

Available online at www.sciencedirect.com



ARTIFICIAL
INTELLIGENCE

Engineering Applications of Artificial Intelligence 17 (2004) 159-167

www.elsevier.com/locate/engappai

Evolving the neural network model for forecasting air pollution time series

Harri Niska^{a,*}, Teri Hiltunen^a, Ari Karppinen^b, Juhani Ruuskanen^a, Mikko Kolehmainen^a

^a Department of Environmental Sciences, University of Kuopio, P.O. Box 1627, Kuopio FIN-70211, Finland
^b Finnish Meteorological Institute, Sahaajankatu 20 E, Helsinki FIN-00880, Finland

Abstract

The modelling of real-world processes such as air quality is generally a difficult task due to both their chaotic and non-linear phenomenon and high dimensional sample space. Despite neural networks (NN) have been used successfully in this domain, the selection of network architecture is still problematic and time consuming task when developing a model for practical situation. This paper presents a study where a parallel genetic algorithm (GA) is used for selecting the inputs and designing the high-level architecture of a multi-layer perceptron model for forecasting hourly concentrations of nitrogen dioxide at a busy urban traffic station in Helsinki. In addition, the tuning of GA's parameters for the problem is considered in experimental way. The results showed that the GA is a capable tool for tackling the practical problems of neural network design. However, it was observed that the evaluation of NN models is a computationally expensive process, which set limits for the search techniques.

© 2004 Elsevier Ltd. All rights reserved.

Keywords: Feed-forward networks; Time series forecasting; Parallel genetic algorithms; Urban air pollution

1. Introduction

The forecasting of air quality is one of the topics of air quality research today due to urban air pollution and specifically pollution episodes i.e. high pollutant concentrations causing adverse health effects and even premature deaths among sensitive groups such as asthmatics and elderly people (Tiittanen et al., 1999). A wide variety of operational warning systems based on empirical, causal, statistical and hybrid models have been developed in order to start preventive action before and during episodes (Schlink et al., 2003). In recent years, the considerable progress has been in the developing of neural network (NN) models for air quality forecasting (Gardner and Dorling, 1999; Kolehmainen et al., 2001; Kukkonen et al., 2003).

Despite the latest progress, there still exist some general problems that must be solved when developing a NN model. In the air quality forecasting, especially, the selection of optimal input subset (Jain and Zongker, 1997; John et al., 1994) becomes a tedious task due to high number of measurements from heterogeneous

*Corresponding author. Fax: +358-17-163191. *E-mail address:* harri.niska@uku.fi (H. Niska). sources and their non-linear interactions. Moreover, due to a complex interconnection between the input patterns of NN and the architecture of NN (related to the complexity of the input and output mapping, the amount of noise and the amount of training data), the selection of NN architecture must be done simultaneously. These aspects requires the formulation of search problem and the investigation of search techniques which are capable of facilitating model development work and resulting more reliable and robust NN models.

In this context, the evolutionary and genetic algorithms (GA) (Holland, 1975) have proven to be powerful techniques (Yao, 1999) due to their ability to solve linear and non-linear problems by exploring all regions of the state space and exploiting promising areas through genetic operations. The main drawbacks related to the using of GAs for optimising NNs have been high computational requirement and complex search space (Miller et al., 1989), which are due to the randomly directed global search and the stochastic nature of NNs. In order to overcome these problems, there have been considerable efforts to find the computationally efficient set of control parameters (De Jong, 1975; Grefenstette, 1986; Bäck et al., 1997; Eiben et al., 1999), to utilise

parallel computing techniques (Cantú-Paz, 1995) and to minimise computational burden related to the fitness evaluation of NNs (Yao, 1999). The fitness evaluation has been generally done by using some fitness approximation approach rather than exact computing despite the risk of biased estimates.

The objective of this work was to investigate the capability of coarse-grained GA (migration model; Section 2.3) within the design of NN model for forecasting next day air quality (Nitrogen dioxide (NO₂)) at urban traffic station in Helsinki. The model considered was the fully connected multi-layer perceptron (MLP) which was trained and evaluated with four years of observational data (Sections 2.1 and 2.6) and using the practice discussed later in Section 2.2. The search was focused on the architectural issues of the MLP (Section 2.4), because it is still unclear how these issues affect the capability of MLP to forecast concentrations. In addition, the meta-evolutionary approach was experimentally used for tuning the coarse-grained GA (Section 2.5) in order to maximize search efficiency which was valuable in terms of computational requirements. Finally, the evolutionary design of NNs was repeated multiple times and results were validated and assessed in terms of general and episode (model's capabilities in episodic situations) performance (Section 2.7).

