PREDICTION OF GROUND-LEVEL OZONE CONCENTRATIONS THROUGH STATISTICAL MODELS

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Abstract: This study aims to evaluate the performance of three statistical models: (i) multiple linear regression (MLR), (ii) artificial neural network (ANN) and (iii) multi-gene genetic programming (MGP) for predicting the next day hourly average ozone (O_3) concentrations. O_3 is an important air pollutant that has several negative impacts. Thus, it is important to develop predictive models to prevent the occurrence of air pollution episodes with a time interval enough to take the necessary precautions. The data were collected in an urban site with traffic influences in Oporto Metropolitan Area, Northern Portugal. The air pollutants data (hourly average concentrations of CO, NO, NO_2, NO_x and O_3), the meteorological data (hourly averages of temperature, relative humidity and wind speed) and the day of week were used as inputs for the models. ANN models presented better results in the training step. However, with regards to the aim of this study, MGP presented the best predictions of O_3 concentrations (test step). The good performances of the models showed that MGP is a useful tool to public health protection as it can provide more trustful early warnings to the population about O_3 concentrations episodes.

1 INTRODUCTION

Ground-level ozone (O_3) is one of the air pollutants of most concern in Europe. It is an irritating and reactive component in atmosphere that has negative impacts on human health, climate, vegetation and materials (Pires et al., 2008a). O_3 is the result of three basic processes: (i) photochemical production by the interaction of hydrocarbons and nitrogen oxides under the action of suitable ambient meteorological conditions (Guerra et al., 2004; Zolghadri et al., 2004); (ii) vertical transport of stratospheric air, rich in ozone, into the troposphere (Dueñas et al., 2002); and (iii) horizontal transport due to the wind that brings O_3 produced in other regions. Air pollution modelling and prediction take a great importance in preventing the occurrence of air pollution episodes with a time interval enough to take the necessary precautions. With regards to the prediction of O_3 concentrations, several studies have been published (Al-Alawi et al., 2008; Ozdemir et al., 2008; Sousa et al., 2007). Artificial Neural Networks (ANN) are often used and presented good performances due to the nonlinearity that is associated to the O_3 formation. As far it is known, no study was performed to evaluate the performance of MGP for predicting O_3 concentrations. In this study, the aim is to compare the performances of three models for predicting the next day hourly average O_3 concentrations during seven days. The models developed were: (i) multiple linear regression (MLR); (ii) feedforward ANN; (iii) multi-gene genetic programming (MGP).

2 MODELS

MLR is an extension of the simple linear regression model for data with multiple predictor variables and one outcome. Thus, this statistical model assumes that the best approach to estimate the dependent variable from the explanatory variables is to find the linear combination of these variables that minimizes the sum of squared errors (Pires et al., 2008b).

ANN models are characterized by a set of processing neurons with an activation function that are distributed in layers (input, hidden and output layers). The neurons in the different layers are linked

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by synapses, each one storing a weight value. These weight values are modified during the training step of ANN model, minimizing the value of a selected objective function. One of the problems of the training step is the overfitting. A high number of iterations lead to decrease the error in the training set, but the achieved model presents a large error when applied to a new set. The method often applied to solve this problem is the early stopping (Nguyen et al., 2005; Özesmi et al., 2006). Using this method, the data should be divided into three sets (Chiang et al., 2004): (i) training set, used to determine the model parameters; (ii) the validation set, used to evaluate the performance of ANN model during the training step and to stop it when the validation error starts to increase; and (iii) the test set, used to evaluate the ANN performance when applied to a new set.

MGP is based on the principles of the simple genetic programming (GP) algorithm (Koza, 1992). The models are also encoded in tree structures (tree expressions). The initial models (first generation) are created randomly and are modified following an iterative process, using genetic operations (selection, crossover and mutation). The tree structures are continuously evaluated and the fittest ones are selected to the next iteration (elitism). This procedure leads to optimize the model structure and parameters, simultaneously. The iterative process stops when a termination criterion (the achievement of the maximum number of generations or a desired training error) is satisfied. Figure 1 summarises the GP procedure. The main differences between GP and MGP are: (i) a model is composed by several tree structures, called genes, and not a single one (see Figure 2); and (ii) the output value is calculated

