layers are connected through a hidden layer. There may be one to several hidden layers between the input and output layers (Monge Sanz and Medrano Marqués 2004). In mathematical form, the adaptive procedure of a feed forward MLP can be presented as (Bandyopadhyay and Chattopadhyay 2007)

$$w_{k+1} = w_k + \eta d_k .$$

The positive constant η is called the learning rate. The direction vector d_k is the negative gradient of the output error function E . Mathematically it is denoted as

$$d_k = -\nabla E(w_k) .$$

The optimal weight matrix obtained this way is applied to the test set to investigate the viability of the model. Details of the MLP are available in the literature that include Rojas (1996) and Yagnanarayana (2004). Gardner and Dorling (1998) presented a review of the application of MLP in atmospheric studies.

Implementation procedure

The basic aim of this paper is to generate autoregressive neural network (AR-NN) (Dorffner 1996) for daily total ozone concentration over Kolkata. Prior to developing the AR-NN model, the autocorrelation function is computed for the daily TO over Kolkata. From the high value of the lag-1 autocorrelation coefficient (0.87) it is understood that the daily TO time series is characterized by serial dependence. However, it is further observed that the autocorrelation function resembles a sinusoidal pattern that does not decay to 0 with increase in lag. This indicates that the time series of daily TO is not stationary. This non-stationarity necessitates the implementation of AR-NN instead of linear autoregression.

A linear autoregressive model of order p can be expressed using p previous values of the time series, including a noise term, ϵ , as follows:

$$x(t) = \sum_{i=1}^p \alpha_i x(t-i) + \epsilon(t) .$$

In the above equation, a linear function F^L can be introduced, in which case the equivalent form of the above equation would be (Dorffner 1996)

$$x(t) = F^L [x(t-1), x(t-2), \dots, x(t-p)] + \epsilon(t) .$$

Replacement of L by MLP leads to the autoregressive neural network (AR-NN) model. This type of approach has been used by Chattopadhyay and Chattopadhyay (2009a) to develop univariate model for monthly total ozone over Kolkata.

In this work, competitive AR-NN models are generated for the daily TO concentration over Kolkata. An artificial neural network, in the form of MLP, is implemented in order to generate the AR-NN models. While developing AR-NN models, three-layered MLPs are developed for various orders of AR-NN. The order of AR-NN is defined as the number of past day TO concentrations considered as predictors to estimate the current day TO concentration. Thus, in general, an AR-NN model with n past values is identified as AR-NN(n). Beginning with single predictor, *i.e.*, AR-NN(1), the order of AR-NN is varied up to 13. Thus, 13 three-layered MLP models are generated. Each of these 13 models is characterized by sigmoid non-linearity and trained by the back propagation method explained earlier. An extensive variable selection method through multiple linear regression is implemented while developing the AR-NN models. Choosing the minimization of least square error as the stopping criteria, the optimum size of the hidden layer is identified in each model and predictions are produced by validating it over the test cases. For each model, the coefficient of determination (R^2) (Wilks 2006) and Willmott's index (WI) (Willmott 1982) are computed to assess the prediction potential of each model.

3. STATISTICAL SKILL ASSESSMENT

In Section 2, the method of implementing the ANN in generating a predictive model for total ozone in autoregressive manner has been discussed. The model has been abbreviated as AR-NN model to focus its univariate nature. After generating the thirteen AR-NN models for the daily total ozone concentration over Kolkata, the models have been assessed statistically in the present section with respect to their prediction capacity. The most popular and conventional statistic for testing the goodness-of-fit of a model to the observation is the Pearson correlation coefficient. However, in meteorological modeling, the shortcomings of the correlation coefficient have been discussed in Willmott (1982) and Willmott *et al.* (1985), where an alternative index was proposed to assess the suitability of a model to the observations. In subsequent works, this index started to be mentioned as Willmott's index of agreement (*e.g.*, Badescu 1994, Cannon and Whitfield 2002). In Fig. 1, the Willmott's indices (WI) for all of the thirteen models are presented. Closeness of WI to 1 indicates a good model. In Fig. 1 it is observed that in all of the thirteen models, the WI is above 0.90. This indicates that all of

