Stoch Environ Res Risk Assess (2005) 19: 241–248
DOI 10.1007/s00477-004-0228-y

ORIGINAL PAPER

Sung Eun Kim · Ashok Kumar

Accounting seasonal nonstationarity in time series models for short-term ozone level forecast

Published online: 9 February 2005

Abstract Due to the nonlinear feature of a ozone process, regression based models such as the autoregressive models with an exogenous vector process (ARX) suffer from persistent diurnal behaviors in residuals that cause systematic over-predictions and under-predictions and fail to make accurate multi-step forecasts. In this article we present a simple class of the functional coefficient ARX (FARX) model which allows the regression coefficients to vary as a function of another variable. As a special case of the FARX model, we investigate the threshold ARX (TARX) model of Tong [Lecture notes in Statistics, Springer-Verlag, Berlin, 1983; Nonlinear time series: a dynamics system approach, Oxford University Press, Oxford, 1990] which separates the ARX model in terms of a variable called the threshold variable. In this study we use time of day as the threshold variable. The TARX model can be used directly for ozone forecasts; however, investigation of the estimated coefficients over the threshold regimes suggests polynomial coefficient functions in the FARX model. This provides a parsimonious model without deteriorating the forecast performance and successfully captures the diurnal nonstationarity in ozone data. A general linear *F*-test is used to test varying coefficients and the portmanteau tests, based on the autocorrelation and partial autocorrelation of fitted residuals, are used to test error autocorrelations. The proposed models were applied to a 2 year dataset of hourly ozone concentrations obtained in downtown Cincinnati, OH, USA. For the exogenous processes, outdoor temperature, wind speed, and wind direction were used. The results showed that both TARX and FARX models substantially improve one-day-ahead forecasts and remove the diurnal pattern in residuals for the cases considered.

S. E. Kim (✉)
Department of Mathematical Sciences,
University of Cincinnati, ML 0025,
Cincinnati, OH 45221-0025, USA
E-mail: kim@math.uc.edu
Tel.: +513-556-4072
Fax: 513-556-3417

A. Kumar
Department of Civil Engineering,
University of Toledo, Toledo,
OH 43606-3390, USA
E-mail: akumar@utnet.utoledo.edu

Keywords Ozone forecast · Nonstationary · Functional coefficient autoregressive · Threshold model · Exogenous process

Introduction

Air pollution is a widespread problem in the US, with over 100 million individuals in 114 different areas exposed to levels of air pollution that exceed one or more health-based ambient air quality standards. Ground-level ozone, which is a major element of urban smog, is one of the most complex, difficult to control, and pervasive pollutants. Ozone concentrations can reach unhealthful levels when the weather is hot and sunny with very low wind speed or calm condition. The potential environmental impacts of ground level ozone include human health injury and harmful affects to vegetation and material (e.g. Meng et al. 1997; Seinfeld 1998).

Air pollution forecasts, if reliable and accurate, could play an important role as part of a local air quality management system working along with traditional emission/concentration based control approaches. The critical periods are determined from the air pollution forecasts using weather related data in the area. From a technical point of view near real time forecasts and, at least, a forecast to be available for one day in advance are needed. The purpose of this research is to develop operational statistical models and their inferences for short-term forecasts of ozone concentrations.

Due to the simple structure and the robustness in forecast, time series models have been widely used in environmental modeling (e.g. Merz et al., 1972; Simpson and Layton 1983; Hui 1992; Damon and Guillas 2002). For a review of the univariate time series models Millionis and Davies (1994) can be consulted. Meteorological adjustments in various ozone modeling have been considered in a number of articles (e.g. Fiester and Balzer 1991; Bloomfield et al. 1996; Davis and Deistler 1998). It is known that hourly ozone concentrations are closely related to meteorological conditions such as ambient temperature, wind speed, wind direction, dew point temperature, and radiation. The lagged meteorological variables in time series models are important to improve the prediction performance.

A frequently encountered problem during the application of an autoregressive type model to environmental data is a persistent diurnal behavior in model residuals. This indicates that there exists nonlinearity in the urban ozone dynamics. For this a nonlinear model can be considered. However, nonlinear modeling is rather complex with too many possible structures and is not suitable for multi-step forecasts. In order to account for the seasonal nonstationarity within the linear dynamic model, we consider the functional coefficient model which allows the regression coefficients to vary with another variable such as 'time of day'. As a special case, we first investigate the threshold autoregressive model of Tong (1983, 1990) which separates the autoregressive model in terms of predetermined threshold regimes. In this study we use time of day to define the threshold regimes so that ozone data can be modeled linearly within each of 24 h of day. Functional changes of regression coefficients over the threshold regimes are investigated and finally a functional coefficient model where the coefficient functions are polynomial functions of time of day is derived. The model, in comparison with the threshold model, contains only a few parameters without deteriorating the forecast performance.

The data are described in Sec. 2 and the model classes and test statistics for nonlinearity are presented in Sec. 3. Model evaluation parameters are given in Sec. 4. Section 5 presents an empirical application of the proposed models to the Cincinnati ozone data. Model identification, comparison, and the performance of short-term (one-day-ahead) forecast are given in Sec. 5. Concluding remarks are given in Sec. 6.

