Visual-FIR for ozone modeling and prediction

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Abstract. Air pollution is one of the most important environmental problems in urban areas, being extremely critical in Mexico City. The main air pollution problem that has been identified in Mexico City metropolitan area is the formation of photochemical smog, primarily ozone. The study and development of modeling methodologies that allow the capturing of time series behavior becomes an important task. The present work aims to develop Fuzzy Inductive Reasoning (FIR) models using the Visual-FIR platform. FIR offers a model-based approach to modeling and predicting either univariate or multivariate time series. Visual-FIR offers an easy-friendly environment to perform this task. In this research, long term prediction of maximum ozone concentration in the centre region of Mexico City metropolitan area is performed. The data were registered every hour and include missing values. Two modeling perspectives are analyzed, i.e. monthly and seasonal models. The results show that the models identified capture the dynamic behavior of ozone contaminant in an accurate manner.

Keywords: Hybrid fuzzy systems, environmental modeling, long-term prediction, ozone models

1 Introduction

The main air pollution problem that has been identified in Mexico City Metropolitan Area (MCMA) is the formation of photochemical smog, primarily ozone, O_3. Ozone is not a pollutant emitted from a pollution source, but a secondary contaminant. It is formed in the presence of solar light, volatile organic compounds, VOC, and nitrogen oxides, NO_x. Ozone is a highly reactive form of molecular oxygen.

High levels of ozone causes eye irritation, respiratory disorders, crop damage and increased deterioration rate of material. Ozone levels in Mexico City are very high although they have been reduced slightly in the last years. The Mexican standard of ozone (0.11 ppm, hourly average) is exceeded around 61% of the days in the year with concentrations up to 0.29 ppm (GDF, 2005). Unlike the majority of the cities in the northern hemisphere where the troposphere ozone phenomenon is only present during the summer days the MCMA presents favorable conditions for the formation of O_3 throughout the year.

In these circumstances, it is extremely important and useful to provide early warnings of high levels of ozone concentration so that the authorities can react as fast as possible. To this end, it is necessary to have accurate and reliable forecasts of future high ozone levels. Therefore, the construction of ozone models that capture the behavior of this gas in the atmosphere is of interest not only for environmental scientists but also for government agencies.

There are many different models available for local scale predictions of air quality and for ozone level forecasting. Some of these use classical methods based on numerical algorithms and statistical approaches (Comrie, 1997; Soja and Soja, 1999; Koçak et al., 2000; Chenevez and Jensen, 2001; Slini et al., 2002; Lengyel et al., 2004; Lu et al., 2004; Sousa et al., 2006; Gómez-Sanchis et al., 2006). Others use the chemical/physical knowledge (Stohl et al., 1996). In recent years other paradigms such as neural networks (NN) (Wieland and Wotawa, 1999; Abdul-Wahab and Al-Alawi, 2002; Wang et al., 2003; Wang and Lu, 2006), decision trees or association rules (Wotawa and Wotawa, 2001; Rohli et al., 2003) have been used for the same purpose. It can be found, also, in the literature modeling efforts that use fuzzy logic (Peton et al., 2000; Gómez et al., 2003; Onkal-Engin et al., 2004; Ghiaus, 2005) or hybrid NN and fuzzy logic approaches (Morabito and Versaci, 2003; Heo and Kim, 2003; Yildirim and Bayramoglu, 2006).

In almost all the previous mentioned studies, the contaminant modelled was ozone. Ozone is the pollutant that has received more attention in the literature from the modelling and prediction perspective, due to the harmful effects that cause in humans and the increasing levels of this contaminant in big cities. Both, daily and hourly models are found in the literature. However, daily models are more common and a small number of works deal with hourly models. Another interesting aspect is the prediction term, i.e. short vs. long term prediction. In this paper we understand by short term predictions those that forecast a single value (hourly or daily) at each prediction step and by long term predictions those that forecast a set of values (hourly or daily) at each prediction step. Notice that when long term prediction is performed previously predicted values of ozone are used to forecast the next value of this contaminant, if the model contains as input the variable ozone. Almost all the works present short term prediction models. However, from our point of view, long term prediction models are more useful when the goal is to prevent possible environmental contingencies.

