



Development of missing data prediction model for carbon monoxide

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Abstract

DUERBRLGELVRIWKARVWLPSRUWDSROOXWDDVVLHHLVVBFBWIRU\$,FDOFXODWLRQ
7KHHRULWLVSDUDPRXQWRXUWKDWWKHVPLVVLQDWDRI2GXULWKEDQVVL7KHBUH
DPEHVRIFFXUUEMVKDWPDFRWULEXWMMR WKRLVVLGDWDSUREOPV VXFKDVLQELOLWRIWKH
LQWUXPWR UFRUG FHWDLSDUDPWHV, QRI WKLVIDFW D 2SUBLFWLRQRGB BV WR EH
GMRBWRDGGUMVWKLVSUREOPGDWDVWRIPWRURORIFDODQDLUSROOXWDDVVOXVREWDLG
IURPWKHU4XDOLWLVLRSDUWPWRIRUREB0DODVLD2WRWDORIGDWDVWV
2XVBRGMRSWKFRGBXVLQDLWLWDDQVVL6B/KURXKDUWLILFLDORUDOWZUN\$1
6\$KRB SDUWLFXODWRDWWH30 DQRR2 2WKRRVWLQFLDWLQXW DULDEOMIRU
PLVVLQDWDSUBLFWLRQRGBRI27KUHGGGMMWKRSLPXP2PEHWRGMRSWKH
\$1 PRGB ZWK WKDQXRI5 EXDO WR %RWK PRGBV DUWLILFLDORUDOWZUNFDUERQ
PRQLGBOO SDUDPWHV \$12\$ DQ DUWLILFLDORUDOWZUNFDUERQRRLGGBNRXW
\$122VKRB KLBQXRI5 DQ DQOR2OXRI506DQ
UMSFWL27YKMBQXMLQLFDWBSWKDWWKFRGBVPLKWRQFRSORKARVWVLQFLDW
LQXW DULDEOMWRUBUMWKBUDWKHVKDQVLDQOOLQXW DULDEOM

Keywords: 3UBLFWLRQRGBFDUERBRLGSDODVLDVQLWLWDDQVVLPLVVLQDWDPRGB
3BELW8703UMVSOULKWVUMHB

INTRODUCTION

Air pollution imposes severe environmental challenges as well as prominent health risks to human (Najafpoor *et al.*, 2014). The worst air pollution problem usually takes place at urban areas of both developed and developing countries (Hassanzadeh *et al.*, 2009) which indirectly affects the quality of life as well as public health. Air pollutions are mostly produced by natural activities such as volcano eruptions and human activities, owing to the industrial processes, production of energy from power plants, residential heating and open burning (Najafpoor *et al.*, 2014; Afroz *et al.*, 2003). In addition, the fuel burning vehicles in urban area have worsened the air quality (Wang & Lu, 2006). Consequently, the human health and environment may be affected by the air pollution and in the long term, air pollution has a tendency to intensify the threats to earth.

Incomplete combustion of hydrocarbons contributes to the presence of carbon monoxide (CO) (Levy, 2015), which associated to cardiovascular diseases, daily mortality and morbidity (Chen *et al.*, 2011). In a homogeneous environment, air pollutant levels including CO at each fixed monitoring stations are indicated by the applied measurements. Nevertheless, the dispersion of the actual pollutant contents is still unknown, owing to substantial influences of the prevailing conditions of dispersion, emission sources distribution and the region topography (Zoroufchi & Fatehifar, 2015) and thus, affecting the exact concentrations of the measured air pollutants.

Besides PM₁₀, the development of CO missing data prediction model is important due to the fact that this pollutant is one of the leading contributors to the air pollutants and produced from most of the sites (Azid *et al.*, 2016 & Mohamad *et al.*, 2015). According to Awang *et al.*, (2015) PM₁₀ and CO are being grouped into the same component,

indicating that CO is as important as PM₁₀ and may come from the same sources since it is being grouped together with PM₁₀.

Missing data is a common occurrence in air pollution studies. Failure of equipment and anomalous measurement are the reasons for this missing data (Chen *et al.*, 2016). Researchers are opted to remove the missing data prior to statistical analysis. However, this action can reduce the data size. The data becomes unrepresentative with the removal of massive missing data and subsequently, unreliable result will be produced. Hence, imputing the missing values can be the alternative way to evade unreliable or ravage result on the statistical interpretation.