Data

The Greater Cincinnati area is currently not in compliance with National Ambient Air Quality Standard (NAAQS) for ozone, which was set in 1997. The Hamilton County Department of Environmental Service (HCDOES) monitors ozone levels in the Greater Cincinnati area from seven monitoring stations in the southwest Ohio covering four counties. Data used in model fitting are based on hourly ozone records (in parts per billion) from the monitoring station (Taft station, AIRS code 39-061-0040) near downtown Cincinnati from April 1 to October 31, 2001. Ambient temperature, wind speed, and wind direction are also available from the station. Ozone records are only available since 1999 and meteorological data since 2001. For the purpose of evaluating the performance of short term ozone forecast, 2002 data from the same station are used. Thus, the evaluation uses an independent data set.

Notice that data are of high-quality with ignorable number (0.8%) of missing measurements. There is no evidence of a systematic pattern in missingness. The missing values are replaced with immediate past observations. As we discuss in Sect. 5 the forecast performance of the proposed model is consistent even with highly missing data cases.

Time Series Models

Reference Model

The reference model presented in this paper is an autoregressive model with an exogenous vector process (ARX). The hourly observed time series y_t with mean μ can be modeled as a regression form:

$$y_t = \mu + \sum_{j=1}^{p} \phi_j y_{t-j} + \boldsymbol{\beta}'\mathbf{x}_t + w_t, t = q+1, ..., n \tag{1}$$

with $\phi_p \neq 0$ where p, the order of the autoregressive part in (1), is a positive integer and error process w_t is assumed to be zero mean white noise process. The exogenous vector $\mathbf{x}_t = (\mathbf{x}_{1t}, ..., \mathbf{x}_{lt})'$ contains l exogenous processes with lags r_1, r_2, ..., r_l, respectively, $\mathbf{x_{kt}} = (\mathbf{x_t}, \mathbf{x_{t-1}}, ..., \mathbf{x_{t-r_k}}), \mathbf{k} = \mathbf{1}, \mathbf{2}, ..., \mathbf{l}$ and $q = \max\ (p, r_1, ..., r_l)$. The order r_1, r_2, ..., r_l may involve seasonal components. The parameter vector β are denoted by $\beta = (\gamma_1, \gamma_2, ..., \gamma_l)'$, where $\gamma_k = (\gamma_{k0}, \gamma_{k1}, ..., \gamma_{kr_k})$, $k = 1, ..., l$. The model can be written as a multiple regression form in which the vector of predictor is

$$\mathbf{z}_t = (1, z_{1t}, z_{2t}, ..., z_{Mt})' = (1, y_{t-1}, ..., y_{t-p}, \mathbf{x}_{1t}, ..., \mathbf{x}_{lt})' \tag{2}$$

with the corresponding parameter vector of

$$\theta = (\theta_0, \theta_1, ..., \theta_M)' = (\mu, \phi_1, ..., \phi_p, \beta)', \tag{3}$$

where M denotes the number of predictors.

For a comparison purpose we also consider the model without exogenous processes (AR model). The order p can be estimated using the iterative procedure of Box and Jenkins (1976) and the order r_1, r_2, ..., r_l can be obtained from the cross-correlation functions (CCF) between the pre-whitten response and each of the pre-whitten exogenous processes (see Box and Jenkins 1976 for detailed discussions). Some alternative optimality criteria, e.g. Akaike's AIC (Akaike 1974) and Schwarz's SIC (Schwarz 1978), can be also used. However, in order to avoid overfitting problems, the procedure by Box and

Jenkins has been suggested in air pollution modeling (Millionis and Davies 1994).

Functional Coefficient ARX Model (FARX)

Prior studies (e.g. Bauer et al. 2001; Fasso and Negri 2002) argued that even with use of high dimensional predictor vectors, the ARX model shows diurnal patterns in residuals that cause systematic over- and under-predictions (see Fig. 2 in Sect. 5). One obvious way to take into account the nonlinearity in the time series is to include time of day, weekend-weekday, and month as nonlinear predictor variables in the model together with other exogenous variables. However, as shown in Sect. 5, this is not very effective for the ozone data used in this study.

A useful class of approach for modeling nonlinear time series is the functional coefficient (or varying coefficient) model by Cleveland et al. (1991) and Hastie and Tibshirani (1993). The model assumes the form

$$y_t = \mathbf{g}(u_t)'\mathbf{z}_t + w_t, \tag{4}$$

where $\mathbf{g}(\cdot) = (\mathbf{g_0}(\cdot), \mathbf{g_1}(\cdot), \ldots, \mathbf{g_M}(\cdot))'$ are unknown coefficient functions of interest. This model enables one to model the nonlinearity in time series by replacing the constant coefficients, θ_0, θ_1, ..., θ_M, in (3) with some smooth functions, $g_0(\cdot), g_1(\cdot), \ldots, g_M(\cdot)$, of a carefully chosen variable u_t. In this application we use time of day $u_t \in \{1,2,\ldots,24\}$, due to the reason mentioned above. This model is called the functional ARX (FARX) model (Chen and Tsay 1993). In recent years, various nonparametric methods have been studied to estimate the coefficient functions; for example, smoothing splines (Hastie and Tibshirani 1993), iterative local constant fitting (Chen and Tsay 1993), local polynomial (Fan and Zhang 1999), and local linear (Cai et al. 2000). However, due to the computational burden and difficulties in calculating multi-step forecasts, the nonparametric methods aforementioned have not taken much attention in environmental monitoring studies. In this paper we consider a simple regression procedure to estimate the functional forms of $\mathbf{g}(\cdot)$. For this, we first fit the least squares regressions

