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A neural network model for short term prediction of surface ozone at Pune

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सार — न्यूरल संजाल तकनीक का प्रयोग करते हुए वायु प्रदूषण की अल्पावधि प्रागुक्ति के लिए एक नई प्रणाली प्रस्तुत की गई। औद्योगिक और मानवोद्भवी कार्यकलापों में वृद्धि के कारण वायु प्रदूषण आज एक गंभीर चिंता का विषय बन गया है। सतह ओजोन को कुल वायुमंडलीय आक्सीकारकों और वायु प्रदूषण का द्योतक माना जा सकता है। अनुकूलन पैटर्न मान्यता की तकनीक का प्रयोग करते हुए एक तीन स्तरीय न्यूरल संजाल निदर्श का विकास किया गया। इस निदर्श द्वारा 12 और 13 बजे (अधिकतम संकेन्द्रण का समय) के मध्य के माध्य सतह ओज़ोन का अनुमान लगाया जा सकता है। निदर्श प्रशिक्षण और स्वतंत्र दोनों अवधियों में सही कार्य कर सकता है। अल्पावधि निदर्शन की क्लासिकी पद्धतियां अधिक विश्वसनीय नहीं हैं। इस पद्धति का प्रयोग अन्य वायु प्रदूषकों की अल्पावधि प्रागुक्ति के लिए भी किया जा सकता है।

ABSTRACT. A new method for short term prediction of air pollution is presented using the neural network technique. Due to increase in industrial and anthropogenic activity, air pollution is a serious subject of concern today. Surface ozone can be considered as a representative of total atmospheric oxidants and of air pollution. A three layer neural network model using the technique of adaptive pattern recognition is developed. The model can predict the mean surface ozone between 12 and 13 hours (hour of maximum concentration). The model can perform well both in training and independent periods. The classical methods of short term modelling are not reliable enough. The method can also be used for short term prediction of other air pollutants.

Key words— Air Pollution, Neural network, Surface ozone, Short term prediction.

1. Introduction

Surface ozone is a secondary photochemical pollutant produced from a variety of natural and anthropogenic precursors that include industrial and vehicular emission of volatile organic compounds and oxides of nitrogen. In elevated concentrations, it has detrimental effects on vegetation, human health and various natural materials (Guicherit *et al.* 1987). Ozone is an important constituent of the atmosphere that maintains the thermal structure of the stratosphere and the troposphere. Many studies (Ramaswamy and Bowen 1994; Rajeevan, 1996; Bojkov, 1983) suggest that an increase in tropospheric ozone leads to the warming in surface temperature. Ozone is considered to be the cause of eye irritation (Ö AdW, 1989) and may affect the respiratory tract (Arndt, 1980) even during short term high concentrations.

The non-linear relationship of surface ozone with solar radiation has been mentioned by Bravo *et al.* (1996). There is a value of solar radiation for which ozone concentration has a maximum. This effect may be due to days with high solar flux having little atmospheric pollution, with little ozone formation and high atmospheric transparency (Bravo *et al.*, 1996). The problem of short term modelling in complex terrian are discussed in details by Bonzar *et al.* (1993). They have also shown that in the case of stable atmosphere and of thermal inversions the failure of dispersion model and the inadequacy of this model for controlling emissions. In this regard they have applied the neural network technique for short term prediction. The results obtained by them are significantly better than those obtained from conventional models.

Neural network techniques have recently become the focus of much attention as they can handle the complex and non-linear problems better than the conventional statistical techniques. Neural network is a simple mathematical input output model which learns the relationship (linear or non-linear) between the input and output during the training period. Neural network model brings out the maximum information available within the data during the training period and reflects these in the independent period. Present paper aims to develop a simple model using neural network technique based on the data which are easily available. The performance of the model is satisfactory both in training and independent period. The Root Mean Square Error during

