A simple neural network model for forecasting daily average surface ozone values measured at Tirunelveli

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Abstract

Ozone (O_3) is a reactive oxidant gas produced naturally in trace amounts in the earth's atmosphere. The ozone molecule is composed of three oxygen atoms, in contrast to normal molecular oxygen (O_2), which makes up roughly 21% of air. Around 90% of the ozone lies in the stratosphere and the remaining lies in the Earth's surface (troposphere).Elevated levels of surface ozone can be phytotoxic and cytotoxic as well. This steady intends to access the amount of surface ozone concentration at a site in Tirunelveli (8.7139° N, 77.7567° E) of southern Tamilnadu. The surface ozone variation marked a clear diurnal cycle with maximum values around 1430 hrs and minimum around 0530 hrs. A Neural Network model was proposed to predict the surface ozone. In this model, the daily average value of surface ozone is forecasted by using the input parameters including temperature (T), wind speed and NO_2 concentration. The data set is randomly divided into three sets namely training, validation, testing. Training set is the largest set (70%) and the remaining sets are assigned to contain 15 % of the samples. The model is developed using feed-forward back propogation multilayer perceptron using three neurons in the hidden layer. The model is carried out in matlab using Levenberg Marquadrt algorithm. The network yielded an accepted value of r = 0.63 between observed and predicted surface ozone levels.

Key-words: *Surface ozone, cytotoxic, diurnal cycle, neural network, neurons, validation*

Introduction

Ozone is a natural constituent of the atmosphere and is present in the stratosphere and troposphere. In the stratosphere O_3 is produced following the photolysis of molecular oxygen. Ozone is also present throughout the troposphere and at the earth's surface and is produced through very different chemical processes. In the troposphere, O_3 is a green house gas. It is a secondary pollutant generated through sunlight driven chemical reactions between NO_X and VOC including CH_4, CO and many other more complex compounds. These gases may be present as a result of emissions within a region and also due to transport into the region of O_3 precursors. Elevated levels of surface ozone can cause potential damage to human respiratory system and can affect the cilia membrane of the lungs [**Krishna Sharma, 2013**]. The rates of these processes and the overall O_3 budget depend on meteorological conditions such as solar intensity, temperature and pressure, and on the concentrations of O_3 precursor emissions and water vapour in the atmosphere. The other major source of O_3 in the troposphere is transport from the stratosphere. Large quantities of chemical compounds are emitted into the atmosphere as a result of anthropogenic and biogenic activities. These emissions lead to a complex spectrum of chemical and physical processes that result in such diverse effects as photochemical air pollution (including the formation of ozone in urban, suburban, and rural air masses), acid deposition, long-range transport of chemicals, stratospheric ozone depletion, and accumulation of green house gases. These compounds are removed from the atmosphere in various ways such as dry and wet depositions, chemical reactions with other compounds either in gas phase or on their surfaces and direct photolysis. During the past decade, an increase of approximately 10% (1% per year) in ozone throughout the height of the troposphere has been demonstrated over Europe [**WMO, 1986, 1990**].An increase in surface ozone increases surface temperature [Sharma, 2016].

Ozone is present in the natural, unpolluted troposphere, and its tropospheric column density is approximately 10% of the total atmospheric (troposphere + stratosphere) ozone column density. [**Logan, 1985; Brühl and Crutzen, 1989; Fishman *et al*., 1990**]. The ozone present in the stratosphere absorbs short-wavelength radiation ($\lambda \leq 290$ nm) from the sun and allows only those wavelengths ($\lambda \geq 290$nm) to penetrate into the troposphere [**Peterson, 1976; Demerjian *et al*., 1980**]. The sources of ozone in the natural troposphere are downward transport from the stratosphere and in situ photochemical production. Losses result from photochemical processes and from deposition and destruction at the earth's surface. The rates of downward transport, production, and losses are estimated to be of the same order of magnitude .The ozone present in the troposphere is important in the atmospheric chemistry because the OH radical is generated from the photolysis of ozone at wavelengths $\lambda<319$ nm [**Levy, 1971; DeMote et al., 1990**]. The formation of OH radicals leads to cycles of reactions that result in the photochemical degradation of organic compounds of anthropogenic and biogenic origin, the enhanced formation of ozone, and the atmospheric formation of acidic compounds. It is recognized that trace gases such as NO, NO_2, CO, VOC's and NMHCs are the precursors of surface ozone. In the unpolluted atmosphere, ozone can be formed by photolysis of oxygen by UV radiation with a wavelength of 240 nm or less [**McElroy, 2002**] in the presence of a third molecule such as nitrogen that serves to absorb energy released by photolysis. The ozone rapidly photo dissociates back into oxygen, but the forward and reverse reaction rates may vary slightly depending on ambient temperature, pressure, radiation intensity and concentrations of trace constituents [**Seinfeld, 1989**].