2. Materials and methods

2.1. Experimental data

The test data selected to be considered in this study was extracted from the APPETISE¹ (Air pollution Episodes: Modelling Tools for Improved Smog Management, http://www.uea.ac.uk/env/appetise/) database. The data set comprised the concentrations of airborne pollutants and meteorological soundings and observations, monitored in Helsinki metropolitan area during the years 1996–1999. The data quality was examined and the fairly small fraction (ranged from 1% to 5%) of missing concentration data was obtained. The missing values were imputed using the hybrid method, i.e., a combination of linear interpolation and self-organizing map (Junninen et al., 2004) which is applied earlier in this domain by Kukkonen et al. (2003) and Schlink et al. (2003). The purpose of data imputation was to allow a consistent and fair model comparison exercise.

2.1.1. Concentration data

The concentration data comprised the hourly concentration of NO_2 , NO_x , O_3 , PM_{10} , SO_2 and CO monitored (processed according to routine quality

control and quality assurance procedures employed by the Environmental Office of the Helsinki Metropolitan Area Council) at the urban air quality monitoring station in Töölö (in Helsinki central). The station under consideration is permanently located (in the middle of a busy junction; not in a street canyon) and represents one of the most polluted parts of the city.

2.1.2. Meteorological data

The pre-processed meteorological data, based on a combination of the data from synoptic stations at Helsinki–Vantaa airport (about 15 km north of Helsinki downtown) and Helsinki-Isosaari (an island about 20 km south of Helsinki), was selected to be used in this study, as it is best representative for the whole of the urban area and contains also relevant derived atmospheric turbulence parameters. The mixing height (the depth of the unstable air in atmospheric boundary layer) and turbulence parameters were evaluated using a meteorological pre-processing model (Karppinen et al., 1997) based on the sounding observations at Jokioinen (90 km northwest of Helsinki) and the routine meteorological observations. For a detailed description of the data sets, the reader is referred to Kukkonen et al. (2003).

2.2. Multi-layer perceptron model

The forecasting of air quality can be considered as a non-linear regression problem between predictors (such as meteorological and air quality variables) and predictand (in this case, hourly concentration). Neural networks, in particular the multi-layer perceptron (Hornik et al., 1989), provide a flexible and non-linear tool for tackling regression problems in the air quality modelling (Gardner and Dorling, 1999). There are arguments, which both support and explain the wide use of the MLP in that domain. Primarily, extremely non-linear relationships exist in the real world and it is inappropriate to attempt to understand these problems using traditional regression. Moreover, it has been shown that the MLP can be trained to approximate any smooth, measurable (highly non-linear) function without prior assumptions concerning the data distribution.

On the ground of these aspects, the MLP was chosen to be considered in this study. The MLP was applied for prediction by training the network to output the next day value of NO_2 (T+24h, where T is the forecasting point) of a forecasted pollutant, given an input vector containing earlier air quality measurements at T+0h and weather observations at T+24h (simulating a weather forecast). In the training early stopping strategy was used instead of using regularisation techniques (Kukkonen et al., 2003) because of lower time requirement. The early stopping was adopted by using the

¹IST 1999-11764, EC framework V programme.

validation set 30/70 to assess the generalisation ability during training. The training was stopped when the validation error increased for five iterations and the weights and biases at the minimum of the validation error were utilised. As the training parameters, 1000 epochs, scaled conjugate gradient back-propagation, sigmoid transfer functions for hidden units and linear transfer function for output were used.

2.3. Coarse-grained genetic algorithm

Parallel techniques (Cantú-Paz, 1995), such as coarse-grained GA (regional/migration model), which support the using of several processors have been developed mainly for decreasing high computational requirements but also for simulating natural evolution in more detail. Compared to the pure GA (Holland, 1975), which operates on fixed-sized population using three main operators: selection, crossover and mutation, the coarse-grained GA divides population into a few subpopulations which are kept relatively isolated from each other. The new operations namely migration and competition between subpopulations are used for exchanging individuals between populations. For more details, please refer to Cantú-Paz (1995).