The main goal of this paper is to identify fuzzy inductive reasoning ozone models for the centre area of Mexico City. This research analyses two different modeling perspectives. On the one hand, the identification of ozone models for a specific month of the year. On the other hand, the identification of ozone models for a specific season of the year. For both studies two experiments have been performed, one using dry season data and the other using wet season data. The number of variables considered, the high frequency of the signals (hourly models) and the fact that it is intended to perform long term predictions, increases the complexity of the application. An additional problem is the presence of missing values in the registered data.

In the next section the data used in this study is presented. Section 3 presents the methodology and section 4 presents the ozone contaminant problem and the results obtained in this study. Finally, a discussion and the conclusions of the work are presented.

2 Data

The data used for this study stems from the Atmospheric Monitoring System of Mexico City (SIMAT in Spanish[1]) that measures contaminants and atmospheric variables from 36 stations distributed through the 5 regions of the Mexico City metropolitan area. The registered variables are O_3, SO_2, NO_2, CO, PM10 atmospheric contaminants, as well as temperature, relative humidity, wind speed and wind direction meteorological variables, 24 hours a day, every day of the year. Whenever, for any reason, a measurement instrument of one of the stations fails, a set of missing values is produced.

This study is centered on the modeling of the ozone contaminant in the centre region (MERCED) of the Mexico City Metropolitan Area (MCMA). The ozone, O_3, measured in parts per million (PPM), is the

[1] http://www.sma.df.gob.mx/simat/

system's output variable. The input variables considered are temperature, TMP, measured in °C, relative humidity, RH, measured in percentage (from 0% to 100%), wind speed, WS, measured in meters per second (m/s), wind direction, WD, measured in degrees (from 0° to 359°) and hour of day, HD, from 1 to 24. The web page of SIMAT [8] offers a data base with meteorological and contaminant registers since 1986 up to date. For this study we used the data measured from January 2000 until March 2006.

The root mean square error (RMS) described in equation 1 is used to determine the validity of each of the models.

$$RMS = \sqrt{\frac{\sum_{i=1}^{N}\left(y_i(t) - \hat{y}_i(t)\right)^2}{N}} \qquad (1)$$

where $\hat{y}$ *(t)* is the predicted output, *y(t)* the system output and *N* the number of samples.

3 Methodology

Fuzzy logic-based methods have not been applied extensively in environmental science. However, some interesting research can be found in the area of modeling of contaminants (Mintz et al., 2005; Ghiaus, 2005; Morabito and Versaci, 2003; Heo and Kim, 2004; Yildirim and Bayramoglu, 2006; Peton et al., 2000; Onkal-Engin et al., 2004), where different hybrid methods that make use of fuzzy logic are presented for this task.

The Fuzzy Inductive Reasoning (FIR) methodology offers a model-based approach to predicting either univariate or multi-variate time series (Nebot et al., 1998; 2003).

A FIR model is a qualitative, non-parametric, shallow model based on fuzzy logic. Visual-FIR is a tool based on the Fuzzy Inductive Reasoning (FIR) methodology (that runs under Matlab environment), that offers a new perspective to the modeling and simulation of complex systems. Visual-FIR designs process blocks that allow the treatment of the model identification and prediction phases of FIR methodology in a compact, efficient and user friendly manner (Escobet et al., 2007). Each block is activated whenever necessary and allows to easily chosen the desired option for each parameter associated to that specific task. In this way, it is extremely easy for the user to “play” with different parameter options studying the effect of them to the prediction accuracy.