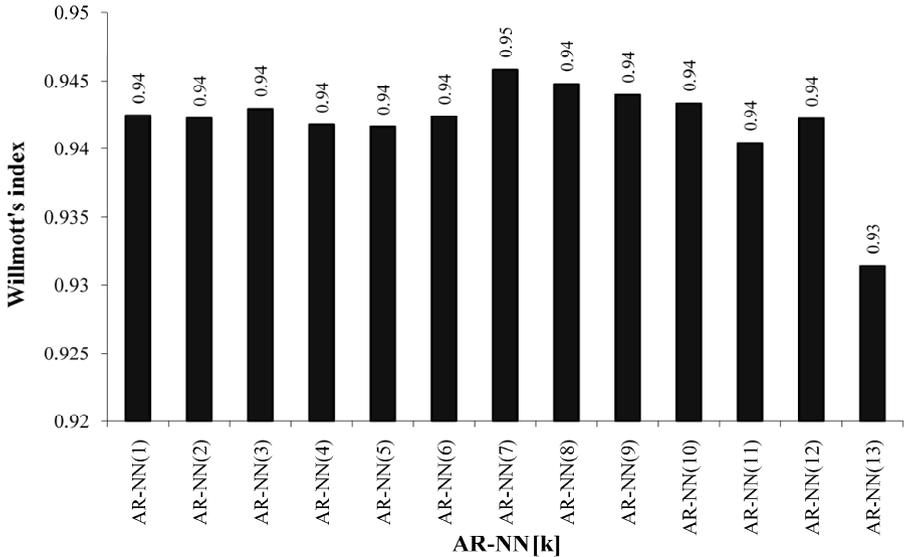


Fig. 1. Willmott's index of daily total ozone concentration over Kolkata for 13 AR-NN models.

the thirteen AR-NN models have significant degree of efficiency in predicting daily total ozone concentration over Kolkata based on the past values of the same time series. The AR-NN(13), that is, the AR-NN model with concentrations of total ozone corresponding to the previous thirteen days has the lowest WI and it differs significantly from the remaining twelve AR-NN models. The maximum value of WI (0.9458) is available in the case of AR-NN(7), which uses the previous seven days' concentrations of total ozone as predictors. It should be mentioned that in the single-hidden-layer multilayer perceptron used to generate AR-NN(7) model, there were 6 nodes in the hidden layer.

To further examine the goodness-of-fit of the AR-NN models, the coefficients of determination (R^2) are calculated for each of the models. Theoretical details of R^2 and its usefulness in judging a predictive model is available in Wilks (2006). The values of R^2 are shown in Fig. 2 for all the thirteen AR-NN models. It is observed that the AR-NN(7) model having 6 nodes in the hidden layer has maximum values of R^2 (0.8144). This agrees with the result obtained through WI. From a closer observation on Fig. 2, R^2 seems to be very similar in the four cases: AR-NN(4) to AR-NN(7). Thus, a further statistical test is implemented to examine the differences among these four AR-NNs. In this step, the following statistics are calculated for AR-NN(4), AR-NN(5), AR-NN(6) and AR-NN(7):

