Scientific paper

Optimization of Neural Networks by SIMPLEX Method Performed on Environmental Data

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Abstract

The aim of the optimization is to find out the optimal parameters for complex system such as synthesis of the compounds, chemical reactions, analytical methods, property of the products or chemical processes. The parameters that we want to determine are the values, which describe the system. The SIMPLEX is one of the most simple and general optimization method. It is used to predict the experiments that in quickest way lead to an optimum.

In this work the SIMPLEX method was used to optimize the parameters of the counter-propagation neural network model constructed for the prediction of the ozone concentration as one of the most outstanding air pollution parameters in the Buenos Aires region. The network was trained with the data available for 980 collected samples; each of them was described by the concentrations of 7 pollutants: CO, SO_2, O_3, NO_x, NO, NO_2, and PM_{10}, and 8 weather related variables: cloudiness, rainfall, insolation factor, temperature, pressure at two locations, and wind intensity with direction. The evaluation function as the optimization criterion of the model was thus the correlation coefficient between the experimental and predicted ozone concentrations.

Keywords: Air quality; SIMPLEX optimization method; Insolation factor; Artificial Neural Networks; Ozone formation; Pollutants

1. Introduction

In the literature, there are many papers devoted to different optimization methods for a variety of complex systems. The applications of optimization algorithms can be found in references.[1–6] In general the optimization procedure allows us that from any state X_s (or point) of the system described in the m-dimensional space $X_s = (x_{s1}, x_{s2}, \ldots x_{sm})$ with the use of an evaluation function $f(X_s)$ the next state of the system $X_{s+1} = (x_{s+1,1}, x_{s+1,2}, \ldots x_{s+1,m})$ can be calculated. The result of the evaluation function $f(X_{s+1})$ should be better than the result of the previous function $f(X_s)$. If $f(X_{s+1})$ is worse than $f(X_s)$, the optimization procedure should direct the procedure towards better X_{s+1} and at the same time offer the criteria needed to stop the optimization.[7]

The standard SIMPLEX method is one of the non-gradient optimization techniques, which are frequently employed in chemistry. Its generalization was provided by Price in the middle of the seventies.[8] He introduced the significant notion that a population of points is considered and from this population the SIMPLEX set is randomly selected. Very important reference focused on SIMPLEX algorithm is also the article writen by Nelder and Mead.[9] In the reference the SIMPLEX is decribed as a numerical method for minimizing an objective function in a many-dimensional space. One of the basic concepts of the SIMPLEX optimization method is that from the initial (or current) set of points (temporary SIMPLEX solutions) a new point (a new solution) is constructed by a reflection of the worst point through the gravity point of the remaining points. The reflection point is used for a conditional updating of the SIMPLEX set, which is initially randomly selected from the population of possible points, i.e. possible experiments. At each step of the optimization process the reflected point updates the set of existing SIMPLEX points so that it conditionally substitutes the point with the

worst value. The value of each point is always determined either by the measurement or using an evaluation function. Dragović et al show in their article[10] the applicability of the SIMPLEX for the optimization of the training parameters of a three-layer feed-forward artificial neural networks with a back-propagation algorithem that was additionally used for prediction of minimum detectable activity of radionuklides in environmental soil samples. The interested reader can find more about the applicability of the SIMPLEX method for other systems in the references.[11–14]

The behavior of the ozone in relation to the other pollutants and weather data, which is investigated in this work has been studied by many authors. Most of the references are focused on the use of different modeling techniques such as Multiple Regression Analysis,[15,16] Partial Least Squares Regression,[17] Principal Component Analysis (PCA)[18] and Artificial Neural Network.[19–21] These methods are applicable to the modeling and analysis of any data where an effect (for example, pollution of the city, damage to plants) is caused by a number of variables with a non-linear influence. To obtain better models, some authors have tried to improve the information content by using the combination of above mentioned statistical methods.[16, 22, 23] Central point of another very interesting article written by Žabkar et al is the applicability of the Q^2 learning method (Qualitatively faithful quantitative learning) on numerical data where the QUIN program was employed to induce a qualitative model for the analysis and prediction of ozone concentrations in the city of Ljubljana and Nova Gorica.[24]