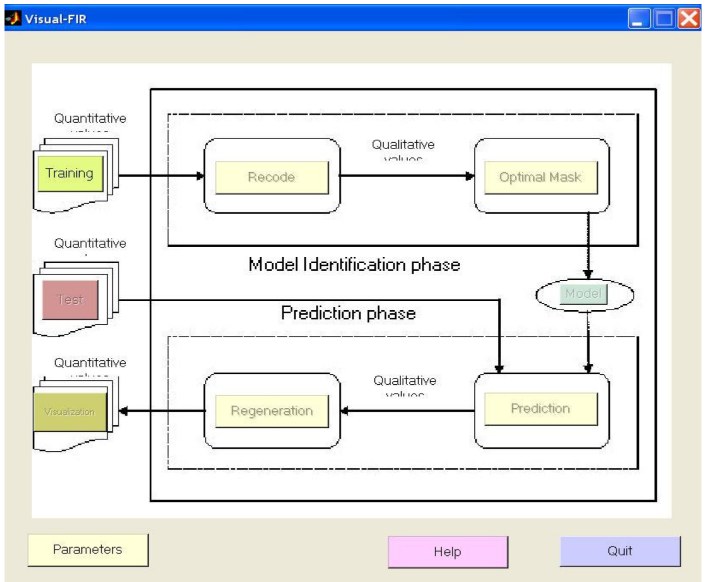

Figure 1: Visual-FIR main screen with the four main processes of FIR methodology, i.e. *Recode*, *Optimal mask search*, *Prediction* and *Regeneration*

The main screen of the new platform is invoked by means of the ***VisualFIR*** command issued from within the Matlab environment. The four main processes of the FIR methodology are then displayed as shown in figure 1. The upper half of figure 1 represents the *model identification phase*, whereas the lower half corresponds to the *prediction phase*, during which the model previously identified is used to estimate the future behavior of the system. The FIR model is composed by its structure (called *mask*) and a set of input/output rules (called *pattern rule base*). In order to get the model it is first necessary to discretize the data by means of the recode button. The *recode* function converts quantitative values into qualitative triples, i.e., class, fuzzy membership, and side values. Then the *optimal mask* function finds causal spatial and temporal relations between variables by using a metric based on the Shannon entropy measure. Once the pattern rule base and the mask are available, a prediction of future output states of the system can take place using the FIR inference engine. The FIR inference engine is based on a variant of the *k*-nearest neighbor rule, i.e., the 5-NN pattern matching algorithm. The forecast of the output variable is obtained by means of the composition of the potential conclusion that results from firing the five rules, whose antecedents best match the actual state. The contribution of each neighbor to the estimation of the prediction of the new output state is a function of its proximity. *Regeneration* is the inverse function of *recode*. It converts qualitative triples into quantitative values. A detailed description of FIR methodology can be found in

(Nebot et al., 2003).

4 Case study and results

In this study two modeling perspectives have been defined. The first one studies the modeling of the ozone behavior during a specific month of the year. The second one is centered on the ozone modeling of a certain season of the year. Each one of these modeling perspectives is presented in detail later on. Next, some modeling aspects that are common to both options are described. The first step after data loading is to convert quantitative values in qualitative triples by means of the recode process of Visual-FIR platform (see figure 1). To this end, it is necessary to specify two discretization parameters, i.e. number of classes per system variable (granularity) and the membership functions (landmarks) that define its semantics. In this study all the variables, except HD and O_3, are discretized into two classes using the EFP method. As known, the EFP algorithm defines the classes in such a way that the same number of data records is included in each membership function. Hour of day (HD) and ozone (O_3) variables are discretized manually into three classes following the recommendation of environmental experts. The landmarks obtained by each variable are shown in table 1. The landmarks described in table 1 are used in both O_3 modeling perspectives, i.e. monthly and seasonal.