$$y_t = \theta^{(\mathbf{j})'}\mathbf{z_t} + \mathbf{w_t^{(j)}}, \tag{5}$$

conditioned on $u_t = j, j = 1,2,\ldots,24$, where $\theta^{(j)} = (\theta_0^{(j)}, \theta_1^{(j)}, \ldots, \theta_M^{(j)})'$ is the vector of regression coefficients at time j. This is the threshold ARX model (TARX) considered in Tong (1983, 1990) with the threshold regimes defined in 24 h of day. The TARX model is a special case of the FARX model (4) where $g_m(u_t) = \theta_m^{(j)}$, $m = 0,1,\ldots,M$ conditioned on $u_t = j$ and the ordinary least squares estimate of $\theta_m^{(j)}$ is an estimate of the coefficient function $g_m(u_t)$. The TARX model is flexible and very effective when the threshold regimes are well defined such that a ozone process can be modeled linearly within each regime of the threshold variable. Bauer et al. (2001) also used immediate past ozone concentrations to define the threshold regimes. As discussed in Sec. 5, by plotting the estimates of $\theta_m^{(j)}$ against j, the TARX model provides a useful insight into the functional form of the coefficient functions in (4) (see Fig. 4).

Testing hypothesis

For practical purpose the TARX model in (5) can be written as

$$y_t = \tilde{\theta}'\mathbf{z_t} + \sum_{\substack{\mathbf{k=1} \\ \mathbf{k \neq j}}}^{\mathbf{24}} \theta'_{\mathbf{k}}\mathbf{z_t}\delta_{\mathbf{kt}} + \mathbf{w_t}, \quad \delta_{\mathbf{kt}} = \mathbf{I}(\mathbf{u_t} = \mathbf{k}), \tag{6}$$

where, $I(\cdot)$ is the indicator function. Conditioned on $u_t = j$, $\tilde{\theta}$ in (6) is equal to $\theta^{(j)}$ in (5) and the model can be fitted easily using 24 regression runs for $j = 1,2,\ldots,24$. The hypothesis for testing varying coefficients can then be formulated as $H_0 : \theta_k = \mathbf{0}$, for all $k \in \{1,2,\ldots,24\}$ and $k \neq j$. For given $q = \max\,(p, r_1, \ldots, r_l)$, the effective number of observations in the regression in (6) is $n-q$. The number of parameter is 24 $(M+1)$ for the full model (6) and $(M+1)$ for the reduced model under H_0. Then, when the model under H_0 is correct, the general linear test statistic

$$F = \frac{(RSS_0 - RSS_1)}{RSS_1}\left(\frac{n - q - 24(M+1)}{23(M+1)}\right), \tag{7}$$

has a central F-distribution with $23(M+1)$ and $n-q-24(M+1)$ degrees of freedom. Here, RSS_0 and RSS_1 are the residual sum of squares under the reduced model and the full model, respectively. Once the test rejects the null hypothesis, it indicates that not all regression coefficients are constant and thus the functional coefficient regression is suggested.

For each fitted model, we also consider two versions of the portmanteau test of goodness of fit. Let $\hat{\rho}_k^2$ be the kth sample autocorrelation coefficient of the residuals from the fitted model, then in the case of white residuals, Ljung and Box (1978) showed that the statistic

$$Q_{\mathrm{LB}} = n'(n'+2)\sum_{k=1}^{h}(n'-k)^{-1}\hat{\rho}_k^2, \tag{8}$$

has an approximate χ^2 distribution with h degrees of freedom. Here n' denotes the number of sample used to calculate $\hat{\rho}_k^2$. Monti (1994) proposed a similar statistic which replaces the autocorrelation $\hat{\rho}_k^2$ with the partial autocorrelation $\hat{\pi}_k^2$:

$$Q_{\mathrm{MT}} = n'(n'+2)\sum_{k=1}^{h}(n'-k)^{-1}\hat{\pi}_k^2. \tag{9}$$

Under white errors, this statistic also has an approximate χ^2 distribution with h degrees of freedom.

Model evaluations parameters

Several model evaluation parameters are considered. The consideration is based on their use in air pollution model evaluation studies. If we denote y_t the observed values, $\hat{y}_t$ the predicted values, $\bar{y}$ the sample mean of observed values, $\bar{\hat{y}}$ the sample mean of predicted values, and p the number of parameters in the model, one can compute:*Root Mean Square Error (RMSE)*

$$\mathrm{RMSE} = \sqrt{\frac{\sum_t (y_t - \hat{y}_t)^2}{n-p}} \tag{10}$$

Coefficient of Determination (R^2)

$$R^2 = \frac{\sum_t (\hat{y}_t - \bar{y})^2}{\sum_t (y_t - \bar{y})^2} \tag{11}$$

Fraction Bias (FB)

$$\mathrm{FB} = \frac{2(\bar{y} - \bar{\hat{y}})}{(\bar{y} + \bar{\hat{y}})} \tag{12}$$

Normalized Mean Square Error (NMSE)

$$\mathrm{NMSE} = \frac{(\bar{y} - \bar{\hat{y}})^2}{\bar{y}\bar{\hat{y}}} \tag{13}$$

Factor of two($Fa2$)

$$\mathrm{Fa2} = \text{fraction of data which satisfy} \quad 0.5 \leqslant \frac{\hat{y}_t}{y_t} \leqslant 2.0 \tag{14}$$