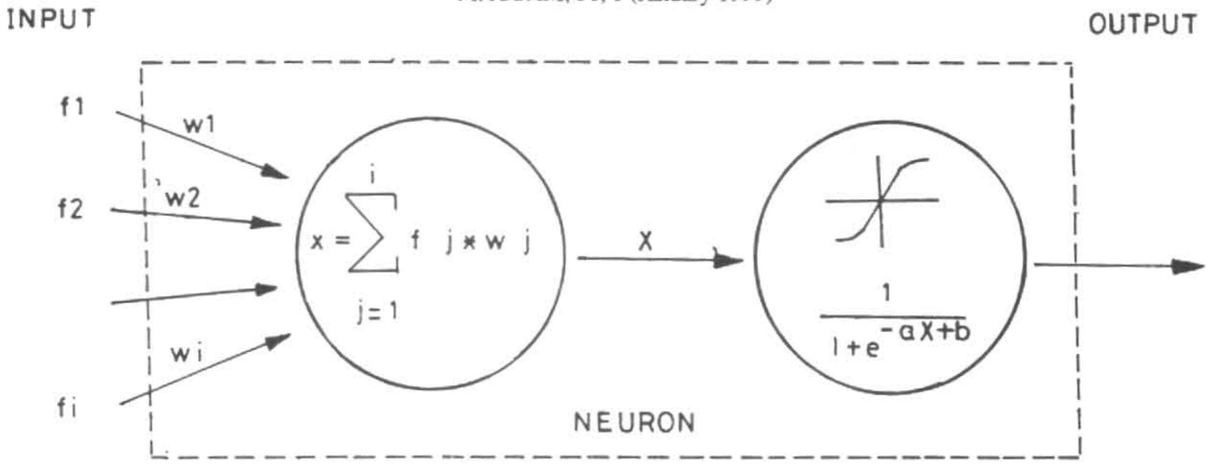

Fig. 1. Schematic representation of a simple neuron

training or independent period is even less than half of the standard deviation of the data (14 nanobar).

2. Area of study and data

In India surface ozone is measured at New Delhi, Pune, Srinagar, Kodaikanal, Trivandrum and Calcutta. Pune has become a fast growing industrial city in recent years. Pune (18° 30′ N, 73° 33′ E) is situated on the Deccan Plateau, on the eastern side of the Western Ghats at a height of 560 m above mean sea level. Due to the increase of population as well as increase in anthropogenic activity, pollution of Pune city has been increasing. It has been found that during the period 1974 to 1983, surface ozone concentration of Pune has shown a slow increasing trend (Tiwari and Peshin, 1995).

Total 731 days of the year 1991 and 1992 of Pune are considered for this study. Daily maximum ozone concentration occurred at Pune between 12 and 13 hours of local time (Tiwari and Sreedharan, 1973). Hence mean surface ozone between 12 and 13 hours are taken.

The following parameters were used to develop the model:

(*i*) Mean surface ozone concentration between 12 and 13 hours as response.

(*ii*) Total solar radiation between 9 and 12 hours as predictor.

(*iii*) Prevailing wind direction at 1130 IST as predictor.

(*iv*) Prevailing wind speed at 1130 IST as predictor.

(*v*) Mean surface ozone concentration between 12 and 13 hours of the previous day as predictor.

(*vi*) Prevailing wind direction at 0530 IST as predictor.

(*vii*) Prevailing wind speed at 0530 IST as predictor.

Since surface ozone concentration has a prominent seasonal or monthly variation, a term which reflects the intra-annual variation is considered in the model as seventh predictor. Mean surface ozone concentrations between 12 and 13 hours for all twelve months and for all 731 days are calculated. It AM_i is the monthly mean value for a particular *i*th month and *A* is the mean value computed from all the data then the value of the parameter *M* for that particular *i*th month is taken as $(AM_i - A)/A$. Value of the parameter for all the months are computed in this way.

Missing data were linearly interpolated to get continuous data of 731 days.