Var.\Cla.	1	2	3
HD	1..12	12..17	17..24
RH	6..64	64..93	----
TMP	10.7..16.7	16.7..28.4	----
WD	0..124	124..360	----
WS	0.06..1.4	1.4..4.82	----
O_3	0.0..0.05	0.05..0.1	0.1..0.2

Table 1: Landmarks used in the recode process for input and output variables

Once the recoded data is available, the *optimal mask* process of Visual-FIR is activated. In the optimal mask screen the mask candidate matrix is created by defining its depth (number of rows) and complexity (number of non-zero values). In this study a depth of 3 and a complexity of 5 are chosen obtaining the candidate matrix shown in equation 2.

	HD	RH	TMP	WD	WS	O_3
t - 2δt	-1	-1	-1	-1	-1	-1
t - δt	-1	-1	-1	-1	-1	-1
T	0	0	0	0	0	+1

(2)

The mask candidate matrix proposed covers a time period of two hours and is used in both modeling perspectives. Notice that the last raw of the candidate matrix is set to “zeros”. Zero values represent forbidden connections. i.e. it is intended to predict ozone levels from past values (one or two hours ahead) of the atmospheric and the contaminant variables and not from its current values. Once the mask candidate matrix is ready, the mask search starts in the optimal mask screen. The optimal masks for each complexity and their associated quality are then show. A genetic algorithm is the default search algorithm used; however, the exhaustive search can be also chosen. In this application the exhaustive search algorithm is used in both modeling options. Next, monthly and seasonal modeling perspectives are presented in detail.

4.1 Monthly Models

Two monthly models have been identified in this study, the first one corresponds to the dry season, i.e. March, and the second one to the raining or wet season, i.e. August.

March Model

In this section a model that captures the behavior pattern of the ozone contaminant in the month of March has been identified. March corresponds to the dry season in Mexico City and the levels of ozone are usually high. The data registered in March from years 2001 to 2005, both inclusive, are used as training data whereas March of 2006 is used as test data to show the performance of the model identified. The total data set contains 3.720 registers, from which 318 are missing values. Missing data is distributed through all the variables except hour of day. In order to avoid the generation of inexistent relationships, a four raw gap of missing values have been added in the concatenation of the Januaries of different years.

Mask (PN)	Complexity	RMS_{test}
(1,6,10,11,18)	5	0.0176
(1,10,12,18)	4	0.0185

Table 2: Masks obtained for the March Monthly Model

Table 2 presents the best masks obtained for complexities 5 and 4 in the optimal mask process of Visual-FIR. The first column of table 2 presents the masks in position notation. The second column shows the complexity of that mask. The last column shows the RMS error (see equation 1) when that mask is used to predict the test data set, i.e. March 2006. Notice that the variables hour of day, wind direction and ozone are selected in both masks obtained, meaning that these variables are very relevant. Wind speed variable is also considered as important to increment the accuracy of the prediction. Notice that the temperature and the relative humidity are not selected, meaning that they do not influence significantly on the ozone behaviour during the dry season.

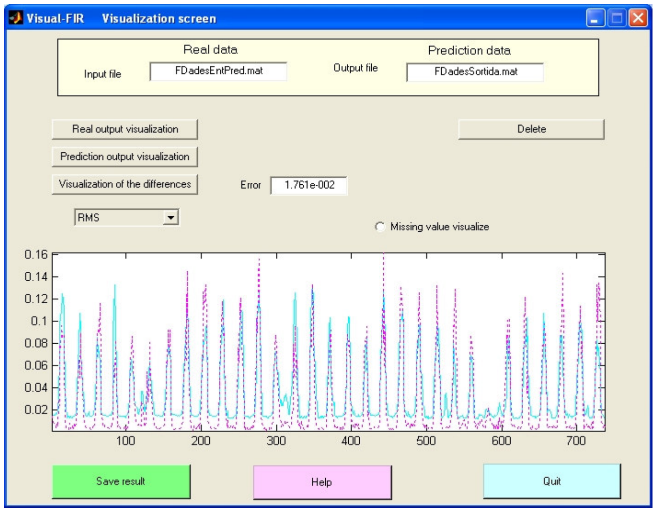

Figure 2: Real vs. prediction signals for March 2006 test data set using mask (1,6,10,11,18) – March Monthly Model