RMSE is an unbiased estimator of the regression error variance and most commonly used statistic in cross-validation schemes. It takes the number of parameters p into account through n-p in the denominator. R^2 is the proportionate reduction of total variation in the time series associated with the use of the model. The remaining three parameters are also introduced to assess the performance of air quality models (e.g. Kumar et al. 1999). FB is the normalized mean bias varying between -2 and $+2$ and has a value of zero for an ideal model. NMSE emphasizes the scatterness of residuals in the entire data set. The normalization by the product in the denominator assures that the statistic will not be biased towards over-predictions or under-predictions. Smaller values of NMSE denote better model performance. Fa2 is defined as the percentage of the predictions within a factor of two of the observed values. The ideal value for Fa2 should be 1. In addition, the percentage of the predicted values within ± 5 and ± 10 ppb of the observed values are calculated to get an idea of the forecasting ability of the models.

Ozone Prediction in Downtown Cincinnati

Model Identification

To identify an initial ARX model, the iterative procedure by Box and Jenkins (1976) is applied to 2001 (April–October) hourly ozone data observed at Taft station. The partial autocorrelation function of the ozone process shows two dominant peaks at lag one and two. This suggests AR with order two (AR(2)) for an initial model. The obvious 24 h correlation shown in the autocorrelation function (ACF) of the AR residuals further suggests the inclusion of the seasonal component of lag 24. For the exogenous processes, the ambient temperature (t) in °F, the wind speed (s) in km/h, and wind direction (w) in degree from north were used. For better physical meaning, the wind direction was incorporated using the west–east component (u) and the south–north component (v) of wind as follows:

$$u = s \times \sin(2\pi w/360), \\ v = s \times \cos(2\pi w/360). \tag{15}$$

To reduce multicollinearities among the predictors and to balance the units, each of the predictor variables was standardized; centered by sample mean and scaled by unit of standard deviation.

The cross-correlation functions (CCF) between the pre-whitten response and each of the pre-whitten exogenous processes have dominant peaks at lag 0 and 2 for both t and s and lag 0 for both u and v. Following model is used as the reference model:

(M1) ARX model with the predictor vector:

$$\mathbf{z_t} = (\mathbf{1}, \mathbf{y_{t-1}}, \mathbf{y_{t-2}}, \mathbf{y_{t-24}}, \mathbf{t_t}, \mathbf{t_{t-2}}, \mathbf{s_t}, \mathbf{s_{t-2}}, \mathbf{u_t}, \mathbf{v_t}). \tag{16}$$

The AR(2) model is also added for comparison. The following two models are also considered within model (M1).

(M2) Polynomial regression with the predictor vector:

$$\mathbf{z}_t = \left(1, y_{t-1}, y_{t-2}, y_{t-24}, t_t, t_{t-2}, s_t, s_{t-2}, u_t, v_t, t_t^2, t_t^3, s_t^2, s_t^3\right). \tag{17}$$

This model is considered based on the curvilinear relations as shown in Figure 1. A third-order model with temperature and wind speed was found based on the minimum RMSE criterion.

(M3) Periodic regression with the predictor vector:

$$\mathbf{z}_t = \left(1, y_{t-1}, y_{t-2}, y_{t-24}, t_t, t_{t-2}, s_t, s_{t-2}, u_t, v_t, t_t^2, t_t^3, s_t^2, s_t^3, h_t, \\ h_t^2, h_t^3, m_t; m_t^2, m_t^3, w_t\right). \tag{18}$$

Here, h_t denotes hour in day, m_t month in year, and w_t a binary weekend indicate variable (1 for weekends, 0 for weekdays). Figure 2 shows that both AR(2) and ARX (M1) models have similar diurnal bias; systematically under-predict during the ascent period and over-predict during the descent period. The ACF plots in

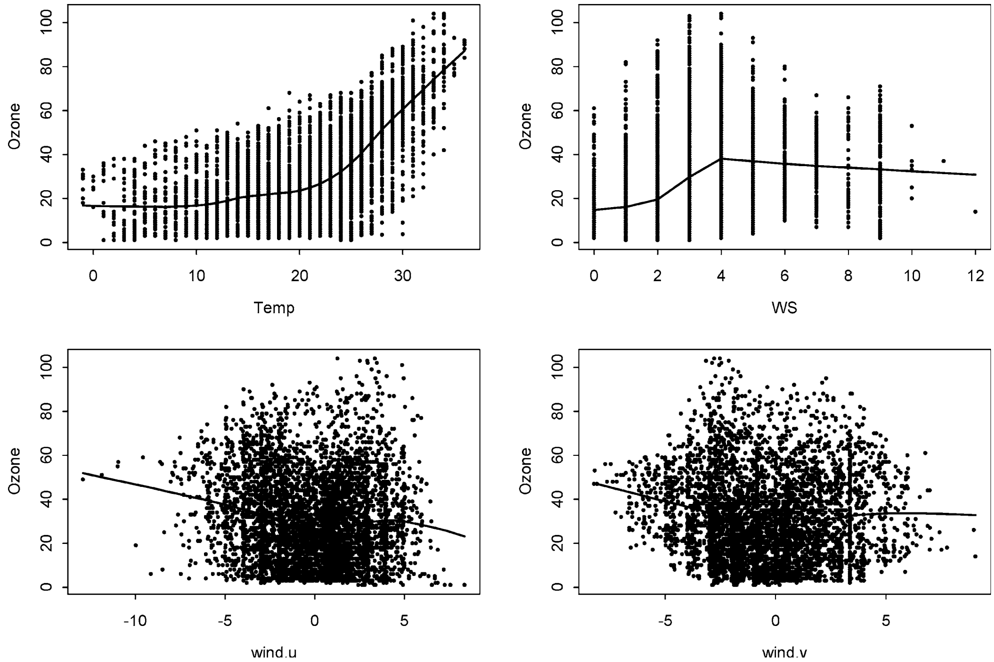


Fig. 1 Curvilinear relation between ozone concentration and meteorological variables with lowess lines superimposed

