Neurocomputing 155 (2015) 62–70

Contents lists available at ScienceDirect

Neurocomputing

journal homepage: www.elsevier.com/locate/neucom

Enhanced radial basis function neural networks for ozone level estimation

Q.P. Ha [a], H. Wahid [b,*], H. Duc [c], M. Azzi [d]

[a] Faculty of Engineering and Information Technology, University of Technology Sydney, Broadway, NSW 2007, Australia
[b] Faculty of Electrical Engineering, Universiti Teknologi Malaysia, 81310 Skudai, Malaysia
[c] Office of Environment and Heritage, PO Box 29, Lidcombe, NSW 1825, Australia
[d] CSIRO Energy Technology, PO Box 52, North Ryde, NSW 1670, Australia

ARTICLE INFO

Article history:
Received 3 July 2014
Received in revised form
5 December 2014
Accepted 15 December 2014
Communicated by K. Li
Available online 8 January 2015

Keywords:
Ozone
Radial basis function network
Learning algorithm
Metamodel
Spatial distribution

ABSTRACT

Assessment of air pollutant profiles by using measurements involves some limitations in the implementation. For this, deterministic air quality models are often used. However, its simulation usually needs high computational requirements due to complex chemical reactions involved. In this paper, a neural network-based metamodel approach is used in conjunction with a deterministic model and some measured data to approximate the non-linear ozone concentration relationship. For this, algorithms for performance enhancement of a radial basis function neural network (RBFNN) are developed. The proposed method is then applied to estimate the spatial distribution of ozone concentrations in the Sydney basin. The experimental comparison between the proposed RBFNN algorithm and the conventional RBFNN algorithm demonstrates the effectiveness and efficiency in estimating the spatial distribution of ozone level.

1. Introduction

Ozone (O_3) is a secondary pollutant gas that is naturally produced in the earth's atmosphere, produced by the chemical reaction between nitrogen oxides (NO_x, $NO_x = NO + NO_2$) and volatile organic compounds (VOCs) under daytime solar radiation. Effort has been paid to the problem of reducing the concentration of ground ozone (also known as tropospheric ozone) that is higher than the national standard. The reason for this concern is that an exposure to ozone that exceeds an allowable level may directly impact human health, causing respiratory problems, heart and lung diseases, and even premature death. Moreover, a long-term exposure to high background ozone levels can also affect living organisms, plant growth and building construction [1,2].

Conceptually, the reaction of ozone is straightforward but the estimation of its spatial profiles becomes complex when dealing with the ozone level not at point values but across a region, as its concentrations are influenced by many factors such as meteorological and terrain conditions. The highest accuracy in the determination of spatial distribution would be achieved if fixed measuring stations could be located at each domain cell. Unfortunately, this is almost impractically as it would involve a high investment cost. It may be overcome by using mobile measurement stations [3,4], but this is generally difficult to be implemented. Therefore, policy makers often use deterministic air quality models to handle the spatial estimation task (see, e.g., [5,6]). However, simulations using dispersion models involve a high computational cost and the prediction results are much dependent on the correctness of model formulation in the development stage, as well as the accuracy of emission inventory data and meteorological data used as inputs.

In air quality modelling, statistical and computational intelligence techniques can be alternatively implemented to reduce the computation burden. For example, an online support vector machine (SVM) was applied to predict air pollutant levels in an advancing time-series based on the monitored air pollutant data [7]. Other methods such as neural networks [8] and neuro-fuzzy [9] have also been used for modelling and control of different air pollutants. A neural network algorithm has been proposed to retrieve the tropospheric ozone column from nadir ultraviolet/visible spectroscopy radiance satellite measurements [10]. From collected stationary information, neural networks have been successfully applied to predict daily ozone levels, see, e.g., [11–14], but mainly on a temporal basis. A comparison for ozone prediction has recently been conducted in [15] to suggest the outperformance of support vector regression models with polynomial kernel functions over neural networks (feed-forward, time delay, and radial basis function) in terms of the root mean squared

* Corresponding author. Tel.: +60 7 555 7169; fax: +60 7 556 6272.
E-mail address: herman@fke.utm.my (H. Wahid).

http://dx.doi.org/10.1016/j.neucom.2014.12.048
0925-2312/

error, where input parameters for training these networks were chosen from available measured air pollutant and meteorological data without taking into account the spatial distribution of the pollutants.

In this paper, motivated by the need of a computationally efficient learning technique to adequately estimate the spatial distribution of air pollutants using a dispersion model, particularly in dealing with the complex problem of the *spatial distribution* of ozone level across a region, we propose a metamodel with an enhanced radial basis function neural network (RBFNN) for improvements of the estimation accuracy. Here, neural networks and the well-adopted air pollution-chemical transport model are integrated to reduce the complexity of the spatial predictions and also to improve reliability via verification with measurement data collected at local monitoring stations. The contribution of our paper is thus twofold with developments of (i) an enhanced RBFNN whose centres, network weights and spread parameters are selected respectively from the integration of the weighted least squares, generalised cross validation, and a reasonably small choice of the standard deviation range, (ii) a metamodel using the proposed RBFNN to provide improved and reliable estimations of the ozone concentration profile distributed spatially over a region.

