TECHNICAL MEMORANDUM

MODELING AND FORECASTING ATMOSPHERIC POLLUTION USING NEURAL AND ABDUCTIVE NETWORKS

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SUMMARY

Monitoring and forecasting atmospheric pollution in rural, urban, and industrial areas is a prime concern for environmental protection authorities worldwide. Such activities have become increasingly important with the increase in industrial and traffic pollution emissions and the rising awareness of the harmful effects of air pollutants on human health, wildlife, and the environment in general. Guidelines, standards, and objectives are set by national and international organizations, including the United Nations' World Health Organization (WHO), regarding permissible pollution levels of various sources of pollution.

Modeling pollution emissions and dispersion has been used to assess current and potential future air quality to allow informed policy decisions to be made. Available emissions and monitoring data can be used to develop emission and dispersion models to forecast future changes based on a range of 'what if' scenarios. Short-term modeling can be used to provide reasonably accurate predictions of next-day pollution levels, thus allowing advance public warning and emergency actions to be taken to avert excessive pollution. Conventional statistical methods have long been used for this purpose, but modern machine learning approaches; e.g. neural networks, can handle a larger number of input variables, require less user intervention and are better in handling nonlinearities and in dealing with data uncertainties and inaccuracies. This Technical Memorandum proposes the use of advanced neural and abductive networks for short-term modeling, analysis, and forecasting of air pollution levels. Compared to neural networks, abductive networks offer a number of advantages, including simplified and more automated model synthesis requiring less user intervention, and analytical input-output model relationships that automatically highlight significant input variables and provide better explanation facilities.

The proposed work should be of interest to environmental protection authorities in the kingdom as well as environmental protection departments of major industrial establishments. Applications include the development of fast and accurate tools for the short-term forecasting of the daily peak, hourly day profile of concentrations of harmful air pollutants. Models can provide advance warning prior to safety thresholds being exceeded for remedial action to be taken. Analytical model relationships derived from historical data can clearly identify influential input variables and their individual contributions to pollution levels. This should provide decision makers with better insight into the problem and enable comparison with previously used statistical or empirical models.

Following a brief introduction in Section 1, the objectives of the work are presented in Section 2. A description of the problem is given and the proposed approach is outlined in Section 3. Section 4 describes various aspects of the proposed work. Relevant CAPS experience in using the proposed approach to solve similar problems is outlined in Section 5.

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SECTION 1 INTRODUCTION

Urban air pollution is a growing problem in many parts of the world. An effective way of controlling pollutant concentrations is through correct management of urban development and traffic. Air quality standards have been introduced that specify maximum concentration levels for various pollutants and the number of times such thresholds are exceeded during a given time interval. In some cases, regulations require the public to get prior warning of increased pollution levels. To implement such strategies, reliable short-term forecasts of pollutant levels are required. The lead time provided by such forecasts allows authorities to take necessary action to warn the public to avoid unnecessary exposure, and to take emergency action to reduce emissions and prevent thresholds being exceeded on the following day. Deterministic (theoretical) models have been proposed for providing such predictions, but they are highly complex, of limited accuracy, and may require data that is not readily available. Statistical methods in the form of univariate time series analysis or multivariate regression analysis have been also used for this purpose. The first category ignores important exogenous effects, such as weather parameters, which degrades model performance. The second approach tends to assume linear relationships for simplicity, while the relationships involved are known to be complex and nonlinear. Moreover, such methods are computationally intensive and require considerable user intervention in determining the appropriate form of the model relationship.

Data-based machine learning modeling techniques offer a better approach to solve this problem. They automatically discover complex and nonlinear relationships that exist between future pollutant concentrations and explanatory inputs such as previous concentration values, weather variables, and social factors, through training on collected data. They utilize abundantly available historical data for offline training and provide fast-executing forecasting models that are suitable for online use. Artificial neural networks have been used for short term modeling of pollution. However, conventional neural networks suffer from a number of limitations, including long training times, difficulty of determining optimum network topology and training conditions, and the black box nature of the resulting models that gives poor explanation facilities. To overcome the above limitations, this Technical Memorandum proposes using advanced neural and abductive network techniques as alternative approaches for the rapid development of accurate and more transparent models for pollution forecasting in various regions of the kingdom. In addition to their use as forecasting tools, the models give insight into the contribution of various emission and meteorological factors to atmospheric pollution in different environments.