It is argued that the parallelisation not only decrease computation time, but also decrease objective function evaluations when compared a single population algorithm (Pohlheim, 2000). Consequently, even a single processor computer can deliver better results by implementing the parallel algorithm in a pseudoparallel. In this context, the utilisation of the parallel GA in the design process of NNs becomes interesting.

2.4. Problem formulation—encoding

An important phase related to the evolutionary search is to define (encode) the problem in a proper manner. This is important because in a poor encoding, the search might be confined in a certain area of the search space and consequently, stuck in a local minimum. Numerous encoding approaches, such as direct where each phenotypic feature is encoded by exactly one genotypic code, and indirect encoding where only some characteristics are encoded, are presented and tested in the evolution of NN models (Yao, 1999). The trend has been towards indirect encoding due to its better scalability for example, but the direct encoding can be suitable for the precise and fine-tuned search of NNs.

In this work, we focused on the search of high-level architecture of MLP namely the inputs and hidden layers. The design of low-level architecture (connections and transfer functions by node), or any other parameters such as learning algorithms were not considered. A combination of direct and indirect encoding was

hid.layers		hid.neurons on	hid.neurons on	model inputs (1-49)			
(1-2)		layer 1 (1-31)	layer 2 (1-31)				
	b ₁	b ₂ b ₃ b ₄ b ₅ b ₆	b ₇ b ₈ b ₉ b ₁₀ b ₁₁	b ₁₂ b ₁₃ b ₁₄ • • • b ₆₀			

Fig. 1. The encoding practice used (parametric binary presentation) where bn is the n bit (0/1). The number of hidden layers is derived from the first bit (0=1 hidden layer, 1=2 hidden layers), the number of hidden neurons is derived via the Gray transformation and inputs selected to the model simply from the bits (0=absence and 1=presence).

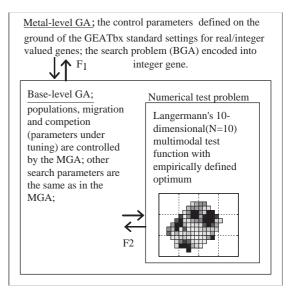


Fig. 2. The tuning of control parameters by using meta-evolutionary technique where F_1 is the fitness function of the meta-level (the number of objective function evaluations) and F_2 the fitness function of the base-level (Langermann's multimodal test function).

utilised by using a parametric binary representation where the number of hidden neurons was within the range of 1–31 on a layer, the number of hidden layers was one or two, and network inputs (the number of inputs varied 1–49) exist (Fig. 1). The Gray coding² was used in the encoding of number of hidden neurons in order to achieve smooth evolutionary landscape.

2.5. Selection of efficient search parameters

For maximising the search efficiency, the optimum distribution parameters (populations, migration and competition) of coarse-grained GA were searched by using the meta-evolutionary approach (Grefenstette, 1986). In this scheme, two genetic algorithms namely a meta-level one (MGA) and a base-level one (BGA) exist; the BGA (parameters under tuning) undergoes evolutionary process which is controlled by the MGA (Fig. 2). The parameters selected for tuning were the

²The Gray coding is a method for transforming a function mapping such that binary representations of consecutive numerical values differ by a single bit.

number of populations (1-10), the number of individuals (1-50) in migration interval (1-50), migration rate (0-100%) of population, competition interval (1-50) and competition rate (0-100%).

2.5.1. Meta-level GA

The MGA complied with the idea of coarse-grained GA with the parameters defined on the ground of GEATbx (http://www.geatbx.com/) standard settings for integer/real-valued optimisation problems (Pohlheim, 2000). Four subpopulations with total population size of 90 were evolved (500 generations) using unconstrained migration (rate of 0.1) every 20th generation (exchanging the best individuals in complete net structure) and mutation with rate of 1 (a mutation per individual) and mutations steps of 0.1 (rough), 0.03 (standard), 0.01 (fine) and 0.003 (very fine). The selection of individuals (BGAs) for recombination was done using stochastic universal sampling (provides zero bias and minimum spread) and the recombination using the discrete recombination of real/integer valued genes.

2.5.2. Base-level GA

The BGA was encoded at the meta-level into the six-dimensional integer-valued gene, in which each genotypic code represented the value of control parameter under tuning. The parameters of the BGA, excluding the parameter under tuning (controlled by the MGA), were the same as in the MGA (for real/integer-valued problem). As the fitness of the BGA (meta-fitness), the average (three independent runs) number of objective function evaluations F_1 for reaching a defined optimum (in a test problem discussed later) was used. The BGA candidates, which were not able to convergence into the optimum within defined 5000 objective function calculations, were penalised with the difference between achieved value and a global minimum of a test problem.