Equation 3 shows the upper mask of table 2, in matrix notation. The model of equation 3 says that the ozone at present time depends on the hour of day and ozone values two hours from now and also on wind direction and speed values one hour in the past. Figure 2 shows the prediction results obtained with FIR mask shown in equation 3. The continuous line corresponds to the real data whereas the dashed line represents the predicted signal. As seen in figure 2 the RMS obtained is of 0.0176, a small value if we take into account that a long term prediction is performed. It is important to notice that the long term prediction uses previously predicted ozone data as past ozone values. We are interested in this research to obtain models that are able to predict ozone behaviour not only one hour ahead, but some days ahead, in such a way that prevention measures can be taken before a contingency takes place. That is the reason why we decided to test the ozone models by predicting the contaminant during a complete month in a unique run. If these models are used in real life a prediction of maximum one week in advance is recommended, due to the fact that the ozone prediction is based on the atmospheric data forecast. The plot of figure 2 shows that the FIR model is capable of properly forecasting the high frequencies of the signal as well as the ozone upper peaks. It is capable of forecasting ozone concentration behaviour in quite an accurate way one month in advance.

	HD	RH	TMP	WD	WS	O_3
$t - 2\delta t$	-1	0	0	0	0	-2
$t - \delta t$	0	0	0	-3	-4	0
t	0	0	0	0	0	+1

(3)

August Model

In this section a model that captures the behavior pattern of the ozone contaminant in the month of August has been identified. August corresponds to the wet season in Mexico City and the levels of ozone are not so high than in the dry season but are still higher than 100 ppm. The data registered in August from years 2000 to 2004, both inclusive, are used as training data, whereas August of 2005 is used as test data to show the performance of the model identified. The total data set contains 3.720 registers, from which 153 are missing values. As before, a gap of missing values are included to separate the data of two consecutive August years in order to avoid unreal relations.

Mask (PN)	Complexity	RMS_{test}
(1,5,8,12,18)	5	0.0180
(1,6,8,18)	4	0.0189

Table 3: Masks obtained for the August Monthly Model

Table 3 presents the set of best masks obtained for complexities 5 and 4 in the optimal mask process of Visual-FIR. The structure of the table is exactly the same of table 2. As happened for the March models, previous instances of the ozone, hour of day and wind speed variables become crucial for the prediction. However, now the relative humidity appears as a relevant feature too, instead of wind direction. This is an interesting finding that makes a lot of sense due to the fact that August is a wet season and therefore the presence of humidity in the air influences directly the ozone levels. The prediction errors of the August models are similar than the ones computed by the March models. The RMS obtained of 0.0180 is again a small value if we take into account that a long term prediction is performed. The prediction plot looks very similar than figure 2.

4.2 Seasonal Models

Two seasonal models have been identified in this study, the first one corresponds to the dry season, i.e. December to March, and the second one to the raining season, i.e. May to August. The data registered in 2005 is used for this study.

Dry Model

The data measured in January, February and April is used as training data, whereas the test set corresponds to the data registered in March. This period is considered the dry season in Mexico City. The total training data set contains 2.141 registers, from which 444 are missing values.

Wet Model

The training data set corresponds to the data registered in May, June and August, whereas the data from July is used as test data set. This period is considered the raining season in Mexico City. The total data set contains 2.214 registers, from which 444 are missing values.