Fig. 3a, b pronounce the diurnal behavior of residuals. Note that model (M3) is expected to take into account the diurnal pattern in the time series.

An ANOVA (Analysis of Variance) table of models is given in Table 1.

It seems clear from RMSE and R^2 that the AR(2) model is clearly inferior to others; this shows the importance of exogenous variables in ozone modeling. Model (M3) shows slightly the better fit than (M1) and (M2) models, but R^2 is increased only by 0.5% and 0.3% respectively. A direct use of the polynomials is not very effective to model the nonlinear relationship between ozone and meteorological variables for (M2) and (M3) models. Based on the results from the portmanteau tests ((8) and (9)) in Table 1, all four models discussed above reject the null hypothesis of white errors. For subsequent modeling we have chosen to focus on ARX model (M1).

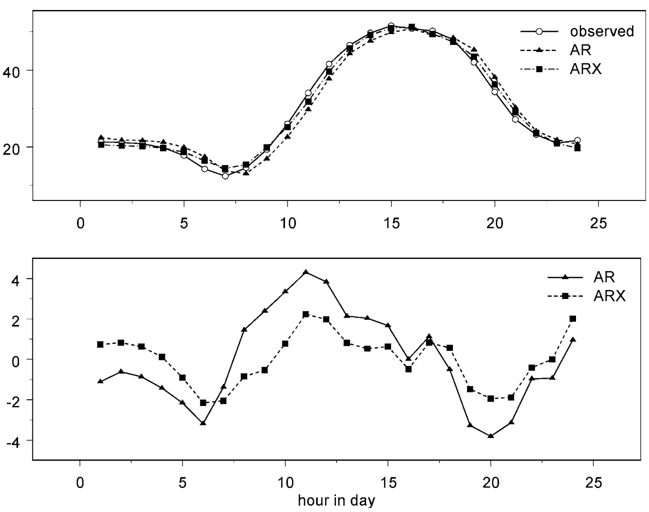


Fig. 2 Hourly mean observed and mean predicted from non-threshold (AR and ARX) models (top) and the corresponding residuals (bottom)

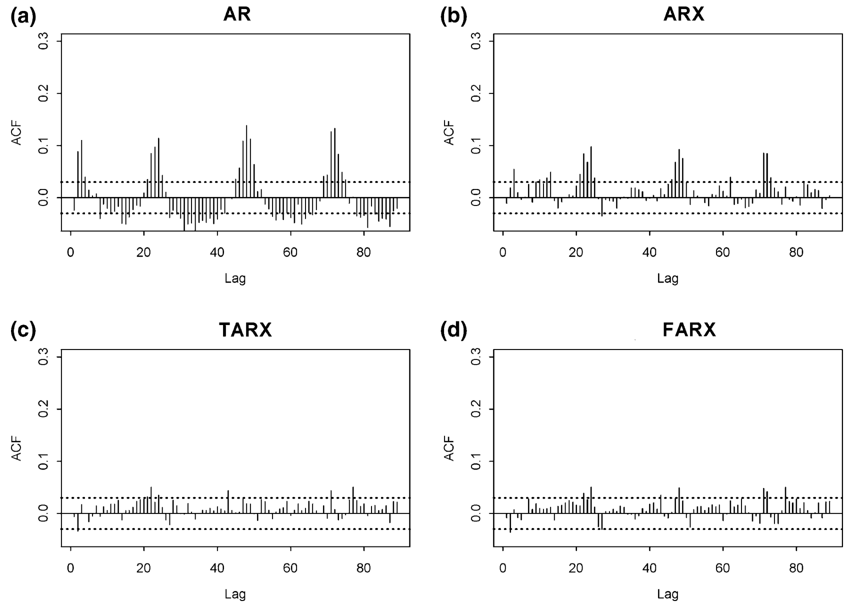
The threshold model discussed in Sect. 3.2 is applied to the ARX model (16) to account for the nonlinearity and the diurnal bias in residuals. As shown in Fig. 2 and 3a, b, the residuals of both AR and ARX models show biases which have diurnal patterns. This motivates the use of time of day as the threshold regimes in the TARX model. The test statistic (7) is $F = 4.557$ with degrees of freedom 230 and 4872. The p-value is less than 0.0001, which strongly rejects the null hypothesis of constant coefficients. The result from the fitted TARX model is summarized in Table 1. The model fits the data significantly better than the ARX model and the diurnal autocorrelation in residuals is almost removed (Fig. 3c). Both portmanteau tests (8) and (9) support this result with the p-values 0.421 and 0.472, respectively.