In the present work about 1000 samples (data records) each presented as a 15-dimensional vector (concentrations of 7 pollutants: CO, SO_2, O_3, NO_x, NO, NO_2, and PM_{10}, and 8 weather related variables: cloudiness, rainfall, insolation factor, temperature, pressure, and wind intensity with direction)[25–28] were used. The first variable x_1, being the ozone concentration, was studied as the response variable of the model. To find the best correlation between the air pollutants and weather conditions the semi-supervised modeling technique, so called counter-propagation neural network[14] was used. The SIMPLEX method was simultaneously employed to obtain the optimal parameters for the training of each selected counter-propagation neural network.

2. Methods and Experimental Section

2. 1. Predictive Kohonen Neural Network

The main goal of Kohonen neural networks (Koh-NN) is to map objects from *m*-dimensional into *n*-dimensional space. The primary neuron for weight modification is chosen by a competition.[14,29] The learning algorithm modifies the weights w_{ji} of the neuron $\mathbf{W_j}$ having the most intense output, or whose weights are most similar to the input signal $\mathbf{X_S}$. At the same time the learning algorithm smoothes the weights in all weight levels (including SOM) by making modulated changes to neurons in a defined "neighborhood" of the $\mathbf{W_j}$. The Kohonen learning is an unsupervised learning. The correction on the i-th weight of the j-th neuron $\mathbf{W_j}$ after the excited neuron $\mathbf{W_e}$ has been chosen by the object $\mathbf{X_s} = (x_{s1}, x_{s2}, \ldots, x_{sm})$ is carried out using the equation:

$$w_{ji}^{new} = w_{ji}^{old} + \eta(t) \times b(d_c - d_j) \times (x_{si} - w_{ji}^{old}) \quad (1)$$

Parameter η determines the rate of learning; it is maximal at the beginning (t = 1, $\eta = \alpha_{max}$) and minimal at the end of the Koh-NN learning procedure (t = t_{max}, $\eta = \alpha_{min}$). The function $b(d_c–d_j)$ in equation (1) describes how the correction of the weights w_{ji} decreases with increasing topological distance between the central neuron and the neuron being corrected. Index *j* specifies individual neuron and runs from 1 to *n*. Topological distance of the *j*-th neuron from the central one is defined according to the topology used for the distribution of neurons in the plane. The minimal distance is zero ($j = c$, $d_c–d_j = 0$), which corresponds to the maximal correction function (b = 1). The maximal distance ($d_c–d_{max}$) to which the correction is applied is shrinking during the learning procedure. The correction function at maximal distance is minimal (b = 0). At the beginning the $d_c–d_{max}$ covers the entire network, while at the end, at t = t_{max}, it is limited only to the central neuron.[14]

In the network there are different types of neighborhood relations. In our case the objects are described by 14 active variables composed of concentration and meteorological data. The missing values were marked with a special key (–9999.), which enables our adapted Kohonen and counter-propagation neural network software to handle the missing data.[30,31]

The concentration of O_3 is regarded as the non-active dependent variable that does not enter the distance calculations and forms the top map (SOM). Although the goal of this study was preliminary exploration of the data (finding relations between the input variables) and not the generation of a model, we have treated the ozone data as the target data and input them on the output side virtually achieving the counter-propagation neural network instead of the Kohonen one. Predictive Kohonen neural network is comparable to the counter-propagation neural network (CP-ANN).[30] The training parameters were chosen by the SIMPLEX method. The top map (SOM) and all weight maps were obtained after 1900 epochs of training. One epoch of the training process was completed after all 980 data records (concentrations and weather data) were sent through the network once all necessary weight corrections in the network were made after the input of each data record. More detailed description of the Kohonen map formation can be found in the textbooks.[14, 29]

2. 2. SIMPLEX Optimization

The SIMPLEX is one of the most simple and general optimization method. It is used to predict the experiments that mostly lead to an optimum on a few steps.