3. Brief review of neural network technique

Neural Networks are signal processing systems that attempt to emulate the behaviour of biological nervous systems by providing a mathematical model of combination of numerous basic blocks called neurons connected in a network. It is remotely analogous to living nervous system and hence its name. One can think of neural networks as an extended form of regression which have the properties of (*i*) adaptivity (*ii*) robustness, (*iii*) ruggedness, (*iv*) speed (*via* massive parallelism), (*v*) nonlinearity and (*vi*) optimality with respect to error. For regression, we assume a functional form first, such as linear or exponential, and then we find the coefficients that minimize some measure of errors, whereas for neural networks, the method itself extract the functional form from the data. As input to the model, a historical set of significant meteorological data is used, whereas the output, ozone concentration is predicted by the model. The network is trained with the past data. By the proper choice of training sets, after the learning process, the trained network is capable of predicting the ozone concentrations as an output according to the inputs and internal structure of the network established during the learning period.

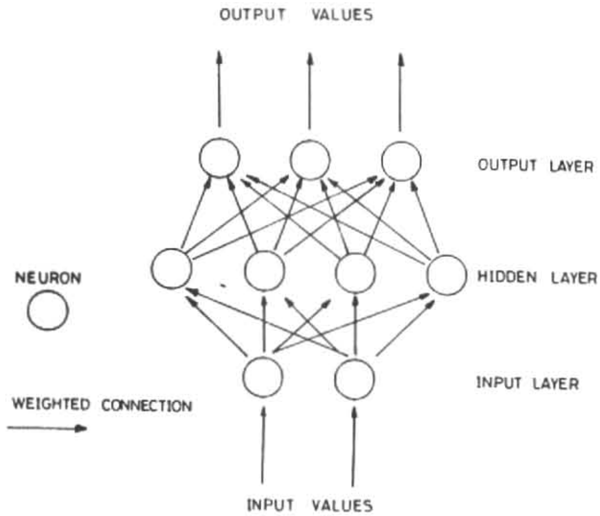

Fig. 2. Typical configuration of a three-layer perceptron neural network

The most common neural network is the feedforward mapping network. It consists of a set of nodes and a set of interconnections between them. A node contains a computational element called neuron (Fig. 1), taking inputs from incoming interconnections (input links) and providing outputs to outgoing interconnections (output links). The units of the neural network are arranged by layers. A unit on one layer takes inputs from the units on the layer below and feeds its output to the units on the layers above. The bottom layer is called input layer whose units take input from the outside and without processing them distribute to the units on the layer above. The top layer is an output layer whose output is the output of the neural network. The layers between input and output layers are called hidden layers. A pattern is defined as a set of input values with the related output values. A typical computational element takes the weighted sum of the input links and passes the result through a transfer function.

The structure of a three layer neural network is shown in Fig. 2. The transfer function used here is the sigmoidal function.

$$Y = [1 + e^{(-ax+b)-1}]$$

Where a determines the slope of the sigmoid and b is the threshold. The process of learning the training set of patterns means the determination of the optimum weights which minimize the mean square error between the outputs in the output layer and the desired values. Most commonly used "back-propagation learning algorithm" (Rumelhart *et al.*, 1986) is used for the training. Initially random weights between ± 0.5 are assigned to each weight as initial guesses. The weights are learned through an iterative process. During learning the weights are updated according to the formula:

TABLE 1

Correlation matrix of the variable in the model

	O_3	PO_3	GR	WS	WD	WS1	WD1
O_3	1.00	0.89	0.40	-0.36	-0.32	-0.50	-0.46
PO_3	0.89	1.00	0.38	-0.32	-0.28	-0.50	-0.47
GR	0.40	0.38	1.00	-0.09	0.13	-0.19	-0.12
WS	-0.36	-0.32	-0.09	1.00	0.21	0.42	0.37
WD	-0.32	-0.28	0.04	0.21	1.00	0.52	0.50
WS1	-0.50	-0.50	-0.19	0.42	0.52	1.00	0.68
WD1	-0.46	-0.47	-0.12	0.37	0.50	0.68	1.00

O_3 : Current Day Ozone Concentration,

PO_3 : Previous Day Ozone Concentration

GR : Total Solar Radiation, WS : Wind Speed at 1130 IST

WD : Wind Direction at 1130 IST, WS1 : Wind Speed at 0530 IST

WD1 : Wind Direction at 0530 IST,

$$\text{New weight change} = \text{Learning rate} \times \text{Error} + \text{Momentum} \times \text{Last weight change}$$

where learning rate and momentum rate are required to get the convergence faster.