SECTION 2 OBJECTIVES

We propose using advanced neural and abductive network modeling techniques to the important area of short-term modeling and forecasting air pollution levels in rural, urban, and industrial areas of the kingdom. The proposed work serves the following objectives:

- Develop transparent and accurate models that predict concentrations and threshold level exceedances for air pollutants.

- Provide advance information on prospective excessive concentrations. This should allow issuing public warnings and taking remedial measures to reduce pollution levels and avert harmful pollution episodes.

- Assist in the decision making process at pollution monitoring and control authorities.
- Compare the structure and performance of resulting models with currently used models and forecasting techniques.
- Improve our understanding of short-term variations in air pollution levels in various regions of the kingdom.
- Determine the factors that influence air pollution concentrations, including emissions, traffic, and various weather parameters, in various regions.
- Introduce the use of modern computational intelligence and data mining techniques for pollution monitoring and control in the kingdom.
- Develop platforms for training junior scientists and engineers in pollution modeling, forecasting and control.

SECTION 3 DISCUSSION OF THE PROBLEM

3.1. Description of the Problem

Monitoring and forecasting air quality is gaining importance due to the increasingly adverse health effects of urban pollution, which can even lead to premature deaths among sensitive population groups such as asthmatics, children and the elderly [1]. This has increased the demand for developing predictive pollution models that can give adequate advance warning of eminent critical pollution episodes for emergency measures to be taken in time to avert safety limits being exceeded. Major sources of atmospheric pollution include: SO_2, NO_2, CO, O_3, hydrocarbons (e.g. benzene, toluene), particulate matter (PM), and lead.

While SO_2 sulfur emissions are generally decreasing in the western industrialized world, they are on the increase in many developing countries [2]. The gas is formed when coal and oil fuel is burned, and during metal smelting and other industrial processes. High SO_2 concentrations affect breathing, alter pulmonary defenses, and aggravate existing respiratory illnesses and cardiovascular diseases. WHO specifies 100-150 $\mu g/m^3$ as safety limits for daily averages of SO_2 particulate matter in ambient air. The 1999 European Community (EC) legislations in this regard specify that an attention level of 125 $\mu g/m^3$ for the mean of hourly values over a day should not be exceeded more than three times a year.

NO_2 is a highly reactive gas that is corrosive to metals and is a strong oxidizing agent. It can be generated directly from combustion processes or as a result of conversion of NO gas in the atmosphere. The gas is toxic to animals and humans, as it forms nitric acid with water in the eye, lung, mucus membrane and skin. Susceptible humans, such as asthmatics, exposed to high concentrations of NO_2 can suffer lung irritation and potentially, lung damage. Health guideline values adopted by WHO are: 200 $\mu g/m^3$ (one-hour mean) and 40 $\mu g/m^3$ (annual mean).

CO pollution is primarily attributed to increased motor vehicle traffic and exhaust emissions in urban areas. Formation of COHb reduces the amount of hemoglobin available for oxygen circulation in the body, which can affect the brain, nervous tissues, heart muscle and other specialized tissues that require large amounts of oxygen to function. As a result of oxygen deprivation, such organs and tissues may suffer temporary or permanent damage. Health guideline values adopted by WHO are: 30 $\mu g/m^3$ (one-hour average) and 10 $\mu g/m^3$ (eight-hour average).

Elevated concentrations of surface ozone present a potential health hazard related to the respiratory tract in humans, and can have adverse effects on vegetation and ecosystems [3]. EC legislations require mandatory public warning in cases where O_3 concentrations exceed certain thresholds [4]. In 2002 the public information threshold was 180 $\mu g/m^3$, while the population warning threshold was 360 $\mu g/m^3$. A variety of operational warning systems have been developed to allow preventive action to be taken ahead of and during pollution episodes [3,4].