Study area and Methods

Initially Surface ozone and Nitrogen dioxide measurements were made as a pilot study in some places of Tirunelveli. Readings were taken and considering the importance of the geographical location, the study area was chosen as **Balabackya Nagar** (8.7139° N, 77.7567° E) It is one of the important traffic prones of the district with high mobile population almost the entire year and no considerable studies have been made on air quality in the past. Figure 1 shows the study area.

Fig.1.Study area

Surface ozone measurements were carried out by using a portable sensitive gas monitor Aeroqual S300 coupled with ozone sensor (figure 2). Its ultra low concentration ozone sensor head measures the ozone concentration from 0.000 to 0.150 ppm with an accuracy of ± 0.001 ppm (from 0 to 0.100 ppm). The measurement unit being either ppm or µg/m3 . The operating temperature range is from - 5°C to 50°C, relative humidity limits are 5% and 95%. The ozone sensor was calibrated against a certified UV photometer.

Fig.2.S 300 monitor

Diurnal variation of Ozone

Diurnal ozone variation is an atmospheric term that relates the variation in the surface ozone that occurs from the highs of the day to the low of the nights. In general it stands for the ozone fluctuations that occur during each day. It is very useful in understanding the various processes that are responsible for the production and destruction of ozone. It is a measure of overall budget of production and loss rates. Generally a well-marked diurnal variation of SOZ concentration occurs in relatively unpolluted air during calm weather. The diurnal variation is characterized by a broad minimum at night, a rapid rise in the morning after sunrise and a sharp maximum near noon [**Donald Allen Widen, 1966**]. The mixing ratios of ozone start increasing gradually after sunrise, attaining maximum values during local noon time [**Nishanth, 2011**].Day time higher ozone levels are mainly due to the photochemical production of ozone [**Naja and Lal, 2002**]. The diurnal variation of SOZ concentration for different seasons over the entire study period is shown in Figure 3.

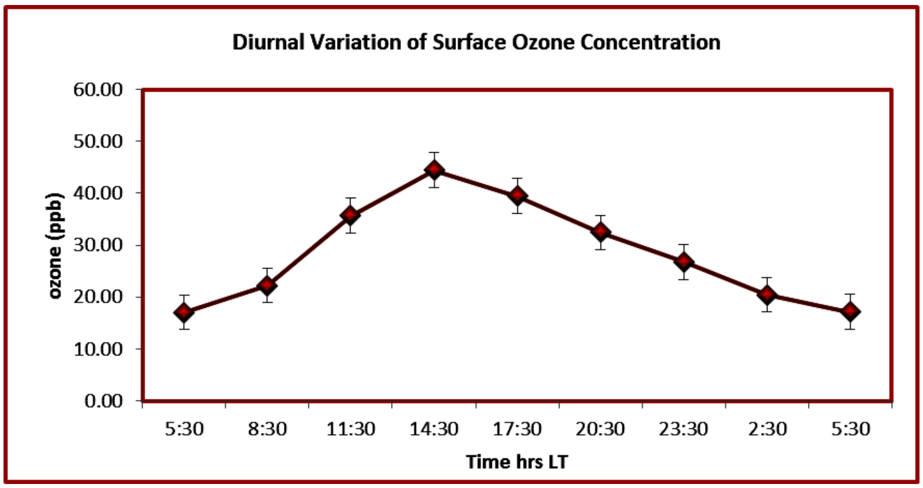

Fig.3.Diurnal Variation

Neural- Network modelling

In general, Neural Networks are simply mathematical techniques designed to accomplish a variety of tasks. Neural Networks uses a set of processing elements (or nodes) loosely analogues to neurons in the brain (hence the same, neural networks). These nodes are interconnected in a network that can then identify patterns in data as it is exposed to the data. In a sense, the network learns from the experience just as people do. Neural networks can be configured in various arrangements to perform a range of tasks including pattern recognition, data mining, classification, and process modeling.

The motivation for artificial neural network (ANN) researches is the belief that a human's capabilities, particularly in real-time visual perception, speech understanding, and sensory information processing and in adaptively as well as intelligent decision making in general, come from the organizational and computational principles exhibited in the highly complex neural network of the human brain. Expectations of faster and better solution provide us with the challenge to build machines using the same computational and organizational principles, simplified and abstracted from neurobiological of the brain. At the heart of every Neural Network is what is referred to as the perceptron (sometimes called processing element or neural node) which is analogous to the neuron nucleus in the brain. The second layer that is very first hidden layer is known as perceptron. As was the case in the brain the operation of the perceptron is very simple; however also as is the case in the brain, when all connected neurons operate as a collective they can provide some very powerful learning capacity.