The remainder of this paper is organised as follows. After the introduction, algorithms for performance enhancement of radial basis function neural networks are developed. The proposed metamodel is then applied to the spatial distribution estimation of ozone as described in Section 3. Section 4 presents the results and discussion for the case study of the Sydney basin in Australia. A conclusion is drawn in the final section, followed by an appendix.

2. Development of RBFNN metamodel

The development of computer models that can be useful for modelling a predefined class of complex systems, or metamodelling, has been subject to intensive research since the last decade. Its objectives are to reduce the cost, time, and amount of effort required during the simulation of intricate processes [16]. Substantial results from the existing works illustrate that using metamodels to locate an optimum solution is often sufficiently accurate in many applications requiring prediction, optimisation and validation. Data-driven methods such as kriging [17], splines [18], support vector regression [19], self-organising maps [20], cluster reinforcement [21], and neural networks [22] are usual methods for metamodelling in complex system identification and pattern recognition. In this paper, the RBFNN is adopted, making use of such advantages [23] as good accuracy, simplicity, high robustness and efficiency, sample sizes, and capability of dealing with different problem types.

2.1. Overview of radial basis function neural networks

The main architecture of the RBFNN consists of three layers: an input layer, a single hidden layer, and an output layer. The neurons in the hidden layer implement a radially activated function to perform a non-linear transformation of input data to approximate output data. There are three common forms of basis functions used in RBFNN, namely Gaussian, multiquadratic and thin plate spline [24]. The Gaussian one is most popular owing to its flexibility of adjusting the function position and shape via the spread parameter. The general output of a Gaussian RBFNN with l inputs, and m outputs which respond to the input vector $x \in \Re^l$ is mathematically represented as

$$\hat{y}_j = f_j(x) = \sum_{k=1}^{N} w_{jk}\phi_k(\|x - c_k\|, \sigma_k), \quad j = 1, 2, \ldots m, \tag{1}$$

where j is the output index, w_{jk} are weights in the output layer, $\phi_k(\cdot)$ is a basis function, $\|\cdot\|$ denotes the Euclidean norm, N is the number of neurons (and centres) in the hidden layer, $c_k \in \Re^l$ is the network centre in the input vector space, and σ_k is the spread parameter for each basis function. With a given number of data samples, the outputs can be evaluated in correspondence to the training patterns according to the following equation:

$$F = \Phi^T W, \tag{2}$$

where F is the $n \times m$ matrix of the network output, Φ is the $N \times n$ matrix of hidden nodes, $W = [w_{jk}]^T$ is the $N \times m$ matrix of network weights, and n is the number of data samples.

For a Gaussian function based RBFNN, the training algorithm involves three main parameters to be set in order to minimise a suitable cost function, namely the centre, the width (i.e., spread), and the network weights. Training strategies can be grouped into two classes: fully supervised training (see, e.g., [25]), and two-stage training (see, e.g., [26]). Supervised training may lead to optimal estimation of the parameters. However, it typically involves the gradient descent method [27], which is computationally expensive. For the latter, the first stage involves the determination of the basis function centres and widths [28], followed by the determination of the output weights in the next stage [29], or a generalised technique [30] is used for growing and pruning radial basis functions.

2.2. Approach for selection of radial basis centres

Among the first methods for the selection of basis centres was the work introduced in [31], employing the subset of the input training data selected randomly. In later approaches, the centres are obtained via a clustering process such as the k-means algorithm or by using the genetic algorithm and fuzzy logic (see, e.g., [32,33]). A more systematic way is via the supervised selection or also known as the forward selection (FS), in which the orthogonal least square (OLS) algorithm is commonly used [26].

Here, we introduce a basis centre selection method which is the integration of the FS method proposed in [28] with the weighted least square (WLS) theory to cope with unequal variances of the observation, as in the case of meteorological data. Typically, a regression of scattered large data of complex systems contains non-constant variances across all data points as of unequal scatter or heteroskedasticity. This is because some observations are known to be less reliable than others in many practical applications. To solve the heteroskedasticity problem, the weighted least squares (WLS) method is more preferable [34] as it outperforms other methods in the ability to handle regression situations in which the data points are of varying quality. For example, in [35], WLS was used to couple with support vector machines to achieve robust estimation. A two-stage WLS regression approach is proposed in [36], to estimate the coefficients of autoregressive with exogenous input models for prediction of hourly cooling-load forecasting with good performance. In this paper, to improve the learning strategy as described earlier in [37], a procedure for selection of the network centres is suggested by considering the regularisation theory, namely regularised and weighted least squares. Moreover, to deal with the ill-posed problem, the learning process is accelerated by making use of the Gram matrix [38]. Apart from that, appropriate ways to estimate several parameters in RBFNN including the network output weights, the least squares weighting factor, the regularisation parameter and the spread parameter are also adopted, in Sections 2.3 and 2.4.

A general objective function for the regularised least squares [39], with the input matrix A and weighting factors H, takes the following form:

$$J(z) = \|Az - b\|^2_{H_b} + \|(z - z_0)\|^2_{H_z}, \tag{3}$$

where the first term corresponds to the original cost function due to the residual error between the estimated output, Az, and the desired output, b, the second term is for regularisation to take into