WHO specifies a maximum limit of 240 $\mu g/m^3$ for 24MA concentration of PM10 before humans are put to serious health risks [5]. 24MA is the value of the 24-hour moving average and PM10 are suspended particulate matter (SPM) with diameter below 10 μm, which are small enough to ingress into the human respiratory track. In Santiago, Chile, a day when this limit is exceeded is considered a pre-emergency situation [5]. Main sources for PM10 pollution include combustion and industrial processes, road dust from vehicular traffic, and black smoke from diesel engines. Statistically significant association has been reported between ambient PM10 and daily mortality [6]. If limit exceedance is predicted, palliative actions can be taken early in the day to reduces emissions. Traffic restriction measures may include speed limits, alternative routing, and incentives to use public transport [3].

3.2. Modeling of Atmospheric Pollution

Short-term forecasts of major air pollutants must be issued to the public and communicated to regulatory authorities concerned on daily basis in many parts of the world. Until recently, such forecasts were generated manually by human experts [7], based on previous pollution measurements, meteorological data, traffic, and other social factors that control the behavior of emission sources. There is a need to automate the forecasting process for improved accuracy, speed, and reliability. An automated system can estimate episode risks, predict short and long term trends, and propose counter measures when necessary [7].

Deterministic, first-principle models have been developed for atmospheric pollution, e.g. [8,9]. Such models embody complex photochemical reaction and atmospheric dispersion mechanisms in mathematical form. Therefore, their implementation is complex, requiring considerable computer and human expert resources [3]. They may need data on emissions that are not readily available, at least not in real time [2]. This approach is not a practical choice for fast prediction of air quality in many online monitoring and control applications.

Pollution time series have been modeled using linear univariate techniques such as the Box-Jenkins ARIMA analysis [10] and Kalman filters [11]. However, environmental pollution processes involve many exogenous inputs on emissions, atmospheric transport and mixing, etc. which limits the accuracy of univariate analysis of the concentration time series alone.
Linear and nonlinear multiple regression analysis can be used to handle multivariate time series

of the variables involved. However, the complex input-output relationships are difficult to understand and handle using traditional regression [12]. It is difficult to determine empirically the correct relationship between the output and the explanatory inputs. Moreover, traditional regression modeling techniques assume normally distributed data [13]. This assumption is highly restrictive in the case of environmental data, which are often not normally distributed and it is difficult to find suitable transforms to normality [13].

3.3. Data-Based Modeling Using Neural Networks:

A recent trend in handling such problems that are difficult to solve analytically has been to resort to machine learning techniques. The availability of large amounts of historical data on measured pollution levels and weather parameters encourages the use of data-based modeling approaches such as neural networks. Such techniques are non-parametric, i.e. the user does not need to explicitly specify the model relationship *a priori*. This enhances their use in knowledge discovery by freeing them from bias or influence by previous assumptions. Complex nonlinear input-output relationships can be modeled automatically through supervised learning using a database of solved examples. Once synthesized, the model can generalize to predict outputs corresponding to new cases, previously unseen during training. Neural networks offer many advantages over conventional modeling approaches, including improved accuracy, reduced development time, increased tolerance to noise, uncertainty, and missing data, reduced need for knowledge on the modeled phenomenon, freedom from assumptions on the probability distributions of input variables, relative ease of updating the model through re-training, and the fact that no programming is needed. Intensive computations are required only once during model synthesis, while predictions by the models synthesized are fast and straight-forward, making them ideal for online use. Ref. [14] shows that neural network models can predict PM2.5 concentrations more accurately than a linear regression model using the same input attributes.

Neural networks have been widely used for modeling and predicting concentrations of many air pollutants, as well as providing automatic warning of eminent critical pollution episodes, see [15] for an overview. Following is a list of selected representative applications:

1. Forecasting hourly concentrations of NO_2 at a busy urban traffic station [12].
2. Forecasting daily average, maximum, and hourly concentrations of SO_2 in industrial and urban locations [2].
3. Forecasting next-hour average concentration of CO traffic pollution [16].
4. Forecasting surface O_3 hourly concentrations one-day ahead at urban and rural sites [4].
5. Forecasting maximum O_3 concentration, threshold exceedance events, and duration of the smog episode above a given threshold [3].
6. Forecasting maximum of a 24-hour moving average (24 MA) of PM10 concentrations 30 hours in advance [5].