	Mask (PN)	RMS_{test}
Dry Model	(1,6, 10,11,18)	0.0155
	(1,5, 12,18)	0.0238
Wet Model	(1,2,6,11,18)	0.0195
	(1,11,12,18)	0.0176

Table 4: Masks obtained for Dry and Wet Seasonal Models

In table 4 the best FIR masks obtained for dry and wet seasons are presented. Table 4 has the same structure of tables 2 and 3. If we look closer to table 4 it can be seen that the best mask (i.e. complexity 5) is exactly the same as the best mask of the March model (see table 2). Here, as happened in March best model, ozone at present time depends on the hour of day and ozone levels two hours in advance and on the wind direction and wind speed values one hour before now. Therefore, this relation, described in equation 3, represents a qualitative patter of ozone behavior in dry seasons. It does not mater if we decide to use a monthly or a seasonal model perspective, the ozone behavior pattern for the dry period remains the same. On the other hand, if we analyze the best mask (i.e. complexity 5) of the August model (see table 3) and the mask of complexity 5 of the wet model (see table 4) it is easily seen that both mask contain the same variables, i.e. hour of day, relative humidity, wind speed and ozone. The difference relays on the time dependencies. In both masks the hour of day relation is presented two sampling intervals back. However, the rest of the relevant variables have different time dependencies in each mask. For example in the august mask, the relative humidity and the ozone variables influence the output one hour into the past, whereas in the wet mask these variables are relevant two hours into the past. The opposite happens with the wind speed variable. Therefore, in wet seasons the qualitative pattern of ozone behavior can be defined only by the variables involve but not for the time dependencies. Figure 3 present the prediction signal obtained when using the masks of complexity 5 (see table 4) for dry seasonal models. As can be seen from this plot, the prediction performance of FIR model is very good.

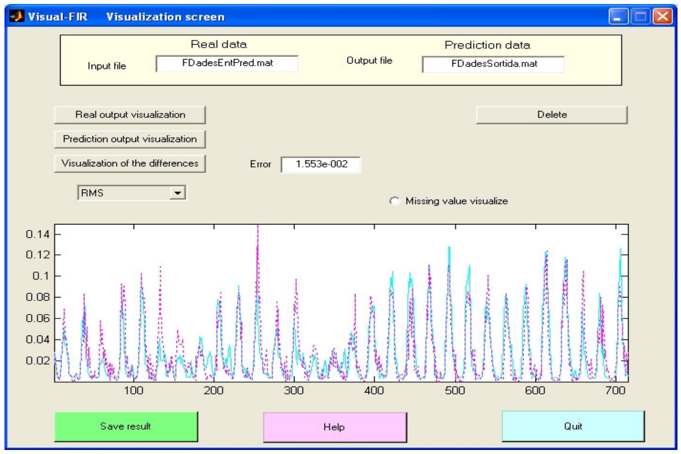

Figure 3: Real vs. prediction signals for March 2006 test data set using mask (1,5,12,18) – Dry seasonal model

5 Discussion and Conclusions

The aim of this paper was to discover behavior patterns of the ozone contaminant in the centre region of Mexico City. Two different modeling perspectives were studied, i.e. monthly models and seasonal models. It has been shown that FIR methodology is capable of capturing the dynamic behavior of the system under study and to accurately predict the ozone signal in the centre region of MCMA. The two modeling perspectives (monthly models and seasonal models) investigated with respect to the causal relations selected lead us to the one and the same conclusion. In both cases, the FIR modeling process identifies hour of day, wind speed and previous values of ozone as the most relevant variables for prediction of future ozone concentration. These results are in agreement with the differential equation models obtained in previous works (Ruiz and Ortiz, 1996). However, we can go further in the conclusions of this research. Not only hour of day, wind speed and ozone past values are relevant to predict future values of ozone contaminant. The FIR models have found that relative humidity is a crucial variable to predict ozone during the wet season, whereas wind direction becomes fundamental to predict ozone levels during the dry season. Therefore, in this research we found two patterns for the ozone behavior, one for the dry season and the other one for the wet season. The next step is to work with other contaminants that reach, also, high levels in MCMA, like small particles (lower than 10 micres). We think that Visual-FIR is a user friendly tool that runs under Matlab that can be used for any researcher, without knowledge of fuzzy logic o qualitative modeling.

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