When the network learns the training set of patterns well enough it can be used for determining the output values for the pattern with unknown outputs (Test period or prediction period).

4. Neural network model for short term prediction of surface ozone

A three layer neural network with one input layer, one hidden layer and one output layer is used to develop the model. The input layer contains seven input units. Before presenting the seven predictors (previous day surface ozone, total solar radiation, wind speed at 1130 hr(IST), wind direction at 1130 hr (IST), wind speed at 0530 hr (IST) wind direction at 0530 hr (IST) and a term for intra-annual variation) into the network, the values of the predictors are normalized and converted between 0.0 & 1.0 (excluding the end points). But a problem arises with the parameters having a circular character, like the wind direction. Because the angle of 2° should have almost the same influence on the network as the angle 358°. Since the wind direction of magnitudes 2° and 358° are almost same but these magnitudes are largely different. This is because of circular nature. This problem is solved by normalizing the circular parameter (wind direction) to a unit circle and taking the sum of cosine and sine of the angle as the input feature.

Another problem in the neural network is how to avoid local minima of the weight sets (Masters, 1993). There are many techniques such as simulated anealing, genetic algo-

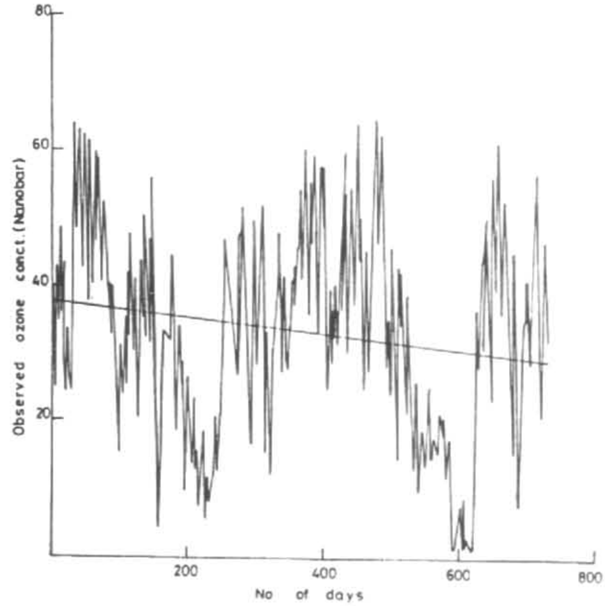

Fig. 3. Behaviour, with respect to time, of the hourly mean surface ozone between 12 and 13 hrs for 731 days during 1991-1992 period

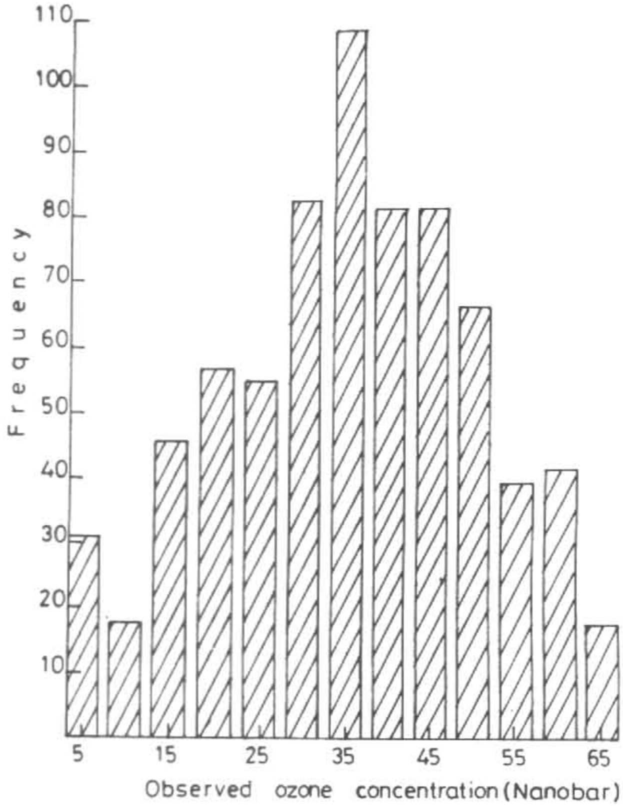

Fig. 4. Histogram of 731 days mean ozone concentration between 12 and 13 hrs during 1991-1992 period, expressed in nanobar

rithm etc. to avoid local minima. In our case we have adopted simulated annealing technique to avoid local minima.

