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An overview of forecast models evaluation for monitoring air quality management in the State of Texas, USA

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Abstract
Purpose – The purpose of this study is to investigate forecast models using data provided by the Texas Commission on Environmental Quality (TCEQ) to monitor and develop forecast models for air quality management.

Design/methodology/approach – The models used in this research are the LDF (Fisher Linear Discriminant Function), QDF (Quadratic Discriminant Function), REGF (Regression Function), BPNN (Backprop Neural Network), and the RBFN (Radial Basis Function Network). The data used for model evaluations span a 12-year period from 1990 to 2002. A control chart of the data is also examined for possible shifts in the distribution of ozone present in the Houston atmosphere during this time period.

Findings – Results of this research reveal variables that are significantly related to the ozone problem in the Houston area.

Practical implications – Models developed in this paper may assist air quality managers in modeling and forecasting ozone formations using meteorological variables.

Originality/value – This is the first study that has extensively compared the efficiency of LDF, QDF, REGF, BPNN and RBFN forecast models used for tracking air quality. Prior studies have evaluated Neural Networks, ARIMA and regression models.

Keywords Air pollution, Environmental management, Forecasting, Ozone, United States of America

Paper type Research paper

Introduction
According to the May 14, 2001 *US News & World Report*, in 2000, more than 141 million Americans lived in communities with severe ozone pollution up from 132 million in 1999. Many of the largest metropolitan areas, such as Los Angeles, Philadelphia, Atlanta, and Houston, are searching for better ways to manage ambient ozone in their atmosphere. Some of the cities are enforcing regulations to adopt complex and expensive technologies to reduce nitrogen oxides (NOx) from diesel engines (Peckham, 2003) which are an effective agent for producing ground level ozone. Besides, big cities are also discouraging use of personal vehicles by putting high tax on vehicle usage and spending big amounts to foster public transportation systems to reduce pollution caused by vehicles. If a

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metropolitan area exceeds the ozone threshold set by the US Environmental Protection Agency (EPA), it is considered a non-attainment area. If the eight-hour ozone level is less than 85 ppb (parts per billion), the day is classified as a non-ozone alert day. Otherwise, the day is classified as an ozone alert day. State environmental quality managers typically announce, on a daily basis, the quality of the air using a color-coding scheme to represent the level of severity.

Non-attainment areas are subject to increased costs and requirements for automobile inspections as well as possible loss of highway funding. According to Case (1999), a new program underway in seven non-attainment areas, including Chicago and Washington, DC, focuses on company fleet vehicles. In these areas, approximately 30 percent of light duty vehicles purchased as replacements and 50 percent of heavy-duty vehicles will need to meet low emission standards or be powered by alternative fuels, such as compressed natural gas, ethanol or electricity. According to McCubbin and Delucchi (1999), motor vehicles have significantly larger health costs than previously reported. Diesel vehicles cause more damages per mile than do gasoline vehicles, because of greater particulate emissions. Spektor *et al.* (1991) report that the effects of exposing healthy children and adults to ambient air reduced their respiratory function proportionally to increasing concentrations of ozone with no apparent threshold for this response.

A number of researchers such as Elders (1992), McCollister and Wilson (1975), and Prybutok *et al.* (2000) have investigated models for forecasting daily ozone levels. These models are intended to be tools for air quality managers to take actions to minimize the effect of ozone and to warn citizens to not avoid prolonged exposure outdoors. Early models, such as Wolff and Lioy (1978)'s model, used regression procedures with a few variables, mainly maximum temperature, wind speed, and wind direction. Because of the model's relative simplicity, it could be used to make real time forecasts of maximum ozone levels. For the northeastern part of United States, this model appeared to be reasonably accurate in 74 percent of the cases tested using forecasted meteorological data. Revlett (1978) also developed a model using the variables: non-methane hydrocarbons, NO2, NO, temperature, wind speed, wind direction, sky cover, humidity, and mixing height of chemicals. He concluded that the use of this model for early abatement action was questionable due to the lack of accuracy in forecasting all of these variables.