3.4. Limitations of Conventional Neural Networks

In spite of the wide-spread use of feed-forward neural networks trained with error back-propagation for pollution modeling and forecasting, the technique suffers from a number of limitations. These include slow convergence, the possibility of getting stuck in a local minimum, and the difficulty of determining optimum network topology and training parameters [2]. There are many choices to be made in determining numerous critical design parameters with little guidance available. Designers often resort to a trial and error approach [2,16], which can be tedious and time consuming. Such design parameters include the number and size of the hidden layers, the type of neuron transfer functions for the various layers, the training rate and momentum coefficient, and training stopping criteria to avoid over-fitting and ensure adequate generalization with new data. In environmental applications, a large number of inputs can be measured, and it is often necessary to select a smaller subset of good predictors to build a model with adequate performance. Genetic algorithms (GA) have been proposed to search for an optimum subset of inputs and optimum values for architecture and training parameters for the neural network model [4]. This approach suffers from long computation times. The early stopping criterion, often implemented to avoid overfitting, requires a dedicated cross validation test set, which reduces the number of examples used for actual training.

Another limitation is the black box nature of neural network models, which makes them lack on explanation facilities, providing little insight into the modeled relationship and the relative importance of various inputs [17,18]. The acceptability of, and confidence in, pollution models for decision making in an operational environment appear to be related to their transparency and their ability to justify results to human experts and decision makers [18]. Simplified analytical models that relate significant inputs to model output in equation form have been found very useful in environmental studies [19]. Such equations could trigger hypotheses on the modeled phenomenon, which can then be verified by further experiments, thus aiding scientific enquiry. Generating manageable analytical expressions from neural network models is a tedious process involving network pruning through iterated removal of weak weight links and testing the resulting network for adequate performance [19].

3.5. Proposed Approach

To overcome limitations of conventional neural networks, we propose using abductive networks [20] and advanced predictor and classifier neural network tools that train quickly and generalize well for new data. These tools optimize the number of hidden neurons automatically, and therefore do not require much user intervention. They also provide ranking of the input variables according to their predictive importance in the generated model. The tools do not require a dedicated cross validation set to determine when to stop training, and therefore fully utilize available data for training.

Abductive networks have been used at CAPS for forecasting the monthly domestic energy consumption at the Eastern Province over one year [21], short-term load forecasting [22], forecasting the minimum [23] and maximum [24] daily temperatures, as well as hourly temperature profiles [25]. Other application areas at CAPS include automatic identification of radioisotopes in gamma spectroscopy [26] and monitoring of vibrations in rotating machinery [27]. Applications in oil prospecting and production include estimating porosity from wire line well logs [28] and predicting the pressure-volume-temperature (PVT) reservoirs characteristics [29].

Compared to neural networks, abductive networks offer the advantages of faster model development requiring little or no user intervention [20], faster convergence during model synthesis without the problems of getting stuck in local minima, automatic selection of relevant input variables, and automatic configuration of model structure [30]. With the resulting model represented as a hierarchy of polynomial expressions, analytical model relationships can be derived. These provide insight into the modeled phenomena, highlight contributions of various inputs, and allow comparison with previously used empirical or statistical models. Such analytical model relationships have proved useful in environmental investigations [19]. The technique automatically avoids over-fitting by using a proven regularization criterion based on penalizing model complexity [20], without requiring a dedicated validation data set during training, as is the case with many neural network paradigms.

A database consisting of an adequate number of solved examples is required to develop and evaluate the abductive network model. The dataset should include input variables that are likely to influence the output parameter to be modeled, as well as corresponding values of the output parameter. The model is synthesized through training on a training dataset and is then evaluated by examining its performance on a separate evaluation data set. Model performance will be validated using a variety of performance measures. The proven model can then be tried for pollution forecasting in the real environment.