The most important value in the optimization procedure is the evaluation function or optimization criterion (OC). It depends upon one (simple evaluation function) or more (complex evaluation function) properties of the system.

To get the numerical value of the evaluation function for a defined system response variables have to be measured or a mathematical model, which predicts the properties of the system, has to be found and incorporated into the optimization process.[11]

SIMPLEX optimization method works best with relative low number of variables (3 to 20).[11, 14, 32, 33] The idea of SIMPLEX optimization is to obtain from a given set of points $\{\mathbf{X_i}\}$ in the *m*-dimensional space a new point **B** by reflecting the worst point **T** of the entire set $\{\mathbf{X_i}\}$ through the gravity point **G** of the set without the worst point. By omitting the worst point **T** and adding the new "best" point **B** to the set $\{\mathbf{X_i}\}$ the SIMPLEX is "crawling" in the m-dimensional space towards the optimum (Figure 1).

The mathematical formula for the calculation of the new point **B** is given in the following way:

$$\mathbf{B} = \mathbf{G} + a\,(\mathbf{G}–\mathbf{T}) = \mathbf{G} + a\mathbf{G} – a\,\mathbf{T} = (1 + a)\mathbf{G} – a\mathbf{T}$$

$$\text{If } a = 1 \qquad \mathbf{B} = \mathbf{2G} – \mathbf{T} \tag{2}$$

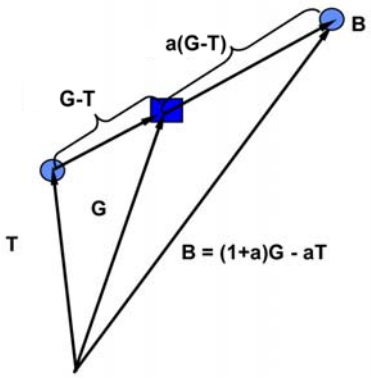

Figure 1: Schematic presentation of the SIMPLEX. B – object with the best response, G – gravity point (average value of all objects without the object with the worst response), T – object with the worst response, a – expansion coefficient (start; a = 1).

Rules for the SIMPLEX algorithm:

1. For a m-variate problem select or generate m +1 initial objects $\mathbf{X_i}$ (SIMPLEX)
2. Measure or calculate OC_i for all objects $\mathbf{X_i}$ in the SIMPLEX
3. Find the object **T** having the worst OC_{worst}
4. Calculate the "gravity object" **G** using m remaining objects $\{\mathbf{X_i}\}$' $\quad \mathbf{G} = (g_1, g_2, \ldots g_m), \quad g_m = (1/m)\,\Sigma'\mathbf{x_i}$
5. Calculate the new object **B** using:
   $B = (a + 1)\,\mathbf{G} – a\,\mathbf{T} \qquad (a = 1)$
6. Drop **T** and include **B** into the SIMPLEX
7. Repeat algorithm at step 3.

When the reflection of the worst point through the gravity point leads no more to the higher value of the OC, but to the lower one, the SIMPLEX must be narrowed. The new object B is calculated by the same equation (2), except the value of the coefficient **a** changes to lower ones (i.e. **a** = 0.5, –0.5). The SIMPLEX is then defined by the following equations:

$$\text{If } a = 0.5; \quad B = (a + 1)\,\mathbf{G} – a\,\mathbf{T} = 1.5\,\mathbf{G} – 0.5\,\mathbf{T} \tag{3}$$