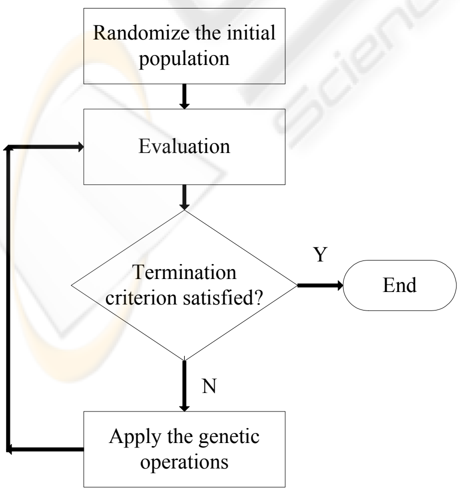
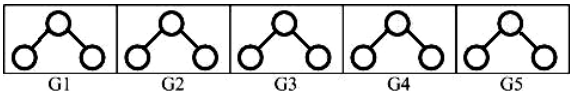


Figure 1: GP procedure.



$$y = b_0 + \sum_{i=1}^{5} b_i G_i$$

Figure 2: MGP model codification.

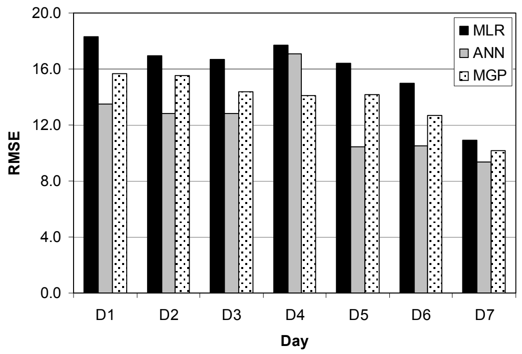
through the linear combination of the outputs of the different genes belonging to the same model (in this study, 5 genes were applied).

3 DATA

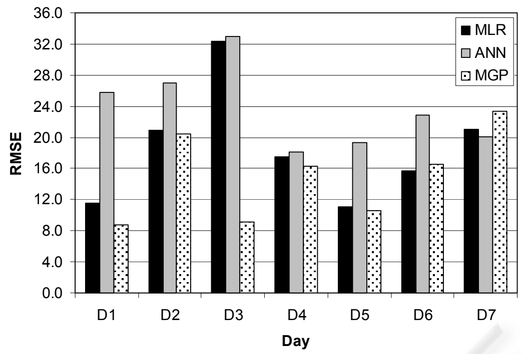
The models considered 10 input variables: the hourly average concentrations (in µg m^{-3}) of carbon monoxide (CO), nitrogen oxides (NO, NO_2 and NO_x) and O_3; hourly averages of air temperature (T), solar radiation (SR), relative humidity (RH) and wind speed (WS); the day of week (DW; the O_3 behaviour is different on weekdays and on weekend). All environmental and meteorological inputs corresponded to the same hour of the previous day. The air pollution data were collected in an urban site (*Antas*) with traffic influences situated in Oporto, Northern Portugal. This site belongs to air quality monitoring network of Oporto Metropolitan Area that is managed by the Regional Commission of Coordination and Development of Northern Portugal, under the responsibility of the Ministry of the Environment. The meteorological data were recorded on the left edge of the Douro River, at an altitude of 90 m approximately. These values are representative of all Oporto Metropolitan Area. The study period was two weeks of May 2004, where high O_3 concentrations were measured and there was no missing data. The last seven days were used for the test period and the corresponded O_3 data of each one (24 data points) were predicted using the data of the seven days before (168 data points). For ANN model, the validation set was 20% of the training data. The input variables were Z standardized to have zero mean and unit standard deviation.

4 RESULTS AND DISCUSSION

The determination of MLR models only considered the regression parameters considered statistically significant. The statistical significance was evaluated through a t-test with a significance level of 0.05. The MLR models were determined using a



(a)



(b)

Figure 3: Performance indexes for training (a) and test (b) periods.

VBA subroutine in Microsoft Excel. In the seven MLR models, the CO, NO, SR, WS and DW were considered the input variables less important in the prediction of O_3 concentrations. Positive correlation coefficients were found between the predicted variable and T, RH and O_3 concentrations of the previous day, while NO_2 showed a negative correlation. NO_x presented positive or negative correlation, when NO_2 or NO was considered statistically significant, respectively.