Enders (1992) examined the behavior of ozone above forests. The author claims that more work needs to be done in this area because of their high biomass, outstanding extent in many countries, and their unique morphology. His research suggested that the biogenic emissions of reactive hydrocarbons from the forests influence the overall ozone level in the air. A number of researchers have used time series techniques for forecasting daily maximum ozone levels (Chock *et al.*, 1975; McCollister and Wilson, 1975; Robeson and Steyn, 1990). The success of these models often was depended upon site characteristics. Prybutok *et al.* (2000) developed forecasting models using 1994 ozone data for the Houston metropolitan area. Their results showed that the neural network model was superior to the regression and Box-Jenkins models in forecasting ozone levels for October 1994.

In this paper, the authors investigate forecasting models using daily meteorological data spanning from 1990 to 2002. These data were obtained from the Texas Commission on Environmental Quality (TCEQ). This research first examined the reported eight-hour ozone level using an X-bar and S-bar control chart. Although control charts are not typically used on meteorological data, they provide a visual display of the data. Shifts in the mean and standard deviation of ozone levels over time were visually inspected. Models used for the forecasting the eight-hour ozone levels and/or color level were the following: Regression, Fisher's linear classification model, the quadratic classification model, and neural network models. A comparison of the performance of these models is presented using data from 1997 to 2002.

Control charts of eight-hour ozone data

If a process is in-control, the parameters of the distribution of the data do not change. If the process becomes out-of-control due to an assignable cause, the parameters of the distribution change and the shape or scale of the distribution change. Detecting when this shift takes place in a time series data set has been the topic of various research papers. If a researcher suspects that a shift has occurred in the process, a common recommendation is to first use a preliminary control charts to visually detect a shift in the process mean and variance (Turner *et al.*, 2001).

Figure 1 displays the eight-hour ozone data for Houston from 1990 to 2002. A subgroup size of ten was selected for these control charts. If there is a shift in the mean of the eight-hour ozone levels or in the standard deviation of these levels, points would continually stay high or low on the graphs. As it appears, the "out-of-control" points appear to occur sporadically, although there is a noticeable cycle in the graphs. This cycle occurs simply because of the seasons of the year. The largest number of "out-of-control" points appears to occur around 200, the summer of 1995. During that summer there were many 100^0 F (38^0 C) days. Interestingly, the following summer (1996), there were no 100^0 F (38^0 C) days and therefore, a noticeable reduction in the number of "out-of-control" days. The conclusion from viewing these charts is that the mean and standard deviation of distribution of the eight-hour ozone data does not appear to have shifted in any substantial way over these years.

Determining meteorological variables contributing to prediction of eight-hour ozone

Using the Houston ozone data from 1990 to 2002 and removing any observations with missing values, a regression model was fit in a step down fashion using a number of meteorological variables. Several variables, which were functions of time, were included.