Though neural network model learns the nonlinear relationship between the predictors and predictand, associationship between the predictors and predictand can not be fully justified by seeing the correlation between the predictors and predictand however their linear relationship can be seen from the Table 1.

Mean surface ozone concentration (nanobar) between 12 and 13 hours of 731 days (1st Jan, 1991 to 31st Dec, 1992) are plotted scatterly in Fig. 3. A trend analysis was made for the data and the straight line shown in Fig. 3 is the fitted trend line which shows a decreasing trend in surface ozone during the period 1991-1992. From the diagram (Fig. 3) we can also see the seasonal variation of ozone concentration with lower values during monsoon period and higher values during premonsoon period which support the earlier study by Tiwari and Sreedharan, 1973.

Fig. 4 gives the histogram of the surface ozone concentration data which shows a near normal distribution of surface ozone with a mean 35 nanobar.

Fig. 5 and Fig. 6 are the scatter diagrams of the total solar radiation and previous day surface ozone concentration *versus* surface ozone concentration respectively. Fig. 5 clearly indicates that the dependence between the two variables are not linear. In the atmosphere containing CO, CH_4, NO_x and non- methane hydrocarbons, *in situ* production of ozone can become very large. These compounds react photochemically in the presence of solar radiation producing ozone that is accumulated in the atmosphere at the surface level and dispersed to the middle troposphere (Tiwari and Peshin, 1995). Since the meteorological conditions that are responsible for the formation and accumulation of ozone tend to generally remain in the atmosphere for several days, previous day surface ozone concentration is used as a predictor (Bravo *et al.*, 1996). It has been reported (Nickerson *et al.*, 1992) that the accumulated ozone or its precursors which present at night are the remnant of the previous day pollution. Wind speed and wind direction have also contribution on the variation of surface ozone concentration (Tiwari and Sreedharan, 1973). Wind is responsible for the transport of precursor gases and atmospheric stability.

Out of 731 days of data (1st January 1991 to 31st December 1992), a set of 730 days of data (2nd January, 1991 to 31st December 1992) is prepared (since 1st January 1991 data does not have previous day ozone concentration). This data set is divided in two sets. Set A contains 1st 650 days (1-650) of data whereas set B contains 80 days (651-730) of data. We have used a three layered Neural Network model in which input layer contains four inputs *viz.* previous

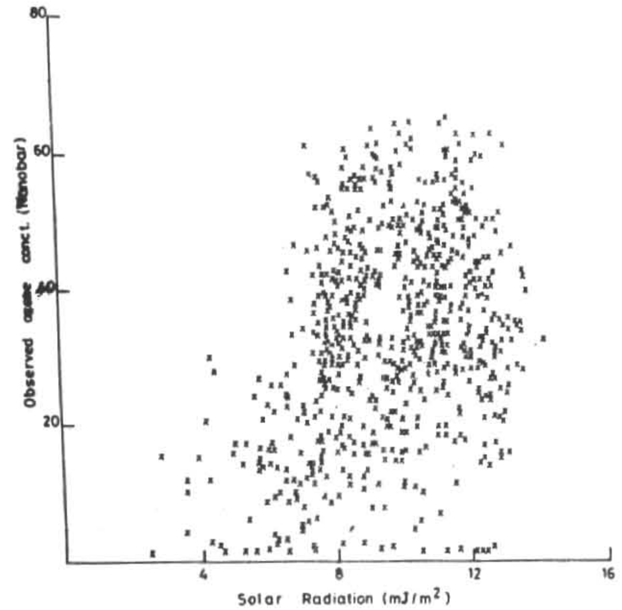

Fig. 5. Scatter diagram of ozone concentration *versus* solar radiation flux between 6 and 12 hours