Input signals are applied to the node via input connection (dendrites in the case of the brain.) The connections have "strength" which change as the system learns. In neural networks the strength of the connections are referred to as weights. Weights can either excite or inhibit the transmission of the incoming signal. Mathematically incoming signals values are multiplied by the value of those particular weights. At the perceptron all weighted input are summed as represented in figure 4. This sum value is than passed to a scaling function. The selection of scaling function is part of the neural network design. Figure shows the structure of perceptron.

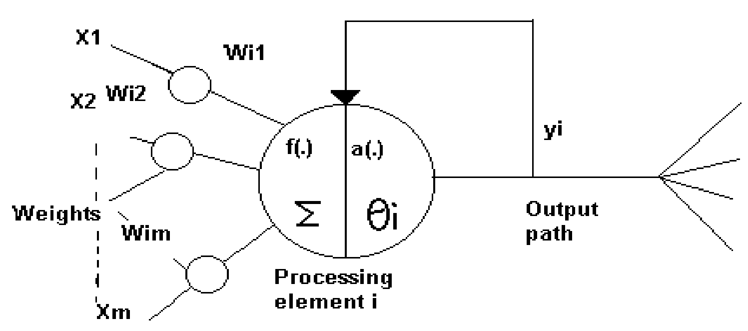

Fig.4.Model biasing

In this model, the daily average values of surface ozone is forecasted by using the input parameters including temperature (T), wind speed and NO_2 .The data set is randomly divided into three sets namely training, validation, testing. Training set is the largest set (70%) and the remaining sets are assigned to contain 15 % of the samples. The training set is a set of samples used to adjust or train the weights in the neural network to produce desired outcome. The validation set is used to find the best network configuration and testing set is to evaluate the fully trained networks. Even though there are many computational functions, the most used function in air quality modeling is the sigmoid function.

The Log Sigmoid function is given as f(x) = 1/(1+e-x). The model is developed using feed-forward back propogation multilayer perceptron using three neurons in the hidden layer as given in figure 5. The model is carried out in matlab using Levenberg Marquadrt algorithm.

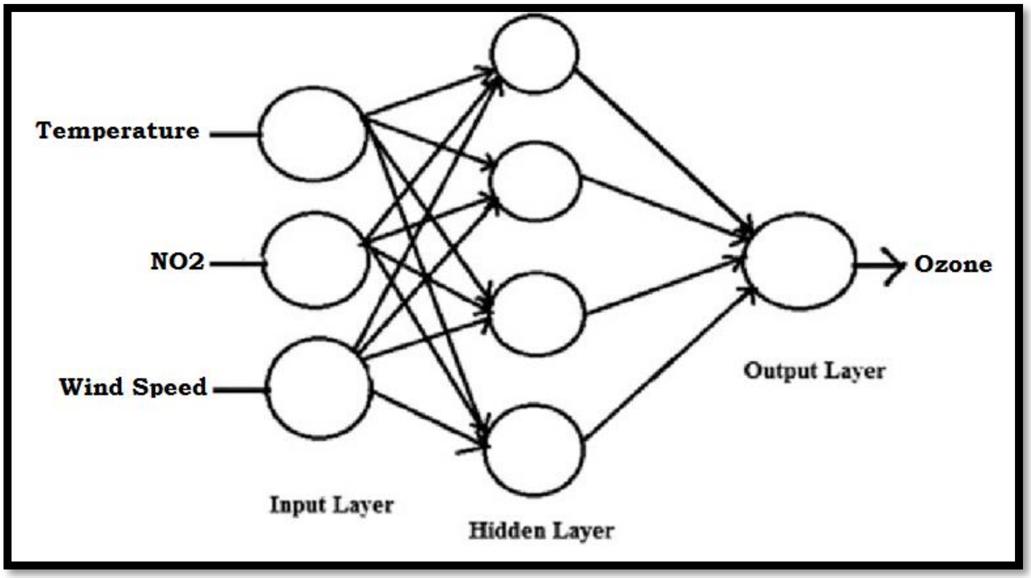

Fig.5.proposed neural network model for ozone

The neural network model is trained using all the input parameters. The model gives an R^2 of 0.635 for all the data points with MSE of 8.476. Figure 6 shows the model results and figure 7 gives the correlation between actual and predicted values of surface ozone.