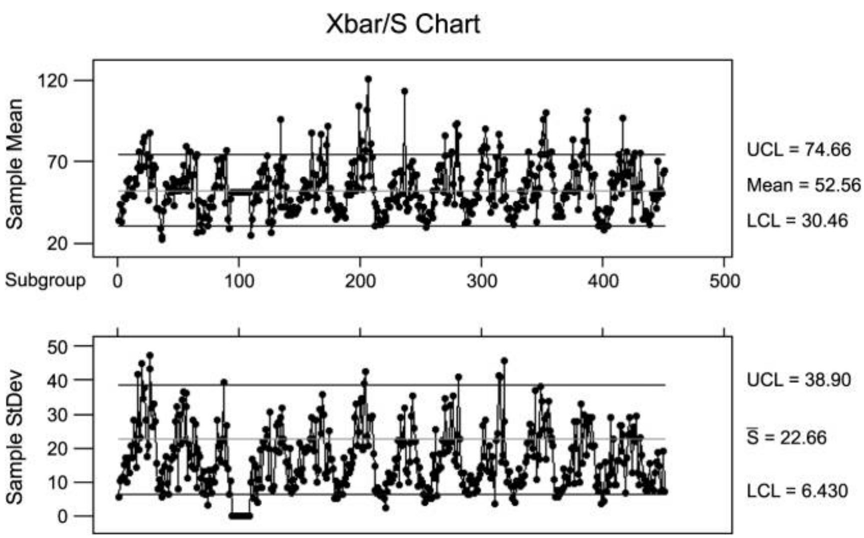

Figure 1. Control charts for eight-hour ozone levels

These variables were cos1 = cos ($2^*\pi^*$time/365), cos2 = cos ($2^*?\pi$ *time/182), and sin3 = sin ($2^*?\pi^*$time/91). They represent cycles of length, one year, 6 months, and 3 months, respectively. Using these variables captures the seasonal effects on ozone levels. In addition, the interaction of the yearly and six-month cycles (denoted by the variable cos1cos2) was found to be a significant contributed and is thus included in the model.

The one-, five-, and ten-day lags of the eight-hour ozone levels were also found to be important contributors to the prediction of the ozone levels and were also included in the model. The variable yestozon is the maximum one-hour ozone from the previous day. The meteorological variables precipation (precip), sun duration (surdur), percentage of sun light (sunperc), maximum daily temperature (maxtemp), minimum daily temperature (mintemp), wind speed variables (denoted by WS), wind direction variables (denoted by WD), and dummy variables formed from the wind speed and wind direction variables were also included. The numbers 9, 12, 18, and 21 represent the 90, 120, 180, and 210 degrees on the compass. A total of 35 independent variables were kept in the final model.

In Table I, an ANOVA table shows the significance of the overall model. The R-square was 61 percent. Table II displays the significance of each variable. While some of the variables were not significant, they were included in the model because they were found to make a difference in the accuracy of future predictions of the less frequently occurring high ozone days. The independent variables included in this regression model make sense from studies that have previously developed models to forecast ozone levels.

Classification methods

Classification procedures derived using the assumption of normal populations predominates in statistical applications because of their reasonably high efficiency across a wide variety of population configurations (Johnson and Wichern, 1992). The linear discriminant rule, also known as Fisher's linear discriminant function, has a simple structure and is based on the assumption of equal population covariance structures as well as normal populations (Fisher, 1936). The quadratic discriminant rule, also known as Smith's quadratic discriminant function, uses a complete set of second order terms and is based on the assumption of unequal population covariance structures (Smith, 1947). The quadratic discriminant rule is an alternative to the linear discriminant rule when the assumption of equal covariance matrices is seriously violated. These two procedures are often referred to as parametric procedures.

Neural networks (NNs), unlike parametric statistical techniques, do not require that a list of assumptions be satisfied. For example, it is not necessary that the functional relationships among independent and dependent variables be specified to a NN. In fact, it is not necessary that a domain specific model exist for a neural network to discern relationships and build its own model (Dutta and Shekhar, 1988). Neural networks are

Table I.
ANOVA for overall regression model with 35 independent variables

		Analysis of variance		
Source	DF	Sum of squares	Mean square	F-value
Model	35	1,641,040	46,887	205.22
Error	4,481	1,023,783	228.47	
Corrected total	4,516	2,664,823		
Root MSE	15.11529	R-square	0.6158	
Dependent mean	54.12731	Adj. R-square	0.6128	

Variable	DF	*t*-value	Pr > |t|
Intercept	1	3.22	0.0013
PRECIP	1	− 2.87	0.0042
SUNDUR	1	10.23	< 0.0001
SUNPERC	1	− 8.38	< 0.0001
YESTOZON	1	− 5.26	< 0.0001
cos1	1	− 1.46	0.1436
cos2	1	− 7.44	< 0.0001
sin3	1	− 1.84	0.0654
MAXTEMP	1	16.53	< 0.0001
MINTEMP	1	− 15.7	< 0.0001
lag1y	1	24.66	< 0.0001
lag5y	1	2.32	0.0202
lag10y	1	2.15	0.0312
cos1cos2	1	2.03	0.0421
lag1sundur	1	− 4.28	< 0.0001
lag1sunperc	1	3.09	0.002
WS12Z	1	5.01	< 0.0001
WS15Z	1	− 6.12	< 0.0001
WS18Z	1	− 4.66	< 0.0001
WS21Z	1	− 5.59	< 0.0001
WD09Z	1	− 0.86	0.3885
WD12Z	1	− 0.25	0.8014
WD18Z	1	− 3.69	0.0002
WD21Z	1	− 1.13	0.2575
wd09zDummyNEast	1	− 0.38	0.702
wd09zDummySEast	1	− 1.82	0.0695
wd09zDummySWest	1	− 2.68	0.0073
wd12zDummyNEast	1	− 1.33	0.1838
wd12zDummySEast	1	− 3.78	0.0002
wd12zDummySWest	1	− 0.24	0.811
wd18zDummyNEast	1	− 1.24	0.2155
wd18zDummySEast	1	2.8	0.0051
wd18zDummySWest	1	− 4.11	< 0.0001
wd21zDummyNEast	1	− 0.11	0.9146
wd21zDummySEast	1	− 0.21	0.8342
wd21zDummySWest	1	− 3.49	0.0005