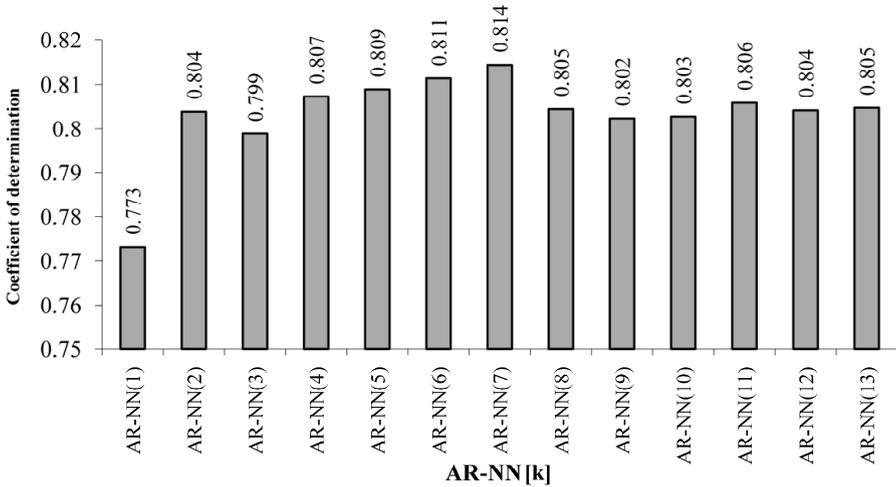


Fig. 2. Coefficient of determination of daily total ozone concentration over Kolkata for 13 AR-NN models.

Table 1

The tabular presentation of the statistics used to assess the AR-NN models

Models	MAE	PE	PY [5%]
AR-NN(4)	6.2772	2.365	0.8917
AR-NN(5)	6.2526	2.3572	0.9002
AR-NN(6)	6.2257	2.3472	0.9031
AR-NN(7)	6.192	2.3344	0.9088
AR(7)	6.5298	2.4645	0.8889
Persistence forecast	7.4577	2.8143	0.8461

- mean absolute error (MAE) (Wilks 2006)
- overall prediction error (PE) (Pérez *et al.* 2000)
- prediction yield (PY) (Chattopadhyay and Chattopadhyay 2009b).

In the case of PY, 5% error has been allowed in each prediction case and the fraction of the set of validation cases has been calculated for which the prediction errors are below 5%. The results are displayed in Table 1. It is observed from this table that AR-NN(7) has minimum MAE, PE and maximum PY among the four AR-NN models producing close values of R^2 . Thus, considering Figs. 1-2 and Table 1, AR-NN(7) is identified to be the best model for univariate forecast of daily total ozone over Kolkata. The observed total ozone time series and those predicted by the AR-NN(7) model are plotted in Fig. 3. In the line diagram, it is observed that in some of the

validation cases, the observed and predicted values are almost coincident. In this figure it is observed that some of the predicted values are found to be deviated significantly from the observed values. The PY has enlightened the deviations statistically.

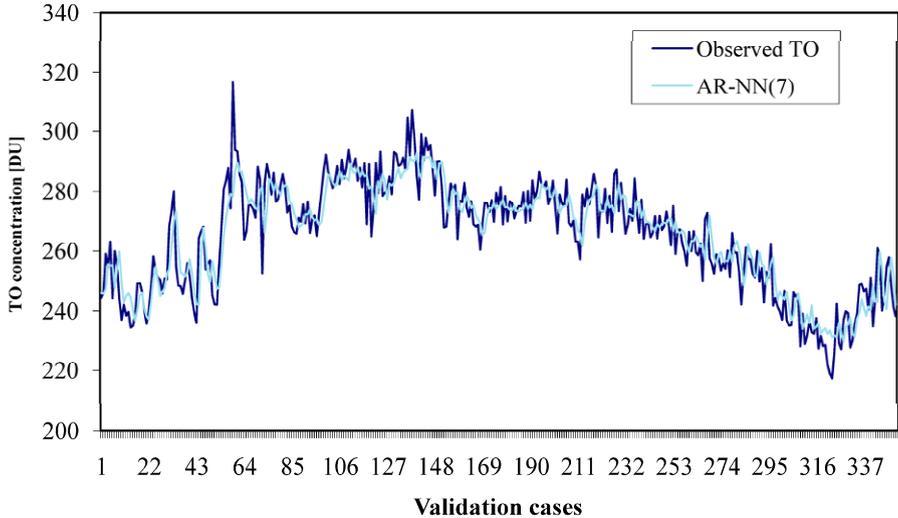


Fig. 3. Schematic plot showing the association between the observed daily total ozone and those predicted by AR-NN(7).