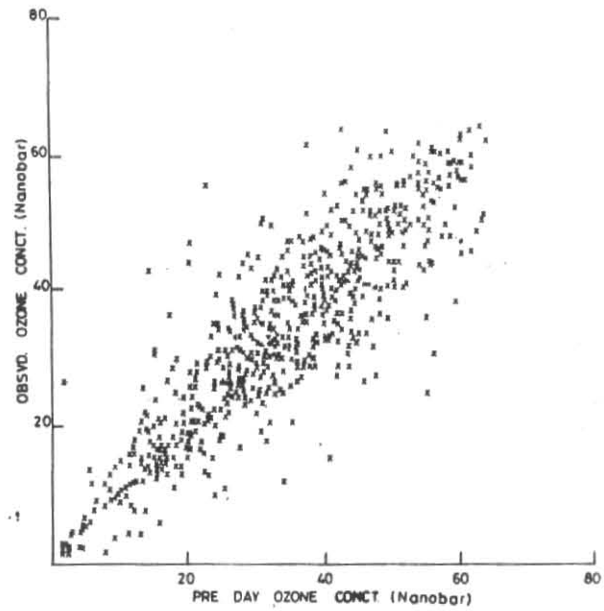

Fig. 6. Scatter diagram of ozone concentration *versus* previous day ozone concentration

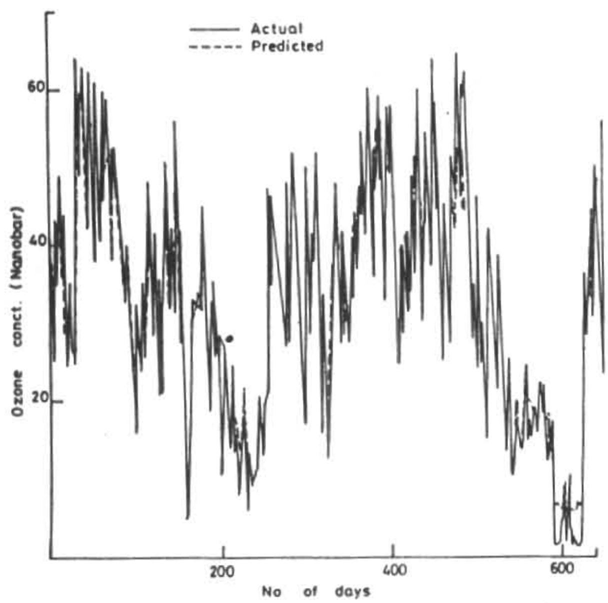

Fig. 7. Performance of the neural network model during the training period

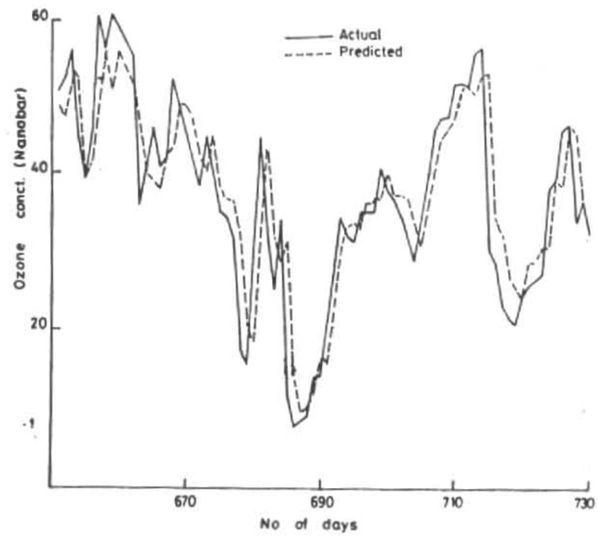

Fig. 8. Performance of the neural network model during the independent period

day surface ozone, total solar radiation wind speed and wind direction (Sin + Cos). The single hidden layer contains five hidden nodes and the output layer contains one output which is the surface ozone of the current day. The network is trained in set A using the method of back propagation (Rumelhart *et al.*, 1986). While training special attention is made to choose the suitable values of the learning process parameters *i.e.*, learning rate, momentum rate and also minimum average error. Too much training (*i.e.*, sufficient small value of error) may overfit the data. Set B (651-730 days) is used for testing the validation of the forecast. Table 2 gives the details of the network feature. Fig. 7 gives the performance of the model during the training period (set A).