2.5.3. Test problem

The use of a real control systems and particularly systems based on the training of NNs at the base-level is impractical due to the requirements of low computation time. However, it is important that a problem at the base-level corresponds to the problem under optimisation in order to achieve valid results. For selecting a feasible test problem, we evaluated a relatively large MLP population with random MLP inputs and architectures, and used Sammon's gradient method (Sammon, 1969) to visualise the form of multidimensional fitness landscape in two dimensions. On the ground of this information, we decided to use the multimodal test function of Langermann (Bersini et al., 1996) to be considered as the test problem at the base-

level.

$$f(x) = -\sum_{i=1}^{m} c_{j} \left(\exp\left(-\frac{1}{\pi} \sum_{j=1}^{N} (x_{j} - a_{ij})^{2}\right) \times \cos\left(\pi \sum_{j=1}^{N} (x_{j} - a_{ij})^{2}\right) \right),$$
(1)

where m=30, N=10 and $0 \le x_i \le 10$. The real valued matrix $A=a_{ij}$ is not presented here due to space requirement; the reader is referred to Bersini et al. (1996).

The global optimum of the function is -1.4, which seemed to be very difficult to reach even by using the huge populations. Also, it was detected, that in most cases, test runs trapped on the local optima of -0.42863 and in some cases, reached the local optima of -0.80600. When the reaching global optimum proved a complex task, the local optima of -0.80600 was considered as the sufficient optimum for the problem. It is probably, that the BGA reaching the proposed optimum (not trapped on -0.42863), have some hill-climbing abilities which can be useful in the real-world case.

2.5.4. Selected parameters

The tuning results indicated that even relatively small populations can be capable of reaching the defined optimum within the given limit of objective function calculations (5000). However, the meta-evolutionary approach proved extremely noisy due to the nature of assessment of meta-level fitness. For the same solution (BGA), one could obtain many different values of the meta-fitness. Therefore, the tuning of control parameter became a largely empirical task, in which the results of the meta-tuning, traditional hand-tuning and the literature were used.

Finally, two subpopulations (15, 15) with total size of 30 with migration interval of 15, migration rate of 10%, mutation (binary) rates of 1 and 2 (mutations per individual), double point crossover (suitable for binary gene) and selection of stochastic universal sampling were chosen to be considered as search parameters. The competition operation between populations was not adopted. The overall size of populations (30) was kept relatively small due to the computational issues and so the risk of poor convergence arises. However, when comparing the population size to some earlier studies (Grefenstette, 1986), the population size near 30 has proven to be adequate.

2.6. Fitness assessment of MLP model

The evaluation (fitness assessment) of MLP models was carried out in straightforward manner by running the real system for each model five times (in order to

minimise fluctuation). The data from the years 1996–1998 was used as training data and data from the year 1999 as model validation data. This approach was computationally expensive due to long training times of NN models. However, it was utilised because it was anticipated to yield more reliable estimates for model fitness compared to approaches based on fitness approximation. In order to get around the computational requirements, we decreased the amount of data used in the training (10% random sample of training data).

The fitness of model was assessed from the observed and predicted values by calculating the index of agreement (IA) (Eq. (2)), which is a dimensionless measure limited to the range of 0–1 and thus, allows the comparison of different models (Willmott et al., 1985).

IA = 1 -
$$\left[\frac{\sum_{i=1}^{N} (P_i - O_i)^2}{\sum_{i=1}^{N} (|P_i - \bar{O}| + |O_i - \bar{O}|)^2} \right],$$
 (2)

where N is the number of data points, O_i the observed value, P_i the predicted value and \bar{O} is the average of the observed data. The final estimate of model goodness (fitness function, F) was then calculated as the average IA of five runs,

$$F = \sum_{i=1}^{N} (1 - IA)/N,$$
 (3)

where N is the number of runs and the IA is scaled to the range from 0 (maximum performance) to 1 (minimum performance).

2.7. Model evolution runs and validation

Finally, the coarse-grained GA with the selected parameters (Section 2.5) was used for evolving the MLP for the forecasting problem (Fig. 3). The starting populations were initialised with the random set of MLP models (see the encoding in the Section 2.4) and 150 generations were executed with elitism. A series of 10 independent runs were performed in order to minimise the risk of poor convergence.