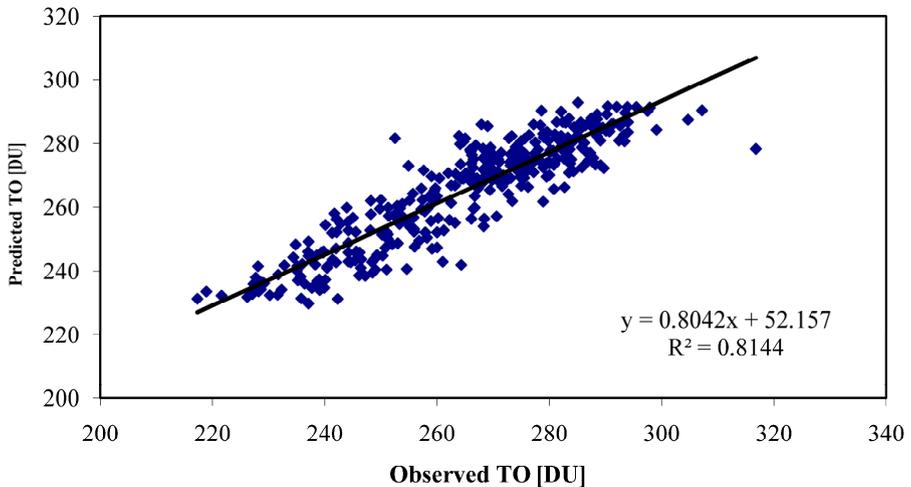


Fig. 4. Scatter-plot showing the association between the observed daily total ozone and those predicted by AR-NN(7).

As a further support to the prediction capacity of the AR-NN(7) model, the corresponding scatter plot has been presented in Fig. 4, which shows that there is a positively sloped cloud of data pairs consisting of actual and estimated data values pertaining to the validation cases. In the same figure, the association between the actual and estimated TO concentrations is presented in terms of the linear regression $y = 0.8042x + 52.157$.

The AR-NN(7) has seven predictors. Thus, to forecast the total ozone concentration on day n , the total ozone concentrations of days $(n-1)$, $(n-2)$, $(n-3)$, $(n-4)$, $(n-5)$, $(n-6)$ and $(n-7)$ are used as predictors. Now, the AR-NN(7) model is compared with the conventional autoregressive model of order 7, *i.e.*, AR(7). The statistics MAE, PE and PY are calculated for AR(7) and are displayed in Table 1. It is found that MAE and PE for AR(7) are larger than AR-NN(7) and PY for AR(7) is smaller than AR-NN(7). Thus, it is found that AR-NN(7) performs better than AR(7).

Since it has already been found that there is a high autocorrelation coefficient at lag-1 (0.87), it is understood that the time series of daily total ozone concentration is persistent (Wilks 2006). Thus, a persistence forecast (Peréz *et al.* 2000) is attempted. The results are displayed in Table 1. It is observed that the persistence forecast model produces higher prediction errors (PE) and lower prediction yield (PY) than the AR-NN(7) as well as AR(7) models.

4. CONCLUDING REMARKS

Autoregressive neural network models are attempted in this paper to model the total ozone time series over Kolkata in daily scale. Prior to the model development, the autocorrelation function for the said time series is observed to indicate non-stationary nature of the time series. Considering the non-stationary behaviour, thirteen competitive orders of the autoregressive neural network models are examined for the time series. The neural networks based autoregressive models are generated in the form of multilayer perceptron. After a thorough statistical investigations, the autoregressive neural network model of order 7 has been identified as the best to represent the daily total ozone time series over Kolkata. It has been further proved that the autoregressive neural network model of order 7 (AR-NN(7)) performs better than the autoregressive model of order 7 (AR(7)) and persistence forecast model. Thus, the crisp conclusion is that the daily total ozone over Kolkata can be predicted based on the seven immediately previous observations of the same as the predictors. Although the AR-NN (7) has a good overall prediction potential, it has been observed that in some cases the prediction errors are above 5%. In future, these errors may be further reduced by applying more advanced ANN learning rules.

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Received 1 June 2010

Received in revised form 1 August 2010

Accepted 21 September 2010