Figure 4 gives the least squared estimates of the coefficients and their 95% confidence limits under the TARX model for each of 24 h of day. The plots well exhibit the curvilinear trends of the coefficient estimates over 24 h of day. The fitted polynomial curves (solid line) with the order of up to four are very close to the *lowess* (locally weighted scatterplot smoothing) lines (dotted line) and well reside within the 95% confidence limits. This suggests the use of the functional coefficient model with polynomial coefficient functions:

$$\mathbf{g}(\mathbf{x}) = \alpha_0 + \alpha_1 \mathbf{x} + \alpha_2 \mathbf{x}^2 + \ldots + \alpha_m \mathbf{x}^m. \quad (19)$$

Here, α_j, $j = 1, \ldots, m$ are the coefficient vectors to be estimated. A stepwise model selection procedure is applied to fit the final model which allows different order of

Fig. 3 ACF of residuals from fitting various models at Taft station



the polynomial for different predictor. Using the final FARX model we can reduce the number of parameters from 240 in the TARX model to only 31, without much deteriorating the prediction performance (Table 2). The ACF in Fig. 3d indicates that the diurnal bias is almost removed. The p-values of both portmanteau tests of 0.133 and 0.160 also show that the residuals are white. In the following section, the proposed models are compared in terms of the one-day-ahead forecast performance.

Forecasting

To explore the forecast performances of the models in Sect. 5.1, the 2002 data at the same station are used. To avoid further complications, it is assumed that meteorological processes are observable or at least predictable from a weather forecasting system. In this sense, forecasting procedures discussed in this section is conditional to known exogenous processes. Due to the autoregressive structure of the models, forecasts can be computed recursively. Table 2 summarizes a comparison of one-day-ahead forecast performances. All models have FB and NMSE values close to zero showing that they are acceptable in terms of unbiasness and scatterness of the mean residuals. Both TARX and FARX models clearly outperform the AR and the ARX model. As regard the TARX and the FARX models, the FARX model is slightly better in terms of R^2 and RMSE, and the TARX model is slightly better in terms of Fa2, ± 5, and ± 10. However, considering the number of parameters, the FARX model is preferred; the extremely large number of parameters in the TARX model results in an overfitting problem by occasionally forecasting negative ozone levels.

Figure 5 draws the hourly profile of one-day-ahead forecasts from various models for the second week of August, 2002; during 2002 the highest peak (120 ppb) was observed at the hour count 3137, which corresponds to 5 p.m., August. 9. Both TARX and FARX models give similar results, so the hourly forecasts from the TARX model is omitted from the plot. The FARX model clearly outperform the constant coefficient models and seems to give a satisfactory forecasting performance. The model well forecasts most of the ozone levels, but still under-predicted the highest peak at 120 ppb. The forecasted daily ozone averages (Fig. 6) from the FARX model appear to agree very well with the observed average on most days. On about 93% (199 out of 213 days) of days there are errors within ± 10 ppb (65% within ± 5 ppb). The temporal pattern of the daily ozone averages is well captured by the model.

To verify the forecast performance of FARX in cases of highly missing data, a portion of 2001 data is removed at random and replaced with immediate past observations. Then, FARX model is fitted for the reconstructed data and the one-day-ahead forecast performance of the fitted model is explored using 2002 data. It appears that FARX model is satisfactory in forecast even with highly missing data cases. With 10% missing data, the forecast error in terms of RMSE increases only by 7.7% (from 10.04 to 10.81). The RMSE value for 20 and 30% missing data increases slightly to 10.96 and 11.26, respectively.

Table 1 Comparison of fitted models

Model	R^2	RMSE	df	Q_{LB} (p-val)	Q_{MT}(p-val)
AR(2)	0.865	6.79	5108	77.7 (.000)	42.4 (.000)
M1 (ARX)	0.911	6.00	5102	47.0 (.000)	30.0 (.003)
M2	0.913	5.92	5098	34.1 (.001)	25.9 (.011)
M3	0.916	5.82	5091	98.8 (.000)	44.6 (.000)
TARX	0.927	5.57	4872	12.3 (.421)	11.7 (.472)
FARX	0.921	5.70	5081	17.5 (.133)	16.7 (.160)