After that, the performance of evolutionary approach was verified by evaluating a reference model and evaluated models multiple times (5) using all the data from the years 1996–1998 in the training (during evolution 10% random sample was used). In the reference model, all variables were included as inputs and parameters were selected based on experience and knowledge (Kolehmainen et al., 2001). The parameters used were 25 hidden neurons, learning algorithm of scaled conjugated gradient back-propagation, the performance function of regularized mean squared error (RMSE), hyperbolic sigmoid tangent for the hidden layers and linear for the output layer.

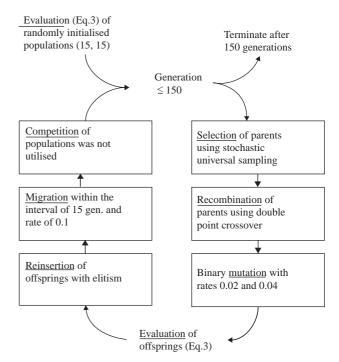


Fig. 3. The main stages and operations in the migration GA used for evolving the MLP models.

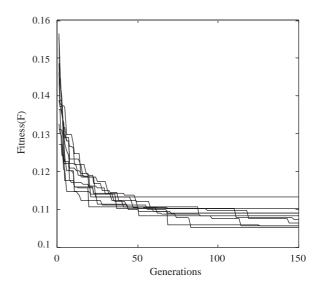


Fig. 4. Convergences resulting in the evolutionary model design.

The performance assessment was performed in the context of general performance (IA) and exceedance performance. The latter was calculated in order to get better understanding of the model's capabilities in the episodic situations. Statistical measures selected for exceedance assessing were the success index (SI) which has been detected to be able to represent performance in exceedance forecasting as well as the overall goodness between predicted and observed data (Schlink et al., 2003) and the fraction of false alarms (FA). In the calculations, the threshold value of $100 \,\mu\text{g/m}^3$ (the national guideline is $70 \,\mu\text{g/m}^3$) was used for an

Table 1 The optimised models achieved in the optimisation runs (1-10). The chosen inputs are marked with 'x' and strongly relevant variables are shaded

Model	1	2	3	4	5	6	7	8	9	10
Model fitness (IA)	0.895	0.893	0.889	0.887	0.890	0.891	0.892	0.894	0.894	0.89
Hid. neurons in layer 1	16	17	19	9	13	30	29	31	31	26
Hid. neurons in layer 2	10	8	12	1	1	0	0	12	0	8
Number of hid. neurons	26	25	31	10	14	30	29	43	31	34
Number of inputs	18	25	21	32	22	19	18	10	21	18
Sine of hour	x	x	x	X	X	X	X	X	X	X
Cosine of hour	x	X	X	X	X	X	X	x	x	X
Sine of weekday	X	X	X	X	X	X	X	X	X	X
Cosine of weekday										
Weekend										
Sine of day of year				X		X				
Cosine of day of year	X								X	X
Sine of week			X	X						X
Cosine of week	X	X	X	X	X					
NO _x	X	X	X	X	X		X			
NO ₂	X	X	X	X	X	Х	X	X	X	X
O_3	X	X	X	X	X	X	X	X	X	X
PM ₁₀	^	Α	A	Α	X	А	Λ	A	Α	Λ
CO CO		X			Α	v				
Pressure		A				X				
Temperature	v	Х		v	v	Х			Х	v
Humidity	X	X	v	X	X	X	v	v	X	X
			X				X	X		
State of ground										
Cloudiness				X						X
Dew point			X	X		X				X
Wet bulb	X	X		X	X				X	
Rain		X		X	X		X			
Visibility		X	X							
Weather										
Weather (1 h)										
Weather (3 h)			X	X		X				
Amount of clouds				X				X		
Type of clouds					X		X			
Low clouds (height)	X	X	X		X	X				
Middle clouds (type)										
High clouds (type)				X						
Wind speed	X	X	X	X			X	X	X	X
Sunshine				X	X				X	
Albedo		X	X	X						X
Solar elevation	X	X	X	x	x	X	X		X	X
Solar radiation		x							X	x
Moisture			X	X						
Inversion (M-O)		X		X	X	X	X		X	
Temperature scale		X		X	100	X	1000	X	200	X
Friction velocity	X	X	X	x	X	x	Х		X	x
Turb. heat flux	X		, a	X		X			X	//
Net radiation	.	X		X	X	X	X		X	
Latent heat flux		Α		X	Δ	A	Λ		X	X
Mixing height				Λ	v		v		Λ	Α
Mixing height2		v		v	X		X			
		X	144	X	X		X		-	
Conv. velocity	X	X	X	X					X	
Temp. gradient		X	X						X	
Wind dir. (sine)	X			X	X	X	X		X	
Wind dir. (cosine)	X	X	X	X	X	X	X	X	X	X