5. Performance of the model during independent period

After proper training the network we have obtained the Root Mean Square Error (RMSE) of the model during

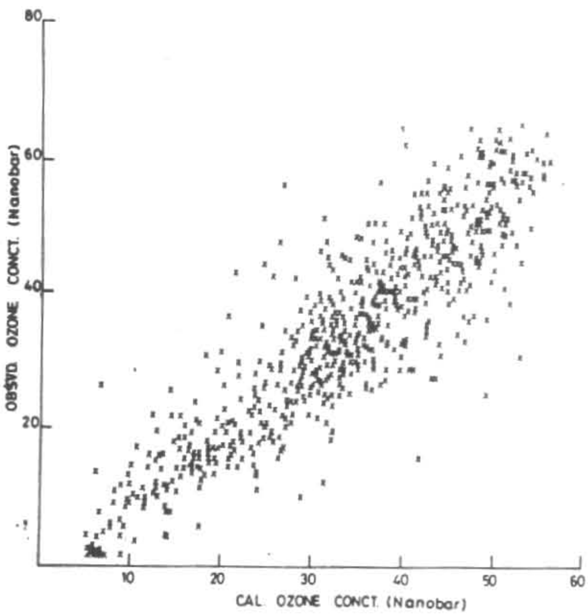

Fig. 9. Scatter diagram of the ozone concentration calculated with the model *versus* observed

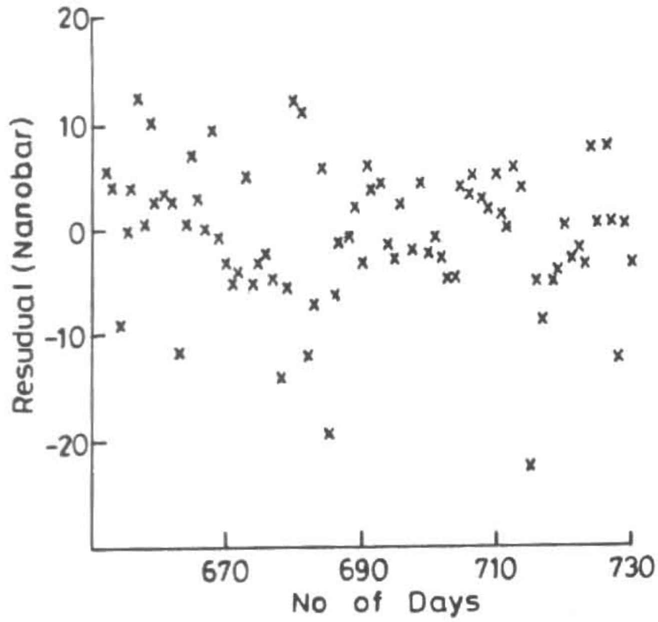

Fig. 10. Residuals of the model (observed value - calculated value) as a function of time during 651 to 730 days (independent period)

TABLE 2

Neural network model architecture

Neurons			*Learning rate*	:	0.3
Input	:	7	*Momentum rate*	:	0.3
Hidden	:	5	*No. of training patterns*	:	650
Output	:	1	*No. of testing patterns*	:	80
			Maximum average error on normalised training patterns	:	0.0057