Table II. Significance level of independent variables included in the regression model

also relatively immune to such problems as multicollinearity, heteroscedasticity, and outliers (Raghupathi *et al.*, 1991).

The most popular neural network for business applications is the "backprop" network (BPNN). This is the label given to neural networks using the backpropagation of error learning algorithm. Generally, these "backprop" use the generalized-delta rule during learning, which is a nontrivial extension of the learning rule for a simple Adaline network (Widrow and Lehr, 1990). This learning rule is generally attributed to Rumelhart *et al.* (1986). It uses a gradient descent algorithm to minimize forecast/classification error. This algorithm often converges slowly and is not guaranteed to reach the global minimum error. Despite these issues, BPNNs have been shown in the literature to be successful and relatively easy to apply to many types of business problems.

Another type of neural network that can be used in classification analysis is the radial basis function network (RBFN). Rather than using supervised training to estimate all parameters in the network, RBF networks have a hidden layer of radial basis function kernel neurons that are trained using an unsupervised clustering algorithm such as K-means (Ceccarelli and Hounsou, 1996). These neurons are known as pattern recognition (or prototype) neurons because they respond most strongly to vector patterns that come closest to matching their own vector pattern. A radial basis function is any symmetric function whose response to a given input is stronger the closer the input is to the kernel of the function (Chen and Lin, 1996). That is, the radial basis functions form spherical receptive fields in for n-dimensional inputs. The radial basis function chosen for the proposed study is Gaussian, which is the most common function, used for this purpose (Neruda, 1995).

Classification models and forecasting results

Since number of prior studies have applied Neural Networks (NN), ARIMA and regression models for forecasting ozone levels in the air and found that neural networks outperforms ARIMA and regression models (Chock *et al.*, 1975; McCollister and Wilson, 1975; Robeson and Steyn, 1990; Prybutok *et al.*, 2000), this study has applied LDF (Fisher Linear Discriminant Function), QDF (Quadratic Discriminant Function), REGF (Regression Function), BPNN (Backprop Neural Network), and the RBFN (Radial Basis Function Neural Network) to identify a better model for forecasting air quality.

All the models are trained using data from January 1992 through December of 1996. The forecasted time period includes data from Jan 1997 to May 2002. A small number of observations with missing values were removed. Ozone alert days and non-ozone alert days are classified according to the US EPA threshold (If the eight-hour ozone level is less than 85 ppb (parts per billion), the day is classified as a non-ozone alert day. Otherwise, the day is classified as an ozone alert day). The results of this classification are presented in Table III.

The classification models were trained to classify each day as a non-ozone day or as an ozone day. The regression model was used to classify a day as either an ozone day or non-ozone day by comparing the predicted value of the model to the threshold value of 85. Since the regression model did so poorly in correctly classifying ozone alert days and did rather well on classifying non-ozone days, the model was evaluated after updating the model with the data up to the day before the prediction. The results of the regression model improved substantially for correctly classifying ozone alert days with the continuous refitting of the regression model with new data.