SECTION 4 STATEMENT OF WORK

The proposed work involves coordination with the client engineers and scientists in identifying a suitable application area, determining relevant input parameters, obtaining the required historical data from client databases, performing data pre-processing to ensure good quality of the training and evaluation data, as well as in integration of the final model with other systems at the client site. Following is a brief description of each task:

4.1. Problem Identification

The proposed technique can be used for modeling and short term forecasting of the concentrations of various air pollutants, including O3, NO_x, SO_x, CO, as well as particulate matter (PM). The system can give advance warning when predicted concentrations exceed specified pollution levels and can also predict the durations of the pollution episode. Consultations with the client would identify a specific application of interest, for which adequate historical data exists for the pollution and weather time series, as well other input attributes that are deemed important for developing the required models.

4.2. Selection of Input Variables

Selection of appropriate input variables for the model synthesis plays an important role in data-based modeling, since the model relationship is derived based on the input-output information provided. It is recommended that only relevant inputs are used, since too many inputs increase training time, lead to complex models that may not generalize well with new data in actual use, and require proportionally larger training sets to avoid the resulting model over-fitting the training data. A smaller subset of effective inputs also reduces the number of measurements required for model implementation, which could reduce cost. Discarding irrelevant or redundant inputs also avoids noise and missing data problems that may be associated with them. In Ref. [5], a linear perceptron model was used to select an optimum subset of 6 inputs from available 13 inputs for forecasting PM10 concentrations. Genetic algorithms were used to select 20 important inputs from a set of 49 variables for predicting hourly concentrations of nitrogen oxides [12]. The abductive network tool to be used in this work automatically selects relevant model inputs according to well-proven optimization criteria. Following is a brief account of typical input variables used in applications reported in the literature:

- Twenty inputs were selected for predicting hourly concentrations of nitrogen oxides [12], including:

    - Timing information, e.g. hour, weekday, etc.
    - Pollution data available at the forecasting point, e.g. for NO_2 and O_3.
    - Meteorological data that determine dispersion conditions, e.g. wind direction, wind speed, temperature, solar radiation, friction velocity.

- Seven inputs were used to predict hourly averages of SO_2 concentrations on the next day [31]:

    - Four hourly SO_2 average concentrations measured every 6 hours on the day preceding the forecasting day.
    - Values of temperature, wind speed, and relative humidity forecasted for the forecasting hour.

4.3. Selection of Data Sets for Model Development

To obtain good forecasting models, the training and evaluation data sets should be a good representation of the problem space. The larger the amount of good training data used, the better we expect the resulting models to be, provided that extending the data set does not introduce incoherencies or inconsistencies that are not explained by the input variables. Also, testing the models on a large set of representative evaluation data increases confidence in the resulting model and improves the statistics of the evaluation analysis performed. Different pollution patterns should be represented fairly in the data to avoid model bias towards patterns seen more frequently during training. Therefore, it is important to include data representing high levels of pollution. Neural network pollution forecasting models have been synthesized using training data from one year [5] up to four years [3,4,12]. Evaluation is usually performed on data for one year.

4.4. Data Preprocessing

Data gathered shall be checked for completeness and absence obvious errors. Missing data values can be substituted through interpolation or the whole data row is discarded. Obvious outliers are treated similarly. Additionally, Data for the input and output variables are often normalized individually to the same range, e.g. 0 to 1, or as Z scores of zero mean and unity standard deviation. Normalization is based on the minimum and maximum values, and the mean and standard deviation values for the individual variable, respectively. An opposite operation restores the predicted output to the original problem space.

4.5. Model Development

Data records available will be split into two portions: A training set containing data for the first *n* years and an evaluation set consisting of the data for the following one or two years. The training set is used for synthesizing a model that describes the input-output relationship. The evaluation set is used to validate the synthesized model on new data previously unseen during training. Two modeling techniques based on neural networks and abductive networks will be used for model synthesis, and their results compared.

4.6. Model Evaluation and Analysis

A variety of performance indices will be used for analyzing the performance of the models on the evaluation data set. These may include:

1. Global fit indices that measure overall fit quality of the forecasted time series, e.g. mean absolute error (MAE), mean absolute percentage error (MAPE), root mean square error (RMSE), indices of agreement [3,12], percentage of variance accounted for (VAF) [3], bias [2], and correlation coefficient between predicted and actual values [8].