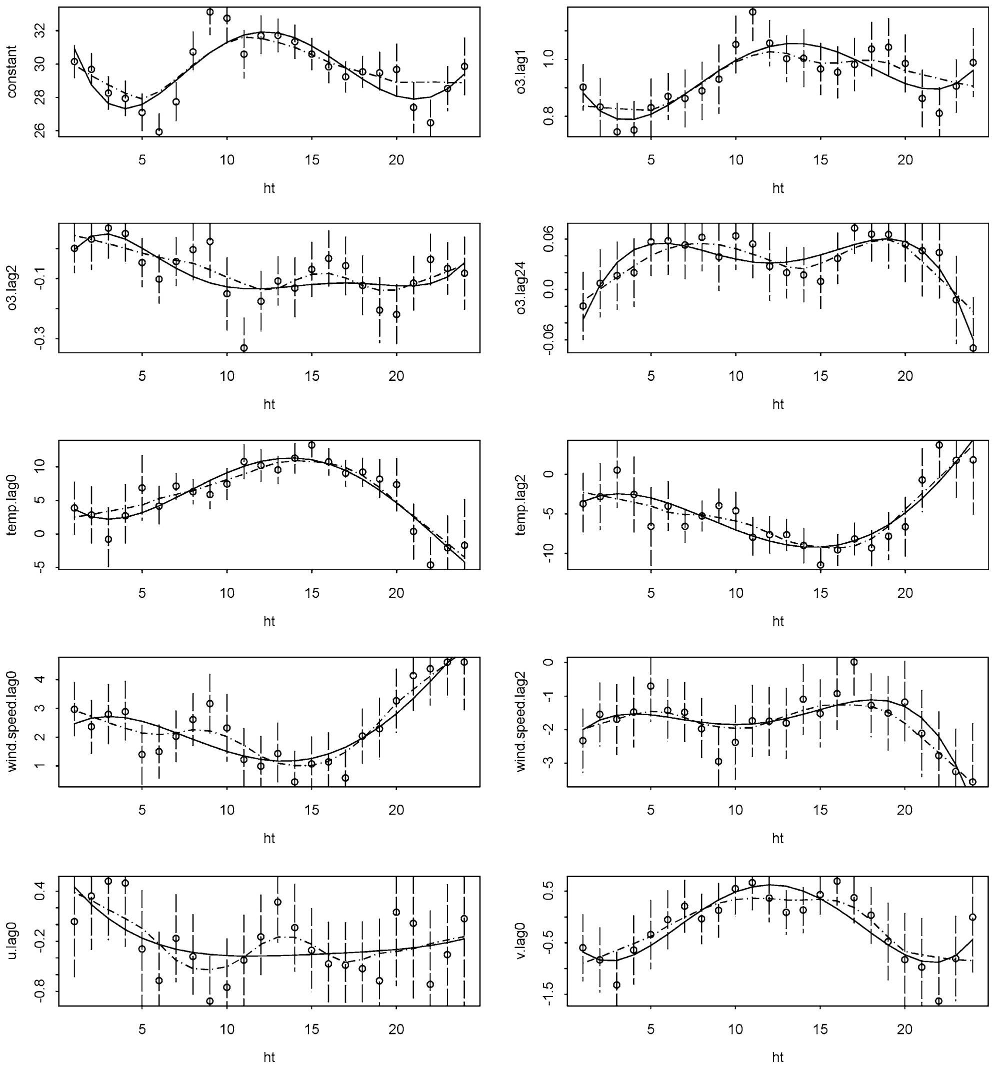


Fig. 4 Coefficient estimates (empty circle) from TARX model with 95% confidence limits (vertical line) against hour in day with polynomial (solid line) and lowess (dotted line) lines superimposed

Conclusion

For regional ozone level forecast, a simple AR model with exogenous variables is reconsidered. Although reduced by introducing lagged meteorological variables (temperature, wind speed, wind direction) in the model, the seasonal nonstationarity in errors is still evident. Direct inclusion of time of day, weekend-weekday, and month as nonlinear predictor variables in the model together with the other exogenous variables failed to remove the nonstationarity. In this paper, a periodic threshold autoregressive models with the 24 threshold regimes defined in 24 h of day (TARX) have been

Table 2 Model evaluation parameters for one-day-ahead forecasts of 2002 hourly ozone level at Taft for different model classes

	AR(2)	ARX	TARX	FARX
R^2	.411	.643	.769	.775
RMSE	17.189	12.82	11.02	10.04
FB	.0231	.0121	.0108	.0119
NMSE	.0005	.0002	.0001	.0001
Fa2	.702	.757	.821	.806
± 5	.232	.314	.391	.387
± 10	.454	.595	.674	.667

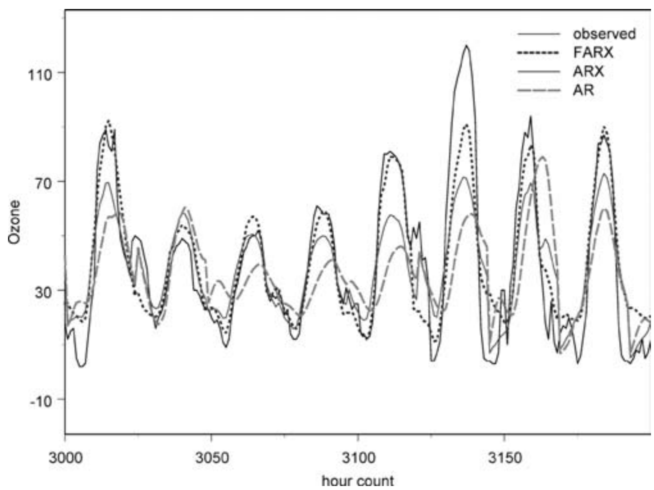


Fig. 5 One-day-ahead forecasts of hourly ozone level for the second week of August, 2002 at Taft station using various models