The BPNN model had 200 hidden layer neurons and used a hyperbolic tangent transfer function for all hidden layer and output layer neurons. Interestingly, the BPNN

Table III.
Classification results using daily ozone data from 1997 to 2002

Classification method	Overall correctly classified observations	Correctly classified non-ozone alert days	Correctly classified ozone alert days
LDF	90.30	94.84	61.28
QDF	86.29	89.79	63.91
REGF	89.45	95.92	0.00
REGF (updating)	90.46	97.30	46.24
BPNN	83.22	83.07	84.21
RBFN	74.71	72.19	90.98

performs noticeably better than the regression or parametric classification models in correctly classifying ozone alert days. This may be more important than correctly classifying non-ozone alert days. The RBFN model had 150 prototype neurons and used a hyperbolic tangent transfer function on all output layer neurons. This model may be quite useful despite its low overall percentage of days correctly classified since the percentage of correctly classified ozone days is quite high. An air quality control engineer would have to determine if this model gives too many "false positives.

Conclusion and discussion

Exclusive dependence on fossil fuel (hydrocarbons) for power generation and transportation systems is causing growing air pollution and green house gas emissions. In the big metropolitan areas, most of the pollutants that come from ozone are created by cars. Large industries account for another significant portion (*EPA Report*, 2008). Nitrogen oxides (NOx) in combination with volatile organic compounds cause the formation of ground level ozone in the presence of sunlight (Granovskii *et al.*, 2007). Elevated levels of ozone can cause asthma and other respiratory disorders, because when it is breathed into the lungs, ozone reacts with the lung tissue (Granovskii *et al.*, 2007). It can also harm breathing passages and makes it more difficult for the lungs to work (*EPA Report*, 2008). According to a US government statistics, ozone air pollution has been associated with at 10-20 percent of all summertime respiratory hospital visits and admissions. Especially children with respiratory problems are at greater risk because of their exposure to the outdoors during summer days.

To protect the citizens from extreme ozone exposure that causes health problems, environmental agencies are trying to identify the ozone action days more accurately. Ozone action days are usually called when forecaster predict days that are conducive to ozone formation (presence of more than 85 ppb in the air). The area's industries and vehicle drivers are asked to voluntarily or involuntarily (through regulatory measures) reduce emissions that cause ozone pollution. Models developed and evaluated in this study can assist the environmental agencies to significantly enhance their capability to identify ozone days more accurately.

The Texas Commission on Environmental Quality (TCEQ) uses correlation studies based on the data used in this study and National Weather Service (NWS) forecasts to predict ozone exceedences. For the years 1997 through 2001, the TCEQ were able to predict exceedences accurately 71.1 percent of the time. Their accuracy on non-exceedence days was better at 85.69 percent. These results, which yield an 82.59 percent overall accuracy rate, leave room for improvement. While NWS forecasts are not archived and were therefore not available for developing the parametric and neural network models used in this study, our study shows that if forecasted meteorological variables are reasonably accurate, the percentage of correctly classified ozone and non-ozone days could be improved by using these models. Also of note, is the tradeoff between accuracy in predicting ozone and non-ozone days. Since the number of non-ozone days is quite large compared to the number of ozone days, the parametric models tend to classify the non-ozone days better than the ozone days. The neural network models, on the other hand, tend to balance the accuracy of classification or, if desired, allow for much higher classification rates of the health-affecting ozone days. The results of our study demonstrate the potential utility of several ozone-forecasting models for forecasting ozone exceedance days for the Houston metropolitan area.

Rising concerns about the effects of air pollution have led to increased attention in the renewable energy sources such as solar power, wind power, biomass, biofuels, hydro-electricity, etc. to limit the amount of ground level ozone in the air. The possibility of generating synthetic or hydrogen fuels by employing only renewable energy is quite good (Granovskii *et al.*, 2007). Pure hydrogen can also be used as fuel for fuel cell vehicles or concentrated as synthetic liquid fuels by means of Fischer-Tropsch reactions (Dry, 1999). In the year 2006, about 18 percent of global energy sources came from renewable energy sources. 3 percent came from traditional biomass, another 3 percent from hydropower followed by water/heating, which contribute 1.3 percent. Latest technologies like: geothermal, wind, solar and ocean energy together provided 0.8 percent of total energy consumes (REN21, 2007). Although renewable energies cost more money than hydrocarbons, they are cost-effective in the long run and provide sustainable development alternatives for humanity.

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