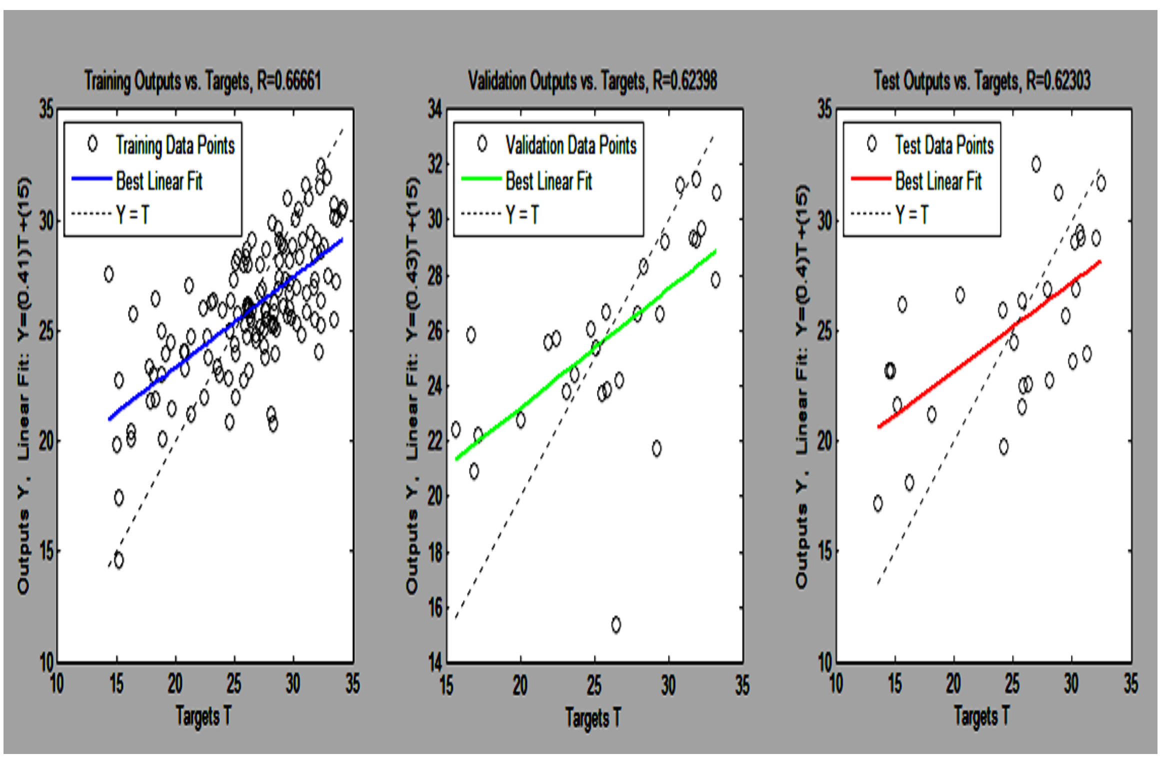

Fig.6.model results

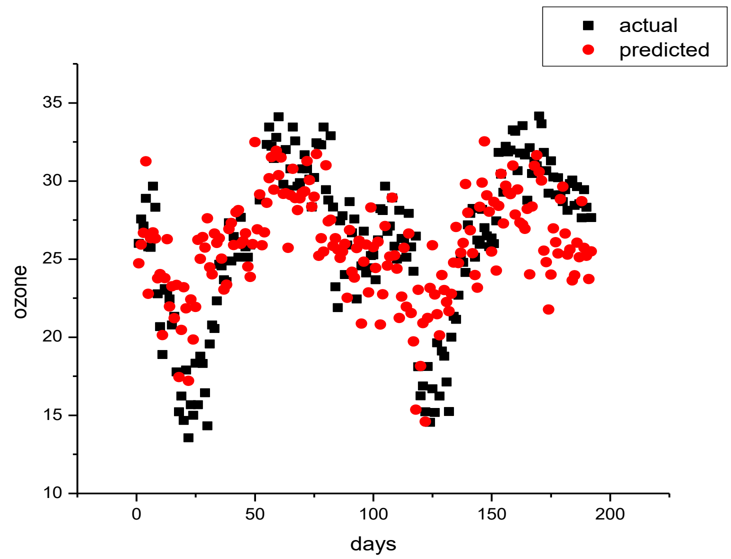

Fig.7.Actual and predicted values of ozone

Conclusion

Surface ozone concentration was measured at a site in Tirunelveli (8.7139° N, 77.7567° E) of southern Tamil Nadu. The surface ozone variation marked a clear diurnal cycle with maximum values around 1430 hrs and minimum around 0530 hrs. Diurnal variation tends to be highly related to sunlight intensity throughout the day. As a result, during early morning hours, when the sun starts to shine, the ozone production rate starts increasing. Moving towards mid-day time, the sunlight being strongest, resulting in high ozone production. Then the concentration seems to be decreasing in late evening hours. A Neural Network model was proposed to predict the surface ozone. In this model, the daily average value of surface ozone is forecasted by using the input parameters including temperature (T), wind speed and NO_2 concentration. The data set is randomly divided into three sets namely training, validation, testing. Training set is the largest set (70%) and the remaining sets are assigned to contain 15 % of the samples. The model gives an R^2 of 0.635 for all the data points with MSE of 8.476.There was a good agreement with the actual and predicted values of surface ozone concentration in the study area.

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