Feedforward ANNs with three layers (10 input neurons, *n* hidden neurons and 1 output neuron) were also determined. Hyperbolic tangent and linear functions were used as activation functions in hidden and output neurons, respectively. The objective function was the minimization of the mean squared error of the training data. The training algorithm was the Levenberg-Marquardt optimization. Different ANN structures were tested, varying the number of neurons in the hidden layer (1 to 10). For each structure, 100 runs were performed. The best ANN model corresponded to the minimum error in the training and validation data. The ANN models were determined using Matlab 7.0. In the seven ANN models, the optimal number of hidden neurons was 5 (1 model), 7 (4 models) and 8 (2 models).

For MGP, several parameters should be defined. The values proposed in this study are usually applied by other authors in GP (Koza, 1992). The population size is the number of individuals in the population; large number of individuals increases the population diversity, but it also increases the computation time effort. The population size was fixed in 200 and the maximum number of generations was 100. The crossover and mutation rates define the probability that an individual is selected for the crossover or mutation operation, respectively; their values were 0.8 and 0.1. The best 10% of the best individuals (20 individuals) were selected for the next generation (elitism). The fittest individuals were the ones presenting the lowest root mean squared error (RMSE; Pires et al., 2008b) in the training period. To avoid early convergence, a new dataset for the evaluation of individuals was created, by random sampling the original data, with replacement when the 20 best individuals of the actual generation were the same of the previous one. However, in the last 10 generations the individuals were evaluated using the original data.

The performances of all models were evaluated using the RMSE. Figure 3 shows RMSE values for all models in the training and test set. ANN presented almost always the lowest training error. However, when applied to a new set (test set), its performance was worse than the others. Table 1 presents the models obtained to predict O_3 concentrations in the first day of the test set. Figure 4 shows the model predictions for the same period. Considering whole test period, MGP presented better predictions of O_3 concentrations.

Considering the flexibility for creating the predictive models, MGP is a promising methodology to estimate environmental complex air pollution problems.

Table 1: Models achieved for the prediction of O_3 concentrations in the first day of the test period (D1).

	Model
MLR	$O_{3\|t+24h} = 41.8 - 20.3 \times NO_{2\|t} + 10.5 \times NO_{x\|t} + 34.5 \times T_t + 8.2 \times RH_t + 6.0 \times O_{3\|t}$
ANN	Structure: (10; 5; 1)
MGP	$O_{3\|t+24h} = 24.1 + 7.6 \times \tanh(\cos(\exp(\cosh(T_t)))) - 3.5 \times \log(T_t) + 24.4 \times T_t - 12.8 \times NO_{2\|t} + 9.5 \times \cosh(T_t - \sin(CO_t))$

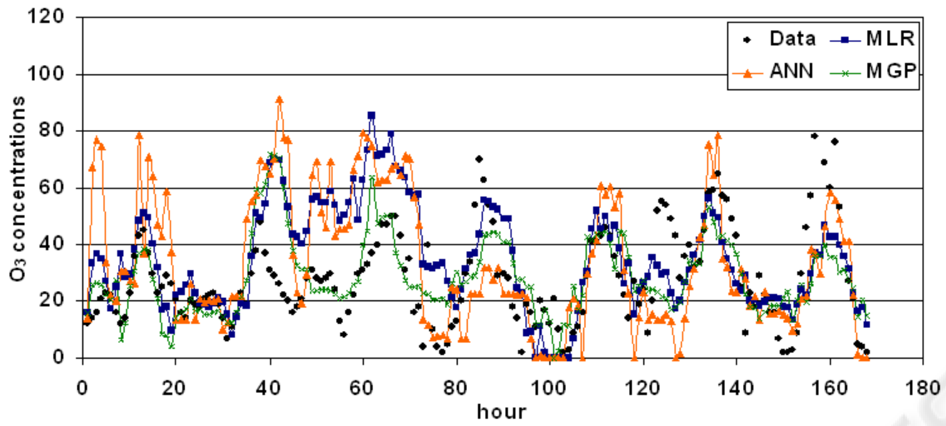


Figure 4: Prediction of O_3 concentrations for the test period.

5 CONCLUSIONS

Aiming the prediction of the next day hourly average O_3 concentrations, the performances of MLR, ANN and MGP were compared. The prediction of seven consecutive days tested the consistence of the models. ANN models presented better results in the training step. However, with regards to the aim of this study, MGP presented the best predictions of O_3 concentrations (test set). The good performances of the models showed that MGP is a useful tool to public health protection as it can provide early warnings to the population about O_3 concentrations episodes.

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