2. Exceedance indices that measure classification performance for critical pollution episodes, e.g. success probability (SP) [2], success rate (SR) [2], false alarm (FA) [2,12], success index (SI) [2,12], area under the receiver operating characteristic (ROC) curve [2], and various forms of skill scores, e.g. Heidke score [5].

Values reported for performance measures in the literature include:

- MAPE = 20% for the 24MA of PM10 concentrations [5].
- MAE = 11.6 $\mu g/m^3$ for tomorrow's maximum ozone concentration [3].
- MAPE = 30% for tomorrow's SO_2 hourly concentrations [31].

Model performance is often compared against baseline forecasts generated using simple methods such as persistence [2]. Performance will also be compared with that of existing models or forecasting methods that may be currently used by the client.

In addition to predicting the modeled output from measured inputs, resulting abductive network models will provide useful information on the modeled pollution phenomena. The model automatically selects input parameters that contribute most to the modeled output and can provide simplified analytical expressions for the model relationship that reveal significant input variables and their relative importance.

4.7. Model Integration

The resulting models can be ported onto computer systems at the client site. Depending on the application, the models may be integrated to operate with other software programs and database applications. In situations where inputs to the model include data acquired online, the model should be interfaced to the software that runs the measurement apparatus. This part of the work requires close coordination with engineers and technicians at the client's site.

4.8. Performance Assessment

Evaluate the performance of the model in realistic operational settings for extended duration. Study the level of acceptance of the new model by the client's work team. Solicit and implement recommendations from the client team for product improvement. Investigate the need for model updating and re-training to accommodate long-term drifts in the training data.

4.9. Documentation

Full documentation will be provided on the data sets used, pre-processing employed, model synthesis, resulting model structures and input-output relationships, model evaluation analysis, and information on model integration.

SECTION 5 RELEVANT EXPERIENCE AT CAPS

CAPS has the expertise and resources to develop machine learning solutions for pollution modeling and forecasting. CAPS researchers have previously used the technique for similar application areas including: forecasting daily weather parameters, forecasting short and medium term electric load and energy demand. Following is a brief description of some relevant applications:

5.1. Modeling and forecasting monthly electric energy consumption in eastern Saudi Arabia using abductive networks [21]:

Abductive networks were used to model the monthly energy consumption in terms of key weather parameters and demographic and economy indicators. Models synthesized on data for five years were used to forecast new data for the 6^{th} year with an MAPE of 5.6%. Compared to regression relationships previously developed on the same data, the models are more accurate, use fewer input variables and are much easier and faster to develop.

5.2. Modeling and forecasting the daily minimum temperature [23]:

Abductive networks were used to model the minimum daily temperature in terms of other 18 weather parameters using data for one year. Evaluated on data of another year, the model predicts the minimum temperature with an error within ± 3% for 99% of the days, as compared to 67% of the days for a regression model. Another model forecasts tomorrow's temperature using the corresponding values for the past three days with the same error bounds for 92% of the days.

5.3. Modeling and forecasting the daily maximum temperature at Dhahran [24]:

Abductive networks were used to model the maximum daily temperature in terms of other 18 weather parameters using data for one year. Evaluated on data of another year, the model predicts the maximum temperature with an error within ± 3% for 97% of the days. Another model forecasts tomorrow's temperature using the corresponding values for the past three days with the same error bounds for 77% of the days.

5.4. Modeling and forecasting tomorrow's hourly temperatures [25]:

Abductive and neural networks were used to model the 24-hour daily temperature profile for tomorrow in terms of today's profile as well as extreme temperature forecasts for tomorrow. Abductive models trained on data for 5 consecutive years give an overall MAPE error of 3.5% when evaluated on the following 6th year.

5.5. Short-term electric load forecasting [22]:

Abductive and neural networks were used for modeling next-day hourly electric loads from a power utility using hourly load and temperature data for 5 consecutive years. Evaluated on the following 6th year, the models give an overall MAPE error of 2.67%.

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