$$\text{If } a = –0.5; \quad B = 0.5\,\mathbf{G} + 0.5\,\mathbf{T} \tag{4}$$

3. Results and Discussion

3. 1. Environmental Data Optimized by SIMPLEX Method

The 15-variable environmental data (7 concentrations: CO, SO_2, O_3, NO_x, NO, NO_2, particulate matter smaller than 10 μm (PM_{10}), and 8 weather data: cloudiness, rainfall, insolation factor (Isf_i), temperature, pressure at two locations, and wind intensity with direction) in a period of 45 days with 1 hour intervals were extracted from a larger data base of concentrations recorded in the minute intervals for the same time period. The monitoring site was located in the City of Buenos Aires in a relatively heavy traffic crossroad of two avenues in the time span from August 11th 2003 0.0 a.m. to September 24th 2003 2.0 p.m. The data required special pretreatment where the hourly content of rain, wind intensity, wind velocity, and cloudiness were concerned.

Due to the fact that multivariate handling of data depends on the normalization of variables the data were normalized with the use of the equation written under and was applied to all 15 variables x_i, $i = 1 \ldots 15$, in a continuous space:

$$x_{ij}^{new} = \frac{x_{ij}^{old} - \bar{x}_i}{\sigma_i} \tag{5}$$

The PM_{10} values were normalized only for the available data, while the (–9999) key for the missing values was kept on place.

The new variable named insolation factor (relative UV radiation) was calculated on the basis of general meteorological data, geographic position of the monitoring site, cloudiness, date, and time of the recording was composed[34]. The relative intensity of UV radiation was modeled by a Gaussian function multiplied by a $cloudiness_i$ with the factor ($1.0 – 0.1 \times cloudiness_i$) in the following

relation.

$$Isf_i = (1.0 - 0.1 \times cloudiness_i)\ e^{-(\frac{i-12}{3})^2} \quad (6)$$

If $cloudiness_i$ is zero, the insolation factor Isf_i follows the Gaussian shape exactly. If on the other hand the $cloudiness_i$ is different from zero the Isf_i is shielded accordingly. Isf_i could be adapted to the geographical altitude of Buenos Aires and to the appropriate months of recording (early spring, August and September).[28]

In present work the SIMPLEX method was used to optimize the parameters employed in the counter-propagation artifical neural network training.

3. 1. 1. Procedure

At first, the data set of all 980 samples was divided into train and test sets using the Kennard and Stone (KS) algorithms.[31, 35, 36] In this way both train and test sets consist of 490 samples. For training artificial neural network train program (ANN-train)[31] and for testing artificial neural network test program (ANN-test)[31] were used. As the evaluation function the correlation coefficient between experimental and test predicted ozone concentrations was applied.

In order to show how the actual optimization procedure runs one movement of a five point SIMPLEX is given below.

1. First, four variables were took into consideration: n_{epoch} (number of epoch), α_{max} (maximal correction factor), α_{min} (minimal correction factor), and NxN (network dimension) are initially chosen at random. Using these four parameters the counter-propagation neural network was built and the correlation factor between the predicted and experimental O_3 was calculated.
2. For 4 variables at least 5 starting points are needed.

The SIMPLEX consists of five points (S_1, S_2, S_3, S_4, S_5) each representing a specific neural network (NN_1, NN_2, NN_3, NN_4, NN_5), which are fully trained by using selected sets of the four parameters. After the training of the neural networks with the training set of data the testing set is applied in all five cases and five correlation coefficients r_1, r_2, r_3, r_4 and r_5 between ozone concentrations are obtained:

$S_1 = (x_{11}, x_{12}, x_{13}, x_{14}) = (\alpha_{max}, \alpha_{min}, n_{epoch}, NxN) =$
$= (0.5, 0.01, 600, 20x20) \Rightarrow r_1 = 0.759$

$S_2 = (x_{21}, x_{22}, x_{23}, x_{24}) = (0.5, 0.01, 400, 10x10) \Rightarrow$
$r_2 = 0.694$

$S_3 = (x_{31}, x_{32}, x_{33}, x_{34}) = (0.6, 0.2, 500, 30x30) \Rightarrow$
$r_3 = 0.791$