exceedance and the SI and the FA were derived as follows:

where TPR = A/M, $(0 \le TPR \le 1)$, FPR = (F-A)/

FA = (F - A)/F, SI = TPR - FPR(4) (5)

$$SI - TPR - FPR$$

$$(N-M)$$
, $(0 \leqslant \text{FPR} \leqslant 1)$,

Table 2
The validation results of the optimised models (1–10) and the reference model when testing models multiple times. The minimum and maximum indices are in bold

Model	IA				SI	SI				FA (%)			
	Min	Max	Mean	Std	Min	Max	Mean	Std	Min	Max	Mean	Std	
1	0.911	0.913	0.912	0.001	0.12	0.19	0.16	0.03	43.8	65.5	55.2	7.8	
2	0.903	0.910	0.907	0.003	0.10	0.23	0.15	0.05	50.0	75.0	65.1	10.0	
3	0.902	0.912	0.907	0.004	0.16	0.23	0.18	0.03	43.5	65.4	56.3	8.3	
4	0.898	0.912	0.906	0.006	0.16	0.24	0.21	0.04	47.1	53.6	49.7	2.9	
5	0.896	0.910	0.905	0.005	0.10	0.23	0.18	0.05	57.1	76.9	65.7	7.9	
6	0.910	0.914	0.912	0.002	0.16	0.19	0.17	0.02	43.8	54.6	47.4	4.4	
7	0.907	0.911	0.908	0.001	0.11	0.19	0.15	0.03	45.0	67.9	54.6	10.1	
8	0.903	0.906	0.905	0.002	0.12	0.21	0.18	0.04	56.5	70.0	60.5	5.5	
9	0.909	0.914	0.912	0.002	0.12	0.19	0.16	0.03	47.1	60.9	54.4	5.9	
10	0.903	0.908	0.906	0.002	0.19	0.28	0.22	0.03	61.0	69.4	65.0	3.9	
REF	0.892	0.902	0.897	0.004	0.05	0.14	0.09	0.03	42.9	78.6	61.9	15.2	

REF-reference model.

where the fraction of correctly predicted exceedances (TPR, true positive rate) represents the sensitivity of model and the false positive rate (FPR) the specificity of model. In the equations, A is the correctly predicted exceedances, M is all observed exceedances, F is all predicted exceedances and N is the total number of observations.

3. Results

3.1. Evolved MLP models

The results obtained in the evolutionary runs are illustrated in Fig. 4 and Table 1. In all the cases, maximum fitness values (Eq. (3)) of evaluated models were of the order 0.11 (IA = 0.89). When considering the architectures (Table 1), remarkable variations can be seen. Particularly, it can be observed that even a relatively small amount of hidden neurons is sufficient in the case of two hidden layers (9–1 and 13–1). This is largely due to the universal approximator theorem (Hornik et al., 1989), which states that a two-hidden layer network may achieve the same accuracy with a single hidden layer neural network with fewer hidden layer neurons. However, the use of two hidden layers did not improve the capability of MLP considerably.

When considering the results in the context of input subsets, strongly relevant, weakly relevant and irrelevant inputs (John et al., 1994) can be detected. As expected, some timing (hour, week day), pollution (NO₂ and O₃ at T+0) variables were selected with high probability due to their strong association with the temporal variation of traffic (the most important source of pollution). Similarly, some meteorological parameters (wind direction, wind speed, temperature, solar evaluation, friction velocity) which determine the atmospheric dispersion

conditions were found to be strongly relevant. Additionally, there was set of weakly relevant variables which were also needed in the forecasting and some irrelevant or disturbing ones (week end, state of ground) which were not needed. Finally, it can be concluded that roughly 20 ± 10 from total of 49 inputs included adequate information for achieving the performance described in the results.