		Input Features		Output Features
1	:	Previous day surface Ozone Concentration	1	Surface Ozone Concentration
2	:	Solar Radiation		
3	:	Wind Speed at 1130 IST (Sin + Cos)		
4	:	Wind direction at 1130 IST (Sin + Cos)		
5	:	Wind Speed at 0530 IST		
6	:	Wind Direction at 0530 IST (Sin + Cos)		
7	:	Intra-annual Variation term		

training as 6.6 nb while the values of the correlation coefficient between the actual and predicted during the training period (set A) is 0.90. The model is then used to give prediction in the independent period (set B). Fig. 8 shows the performance of the prediction by the Neural Network model during test period (set B). The RMSE during test period is found to be 6.5 nb which is even less than half of the standard deviation of the data (14 nb). The correlation coefficient between the actual and predicted values is also found to be 0.9 in the independent period. Fig. 9 shows the residuals (observed ozone - predicted ozone) for the independent period. Fig. 10 is the histogram of the residuals and the fit of a normal curve. A chi square test was made to this fitting giving a value of 2.31. The table value of χ^2 at 5% level for three degrees of freedom is 7.81. Since the calculated value is much less than the table value, the fit is good. This means that the normal distribution is a good approximation for the residuals.

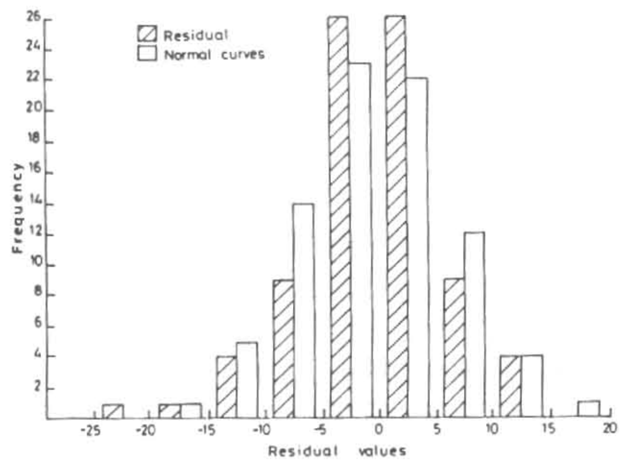

Fig. 11. Histogram of residuals during the independent period and an adjusted normal curve

6. Comparison of the model with persistence

From Table 1 we can see that the previous day surface ozone is highly correlated with the current day surface ozone. This shows a good persistence nature of the surface ozone. To test the neural network model against the persistence, a forecast model which only uses the persistence nature *i.e.*, gives forecast of the present day by using previous day's value was used. The root mean square error for this persistence forecast for the period 651 to 730 days is found to be 7.2 nb which is higher than the RMSE of neural network model of 6.5 nb. Therefore neural network model is better than the persistence forecasts.

7. Conclusions

The variations of surface ozone concentration at Pune are mainly dominated by the variation of the solar radiation and remnant of pollution from the previous day. Wind has also some contribution for the ozone concentration variation. Ozone has a significant seasonal variation with lower values during the monsoon period and higher values during the premonsoon period.

The present model cannot give more accurate prediction due to the lack of consideration of the vertical structure of the atmosphere. The altitude and duration of the thermal inversion, the vertical component of the wind or the intensity and direction of the wind at several altitudes are not being considered here.

Since CO, CH_4, NO_x and non-methane hydrocarbons are mainly responsible for the *in situ* formation of ozone in presence of solar radiation, consideration of solar radiation in the model partly explains these photochemical ozone generation. Good quality of data of these compounds is not available. However, due to consideration of autoregressive nature (previous day ozone) the model takes care of all these compounds to some extent (Nickerson *et al.*, 1992). The present model is based on easily available data as inputs and its performance is significantly good.

Short term prediction model is required for all the important air pollutants (O_3, NO, NO_x, CO, SO_2). It has been discussed by Bonzar *et al.*, 1993 the problem of using statistical and physical models for short term prediction of ambient SO_2 concentration. The same logic is also valid for all the other pollutants. Hence a neural network model is the best way for short term prediction. The present model gives an idea of the measure of air pollution on hour in advance and it could be used in the establishment of criteria for environmental alerts.

The same type of model can be developed for all the major cities and for all important air pollutants where air pollution is a serious problem. But the network architecture will be different for different cities and for different air pollutants. One should be very careful to choose all of these features and also the training set at patterns. The training set should be chosen in such a way to learn "best" from the training pattern to perform "best" in the independent period.

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