$S_4 = (x_{41}, x_{42}, x_{43}, x_{44}) = (0.5, 0.01, 2000, 30x30) \Rightarrow$
$r_4 = 0.786$

$S_5 = (x_{51}, x_{52}, x_{53}, x_{54}) = (0.7, 0.3, 3500, 20x20) \Rightarrow$
$r_5 = 0.767$

$r_2 < r_1 < r_5 < r_4 < r_3 \Rightarrow r_2 = T$ (worst point) $\Rightarrow$ G (gravity point) is calculated from S_1, S_3, S_4 and S_5.

$$G = \frac{1}{m}\sum_{i=1}^{m} x_i \quad (7)$$

$G = \{(0.5, 0.01, 600, 20 \times 20) + (0.6, 0.2, 500, 30 \times 30) +$
$+ (0.5, 0.01, 2000, 30 \times 30) +$
$+ (0.7, 0.3, 3500, 20 \times 20)\}/4 =$
$= (0.575, 0.125, 1150, 25 \times 25)$

New training parameters are calculated by the equation (2):

$\mathbf{B = 2G - T} =$
$= 2(0.575, 0.125, 1150, 25 \times 25) -$
$- (0.5, 0.01, 400, 10 \times 10) =$
$= (0.65, 0.24, 1900, 40 \times 40)$

After **B** is evaluated the neural network is trained with the new set of parameters and the new correlation coefficient (r_6) is obtained. The procedure is continued by excluding the point $\mathbf{X_2}$ (having the worst r) and including the point **B**.

The highest evaluation function was obtained after the fourth step (r = 0.83) with the optimal training parameters: $\alpha_{max} = 0.65$, $\alpha_{min} = 0.24$, $n_{epoch} = 1900$, $N \times N = 40 \times 40$.

Further, these optimized parameters ($\alpha_{max} = 0.65$, $\alpha_{min} = 0.24$, $n_{epoch} = 1900$, $N \times N = 40 \times 40$) were used for mapping achieved with Kohonen network. Based on the 14-variable input and 1 variable output (ozone) data, the clustering of all 980 data records was made. The top map clustering showing ozone concentration was related to the maps of all 14 variables. To make the analysis of the model more evident and understandable the model is explained by using the MATLAB visualization tools (ANN-visual program).[31] Each map is composed of 1600 weights colored according to their relative value revealed in the scale at the bottom of Figure 2. The maps show the relation between the concentrations of ozone, NO_2, and *Isf*, which is negative between ozone and NO_2 and positive between ozone and *Isf*.

A 40 x 40 Kohonen network, using the corresponding data sets, obtained the maps. All maps exposed in Figure 2 were produced using the optimal parameters ($\alpha_{max} = 0.65$, $\alpha_{min} = 0.24$, $n_{epoch} = 1900$, $N \times N = 40 \times 40$), chosen by the SIMPLEX.

On the left side of Figure 2 the top map of the ozone and on the right side the weight maps of NO_2 and Isf_i are shown. Each map is composed of 1600 weights colored according to their relative value revealed in the scale at the bottom of Figure 2.