3.2. Validation statistics

The validation statistics is presented for each model and the reference models in Table 2 and the scatter plots (forecasted versus observed) in Fig. 5. Compared to the reference model, a slight increase in the performances was detected in terms of general performance (IA). When considering the exceedance performances (SI and FA) of the evolved models, a moderate improvement was achieved. However, the consideration of SI and FA proves clearly, that after the optimisation, the capability of MLP for forecasting exceedances was still somewhat poor (SI varied 0.11-0.28) including the large fraction of false alarms (roughly 40–70%). Moreover, Fig. 4 demonstrates that the models clearly underpredicted high concentrations ($> 100 \,\mu\text{g/m}^3$) which can be seen in Table 2 as poor SI indices. Therefore, it can be stated the evolving of model inputs and high-level architecture itself could not improve the performances of the models significantly. However, more robust and reasonable models were produced, that are very important features in practical applications.

4. Conclusions

In this paper a genetic algorithm was tested for designing the multi-layer perceptron model for forecasting urban air pollution. The results showed that GA is

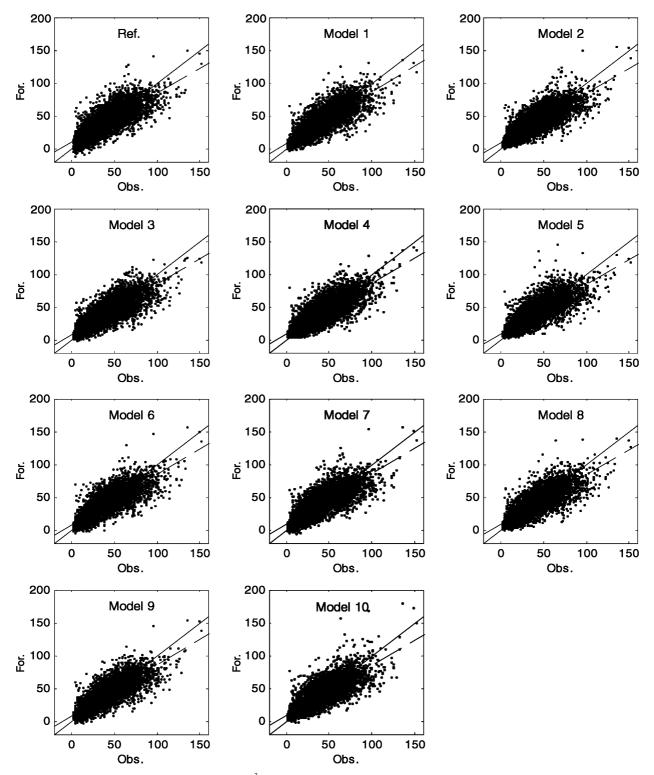


Fig. 5. Plots of forecasted versus observed values ($\mu g/m^3$) by the reference model ("Ref.") and the evolved models (1–10). The plots are further enhanced with a least-squares fitting line (dotted) and a line showing perfect fit (solid).

an applicable technique in this domain; it is capable of searching feasible high-level architectures and particularly reducing the need of computational efforts by eliminating irrelevant inputs. In the case of air quality forecasting this can also imply smaller costs due to the smaller amount of measurements required. No clear connection between architectural issues and performance was found, so it is reasonable to use somewhat simpler architecture instead of complex one in order to minimise the risk of noise over-fitting.

Further research will be focused particularly on the fitness evaluation of NN models, in the context of minimising computational cost. Solutions for that could be a fitness approximation based approach where e.g. a simpler form of model, which can be evaluated quickly during the evaluation phase. Additionally, it was detected that the evolution of MLP inputs and architecture itself did not improve the ability of the MLP to forecast high concentrations significantly, which is largely due to the under-representation of these cases in training data (in this case about 1% of all training instances). Therefore, further work is needed on issues such as boosting, where the frequency of high concentration values is increased, enhancing the error term by using some regularization technique and recurrent neural networks, where the temporal patterns are better considered.

Acknowledgements

This research was funded by the Academy of Finland (FORECAST, Project No. 49946) and utilised the findings and database of EU funded project APPETISE (http://www.uea.ac.uk/env/appetise).