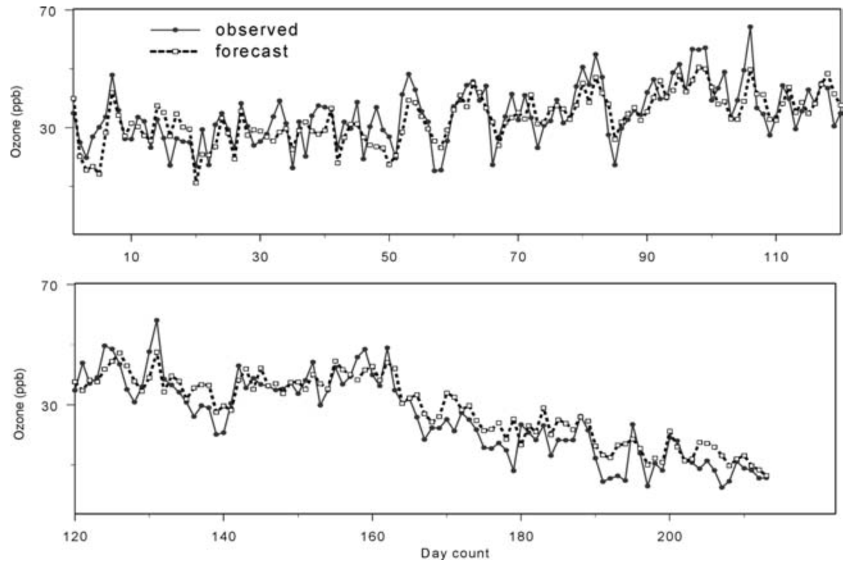


Fig. 6 Comparison of observed and one-day-ahead forecast of daily average ozone concentrations for April to June 2002 (top) and July to October 2002 (bottom)

proposed to enhance fitting and to remove unexplained seasonal autocorrelation in residuals. Application of the proposed model to hourly ozone data in downtown Cincinnati indicates that the TARX model almost removed the persistent diurnal behavior of residuals in the non-threshold models. The model also substantially improved the day-ahead forecasts. Investigation of changing coefficients over 24 h regimes in the TARX model suggests the use of the functional coefficient autoregressive model (FARX) where the coefficient function is a polynomial function of 24 h of day. By using the FARX model, it is possible to drastically reduce the number of parameters without deteriorating the forecast performance. A simple recursive procedure for multi-step forecast requires prior knowledge in current and past values of meteorological variables. In this paper it is assumed that the next 24 h meteorological values are available from a weather forecasting model. The use of forecasted meteorological data may or may not introduce additional error into the ozone forecasts.

Acknowledgements The authors wish to express thanks to Anna Kelley with HCDOES for providing us with the data. Thanks also to the three reviewers who made very helpful comments on this manuscript.

References

Akaike H (1974) A new look at statistical model identification. IEEE Trans Automat Contr AC-19:716–723

Bauer G, Deistler M, Scherrer W (2001) Time series models for short term forecasting of ozone in the eastern part of Austria. Environmetrics 12:117–130

Bloomfield P, Royle JA, Steinberg LJ, Yang Q (1996) Accounting for meteorological effects in measuring urban ozone levels and trends. Atmos Environ 30(17):3067–3077

Box GEP, Jenkins GM (1976) Time series analysis:forecasting and control, revised edn. Holden Day, San Francisco

Cai Z, Fan J, Li R (2000) Efficient estimation and inferences for varying-coefficient models. J Am Stat Assoc 95:888–902

Chen R, Tsay R (1993) Functional-coefficient autoregressive models. J Am Stat Assoc 88:298–308

Cleveland WS, Grosse E, Shyu WM (1991) Local regression models. Statistical Models in S, 309–376, Wadsworth, Pacific Grove

Damon J, Guillas S (2002) The inclusion of exogeneous variables in functional autoregressive ozone forecasting. Environmetrics 13:759–774

Davis MD, Deistler M (1998) Modeling ozone in the Chicago urban area. In: Nychka D, Piegorsch W, Cox LH (eds) Case Studies in Environmental Statistics, Lecture Notes in Statistics. Springer, Berlin

Fan J, Zhang W (1999) Statistical estimation in varying coefficient models. Ann Stat 27:1491–1518

Fasso A, Negri I (2002) Non-linear statistical modeling of high frequency ground ozone data. Environmetrics 13:225–241

Fiester U, Balzer K (1991) Surface ozone and meteorological predictors on a subregional scale. Atmos Environ 25:1781–1790

Hastie TJ, Tibshirani RJ (1993) Varying-coefficient models (with discussion). J R Stat Soc B 55:757–796

Hui K-J (1992) Time series of the analysis of the interdependence among air pollutants. Atmos Environ 26:491–503

Kumar A, Bellam N, Sud A (1999) Performance of industrial source complex model in predicting long-term concentrations in an urban area. Environ Prog 18(2):93–100

Ljung GM, Box GEP (1978) On a measure of lack of fit in time series models. Biometrika 65:297–303

Meng Z, Dadub D, Seinfeld JH (1997) Chemical coupling between atmospheric ozone and particulate matter. Science 227:116–119

Merz PH, Painter LG, Ryason PR (1972) Aerometric data analysis. Time series analysis and forecast and an atmospheric smog diagram. Atmos Environ 6:319–342

Millionis M, Davies TD (1994) Regression and stochastic models for air pollution-I. Review, comments and suggestion. Atmos Environ 28(17):2801–2810

Monti AC (1994) A proposal for residual autocorrelation test in linear models. Biometrika 81:776–780

Schwarz F (1978) Estimating the dimension of a model. Ann Stat 6:461–464

Seinfeld JH (1998) Ozone air quality models:a critical review. J Atmos Pollut Control Assoc 38:616–647

Simpson RW, Layton AP (1983) Forecasting peak ozone levels. Atmos Environ 17:1644–1654

Tong H (1983) Threshold models in non-linear time series analysis. In: Brillinger D, Fienberg J, Gani J, Hartigan J, Krickberg K (eds) Lecture Notes in Statistics. Springer-Verlag, Berlin

Tong H (1990) Nonlinear time series: a dynamic system approach. Oxford University Press, Oxford