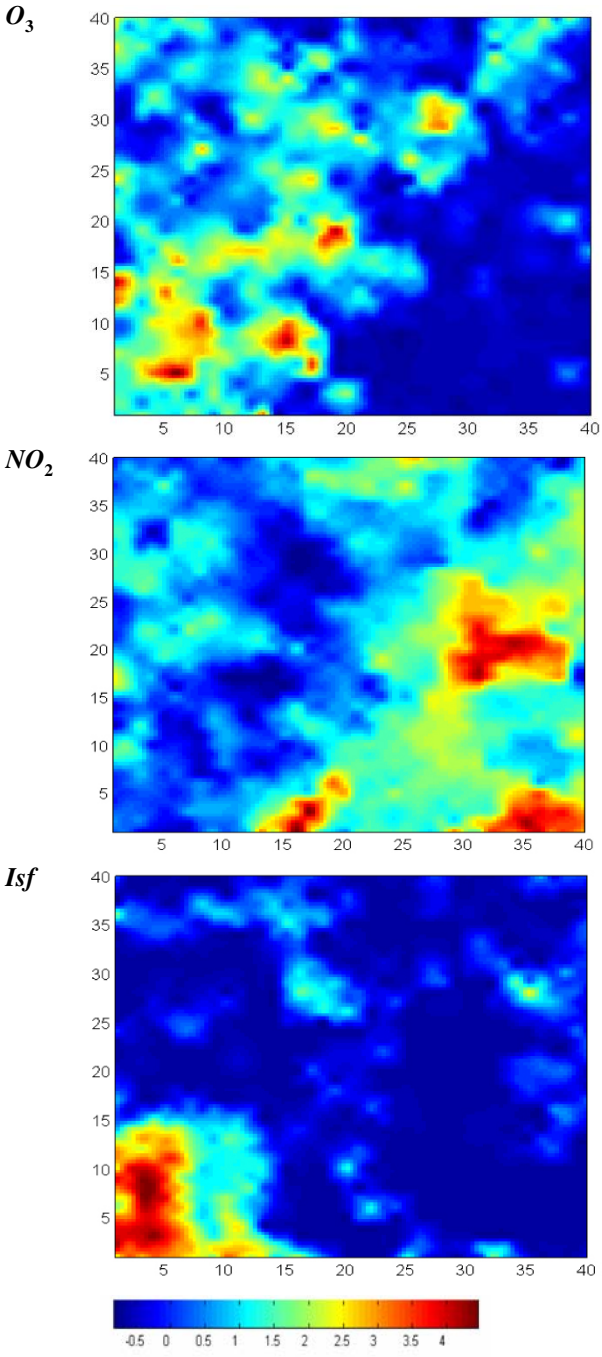

Figure 2: Kohonen self-organizing maps of three variables. The color bar represents particular concentrations for O_3 and NO_2 and relative values for Isf_i

3. 2. Comparison of the Acquisited Data With the Chemistry of These Pollutants in the Air

The results presented above clearly show negative relationship between NO_2, and O_3, and are not completely in accordance with the chemistry of these pollutants in the air, where the concentrations of NO_2 and ozone are generally positively correlated. Most often higher NO_2 concentrations means more ozone and the actual correlations depends not only on nitrogen oxides but also upon volatile organic compounds (VOCs) concentrations.[37, 38] Nevertheless the decrease of the amount of ozone with increasing NO_2 concentration in the atmosphere can be explained by the following reactions:[38, 39]

$$NO_2(g) + h\nu \rightarrow NO(g) + O(g) \quad (8)$$

Namely, the nitrogen dioxide, NO_2, dissociates to NO and oxygen when exposed to a bright light (UV, λ = 328–286 nm) (photoinitiated reaction). The oxygen atom is extremely reactive and readily attaches to a molecule of O_2 forming ozone O_3. This reaction is written as:[38]

$$O(g) + O_2(g) \rightarrow O_3(g) \quad (9)$$

The found negative correlation shows that for any form of mathematical modeling of ozone formation, besides all the relevant variables, the correct time delay between some of them should be taken into the consideration.

In accordance with these findings our next step was to analyze the partition between NO, O_3 and NO_2 formation. To analyze this in details, average minute concentrations data of NO_2, O_3 and NO were calculated from the raw database. In the calculation of averages all five Tuesdays in the period from 11.08.03 to 24.09.03 were considered (Figure 3).