References

- Bäck, T., Fogel, D., Michalewicz, Z., 1997. Handbook of Evolutionary Computation. Institute of Physics Publishing Ltd., Bristol and Oxford University Press, New York.
- Bersini, H., Dorigo, M., Langerman, S., Seront, G., Gambardella, L., 1996. Results of the first international contest on evolutionary optimisation. In: Proceedings of the Third IEEE Conference on Evolutionary Computation, pp. 611–615.
- Cantú-Paz, E., 1995. A summary of research on parallel genetic algorithms. Technical Report IlliGAL No. 95007, University of Illinois at Urbana-Champaign.
- De Jong, K.A., 1975. Analysis of the behaviour of a class of genetic adaptive systems. Ph.D. Thesis, Department of Computer and Communication Sciences, University of Michigan.
- Eiben, A.E., Hinterding, R., Michalewicz, Z., 1999. Parameter control in evolutionary algorithms. IEEE Transactions on Evolutionary Computation 3 (2), 124–141.
- Gardner, M.W., Dorling, S.R., 1999. Artificial neural networks (the multi-layer perceptron)—a review of applications in the atmospheric sciences. Atmospheric Environment 33, 709–719.

- Grefenstette, J., 1986. Optimization of control parameters for genetic algorithms. IEEE Transaction on Systems, Man, and Cybernetics 16 (1), 122–128.
- Holland, J.H., 1975. Adaptation in Natural and Artificial Systems. University of Michigan Press, Ann Arbor.
- Hornik, K., Stinchcombe, M., White, H., 1989. Multilayer feedforward networks are universal approximators. Neural Networks 2, 359–366
- Jain, A., Zongker, D., 1997. Feature selection: evaluation, application and small sample performance. IEEE Transactions on Pattern Analysis and Machine Intelligence 19 (2), 153–158.
- John, G.H., Kohavi, R., Pfleger, K., 1994. Irrelevant features and the subset selection problem. In: Cohen, W., Hirsh, H. (Eds.), The 11th International Conference on Machine Learning. Morgan Kaufman Publishers, San Francisco, CA.
- Junninen, H., Niska, H., Tuppurainen, K., Ruuskanen, J., Kolehmainen, M., 2004. Methods for imputation of missing values in air quality data sets. Atmospheric Environment, accepted for publication.
- Karppinen, A., Joffre, S., Vaajama, P., 1997. Boundary layer parametrization for Finnish regulatory dispersion models. International Journal of Environment and Pollution 8, 557–564.
- Kolehmainen, M., Martikainen, H., Ruuskanen, J., 2001. Neural networks and periodic components used in air quality forecasting. Atmospheric Environment 35, 815–825.
- Kukkonen, J., Partanen, L., Karppinen, A., Ruuskanen, J., Junninen, H., Kolehmainen, M., Niska, H., Dorling, S., Chatterton, T., Foxall, R., Cawley, G., 2003. Extensive evaluation of neural networks of NO₂ and PM₁₀ concentrations, compared with a deterministic modelling system and measurements in central helsinki. Atmospheric Environment 37, 4539–4550.
- Miller, G., Todd, P., Hedge, S., 1989. Designing neural networks using genetic algorithms. In: Schaffer, J. (Ed.), The Third International Conference on Genetic Algorithms and Their Applications, CA, San Mateo.
- Pohlheim, H., 2000. Tutorial for the genetic and evolutionary algorithm toolbox for use with MATLAB (GEATbx) version 3.30, http://www.geatbx.com.
- Sammon Jr., J.W., 1969. A nonlinear mapping for data structure analysis. IEEE Transactions on Computers C-18 (5), 401–409.
- Schlink, U., Dorling, S., Pelikan, E., Nunnari, G., Cawley, G., Junninen, H., Greig, A., Foxall, R., Eben, K., Chatterto, T., Vondracek, Richter, M., Dostal, M., Bertucco, L., Kolehmainen, M., Doyle, M., 2003. A rigorous inter-comparison of ground-level ozono predictions. Atmospheric Environment 37, 3237–3253.
- Tiittanen, P., Timonen, K.L., Ruuskanen, J., Mirme, A., Pekkanen, J., 1999. Fine particulate air pollution, resuspended road dust and respiratory health among symptomatic children. European Respiratory Journal 12, 266–273.
- Willmott, C.J., Ackleson, S., Davis, R., Feddema, J., Klink, K., Legates, D., O'Donnell, J., Rowe, C., 1985. Statistics for the evaluation and comparison of models. Journal of Geophysical Research 90 (C5), 8995–9005.
- Yao, X., 1999. Evolving artificial neural networks. Proceedings of the IEEE Transactions on Neural Networks 87 (9), 1423–1447.