In Figure 3, the delay of peak concentrations between NO (green curve) and NO_2 (red curve) can be observed. For easier representation, we marked the peaks, which consecutively correspond to each other with equal letters. Thus, the peak at 7:35 (which belongs to the NO_2) arises as a consequence of the peak belonging to NO at 6:53. Both peaks are marked with letter A. Equally, the NO_2 peaks at 9:23, 11:07, and 19:28 are the consequences of the NO peaks at 8:07, 9:11, 18:57, marked with B, C,

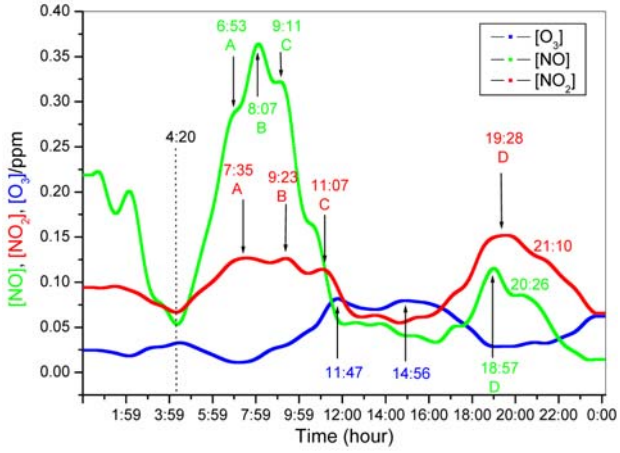

Figure 3: Average minute concentrations of NO, NO_2 and O_3 as a function of time.

and D, respectively. These observations can be explained with the chemical reactions of the formation of NO_2 (and O_3) from NO.

In the first place, the reaction (10) starts inside the internal combustion engines, where consequently several spontaneous reactions of NO_2 formation occur (11–13).

$$N_2(g) + O_2(g) \rightarrow 2NO(g) \quad (10)$$

First possible reaction is direct oxidation of NO to NO_2 (11a). The reaction is rather slow at typical ambient NO concentrations, but it may occur at very concentrated conditions (Torr conditions) for a brief period of time in plumes where the NO concentrations are higher as they exit a stack or tailpipe before significant dilution with the surrounding air has occured:[38, 40]

$$2NO(g) + O_2(g) \rightarrow 2NO_2(g) \quad (11a)$$

However as long as there is any ozone presented in the air the reaction (11a) could be neglected and time delay in NO_2 concentrations compared to NO arises as a consequence of the reaction (11b), which is much faster than the previous one:[39, 41]

$$NO + O_3 \rightarrow NO_2 + O_2 \quad (11b)$$

Second possible reactions, are the conversions of NO to NO_2 in ambient air that involve the chain oxidation of organics initiated primarily by the free radical OH.[41]

These reactions are written as:

$$RO_2 + NO \rightarrow RO + NO_2 \quad (12a)$$

$$\rightarrow RONO_2 \quad (12b)$$

As it is described in the reference,[40, 41] the reaction (12a) predominates over (12b), with (12b) becoming significant for the larger ($\geq C_4$) alkoxy radicals. The alkoxy radical (RO) formed in (12a) undergoes a hydrogen abstraction by O_2 to form HO_2 and an aldehyde;[40] the OH_2 then can oxidise a second NO to NO_2, reforming OH in the process (13):

$$HO_2 + NO \rightarrow OH + NO_2 \quad (13)$$

Thus, in this cycle, two molecules of NO have been oxidized to NO_2 and OH has been regenerated to carry on further oxidations.

Other species that react with NO in ambient air in addition to HO_2, RO_2, and O_3 include OH, alkoxy radicals (RO) and nitrate radicals (NO_3).[41] In accordance with the chemical reactions, therefore it is normal to observe the peak concentrations delay between NO and NO_2 curve (Figure 3).

Additionally, at the late hours of the day (upon 16:00) an interesting change is observed. In Figure 3 and Figure 4 it is shown that after 16.00 the average of NO_2 concentrations start increasing again. It is clear that in the late hours of the day (after 16.00), the insolation factor is lower than during the day and thus the molecules of NO_2 dissociate in lesser amount (Figure 4), moreover repeated increase of the nitrogen pollutans in the air can be again ascribed to the enlarged afternoon traffic.

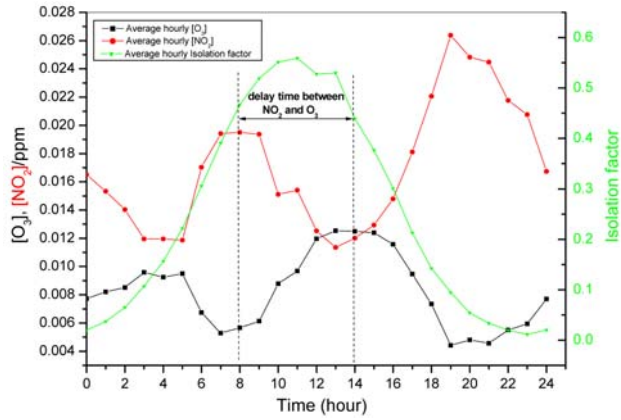

Figure 4: Hourly averages of $[O_3]$, $[NO_2]$ and Isf_i as a function of time.

To resume, Figure 3 and 4 clearly show morning and afternoon increase of NO and consequently NO_2 concentrations, which are connected to the enlarged automobile traffic caused by migration of people to and from work. The increase in ozone concentration during the day is initiated by photochemical reactions enabled by sun light. As long as the level of NO in the air is signifficant and the reaction (11b) can take place the ozone concentrations can not increase. After the decomposition of the NO_2 affected by the sunrise (at about 7 am) (8) and after the concentrations of NO has fallen to a low value, the time delay of the O_3 formation (9) (at about 10 am) is revealed (Figure 4). However in general the correlations between ozone and nitrogen gases are positive with noticable time delay in ozone formation. Such observations are common and can be seen in all urban environment.

4. Conclusions

The general purpose was to analyze the data measured during a surveillance campaign undertaken by the electricity sector with the intention of showing the role of the traffic and power plants to the air quality deterioration in Buenos Aires city.

This study illustrates the usefulness of the SIMPLEX optimization method for rapid determination of the optimal parameters for proper architecture of Kohonen or counter-propagation artificial neural networks and consequently to obtain the best correlation between the pollutants in the air. The most attractive feature of the SIM-

PLEX is to shorten the time needed to get a good result for a desirous complex system. The use of the two-dimensional maps is a good example of how the visualization with the help of Kohonen self-organizing maps improves the analysis of complex data.

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Povzetek

Namen optimizacije je določitev optimalnih parametrov kompleksnih sistemov kot so sinteze spojin, kemijske reakcije, analitske metode, lastnosti izdelkov ali kemijski procesi. Parametri, ki jih želimo z optimizacijo določiti so vrednosti, ki opisujejo sistem. SIMPLEX je ena izmed najenostavnejših in splošnih optimizacijskih metod. Najpogosteje se uporablja za napovedovanje eksperimentov, ki po najhitrejši poti vodijo k optimumu.

V tem delu opisujemo uporabo optimizacijske metode SIMPLEX za določitev parametrov v protitočnih umetnih nevronskih mrežah (counter-propagation artificial neuron networks, CP-ANN). Optimalni model smo uporabili za napovedovanje ozona, ki velja za enega izmed najbolj izrazitih parametrov onesnaženja ozračja na območju Buenos Airesa.

Rezultati, ki jih predstavljamo so pridobljeni iz podatkovnega seta sestavljenega iz 980 vzorcev. Vsak vzorec je opisan s koncentracijami 7 onesnaževalcev zraka: CO, SO_2, O_3, NO_x, NO, NO_2, in PM_{10}, ter 8 vremenskimi podatki (oblačnost, padavine, faktor osončenja, temperatura, tlak izmerjen na dveh lokacijah in intenziteta vetra).

Za cenilno funkcijo, kot optimizacijski kriterij modela, smo uporabili korelacijski koeficient med eksperimentalnimi in napovednimi koncentracijami ozona.