In general, single and multiple imputation methods are the acceptable approaches to generate complete information matrices (Little & Rubin, 1987). One value for each missing one is specifically filled in the former method. For the multiple-imputation, simulated values for each missing data are generated to appropriately determine the uncertainty of the missing data (Junninen *et al.*, 2004) using expectation maximization based (EM) algorithm. Other algorithms are also applicable; however, EM algorithm possesses unique features such as simplicity, power, rapidity (Honaker *et al.*, 2011) and practicality in forecasting the missing air quality data using ANN model.

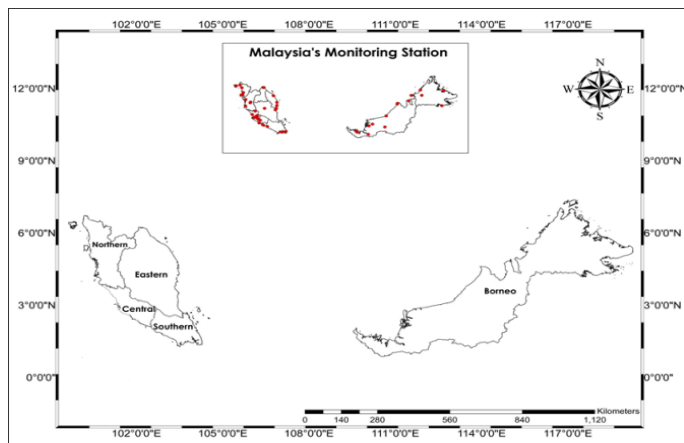
ANN is a non-linear model (Kukkonen *et al.*, 2003) and has been acknowledged as a cost-effective model (Azid *et al.*, 2014) since it is able to discover and ascertain patterns (Zare, 2014), solve complex functions and produce reliable air pollutants prediction. This model can be utilized to assist forthcoming planning with the presence of missing data during the air monitoring, mend air quality management system (Kumar & Goyal, 2011). Besides air quality, ANN model has also been applied for the water quality studies. (Zali *et al.*, 2011) used ANN for

the water quality index (WQI) prediction for Kinta River, Malaysia. Besides that, (Nasir et al., 2011) also applied ANN in their study for WQI prediction model in Juru River, Malaysia.

EXPERIMENTAL

Study area

There are 52 continuous monitoring stations (N06° 25.424' E100° 20.880' to N04° 15.016' E117° 56.166') for ambient air quality throughout Malaysia (Fig. 1). These stations were chosen due to the desired locations in urban, suburban, and industrial area (Azid et al., 2015).



Source: (Kanniah et al., 2016; DOE, 2004)

Fig. 1

Data collection

The air pollutants and meteorological data were obtained from the Air Quality Division, Department of Environment (DOE) Malaysia. The obtained data in this study was entailed daily average observations for most of air pollutants (PM₁₀, NO₂, CO, O₃, NO, NO_x, THC, CH₄, NmHC, SO₂) and meteorological conditions (wind direction, wind speed, temperature, humidity, UVB) from 2010 until 2015. These variables were independently analysed at each monitoring stations. The model equipments for continuously monitoring program (CAQM) on each atmospheric pollutants and meteorological parameters were listed in Table 1.

Variables selection

The best input variables for the CO missing data modelling were selected prior to the designing of the model. Input nodes in ANN were based on the selected input variables, which significantly contributing to the process of forecasting. In addition, high numbers of input could cause reduction of training speed, over-fitting, redundancy and noise variables (Ababneh et al., 2014). Thus, only selected input variables were used for ANN analysis.

One of the methods to select the best input variables for the prediction of CO missing data modelling using ANN model was by applying sensitivity analysis (SA). This method used “leave-one-out” technique to rank the importances of the model input variables by considering their influences on the unpredictability of the model output (Manache & Melching, 2008). This method was carried out manually whereby one-by-one parameters were removed. The R² values of each leave one out parameters were applied to show the differences of R². The percentage (%) contribution of the parameters was determined by applying Equation 1:

$$\% \text{ contribution} = \left(\frac{b_i - a_i}{z_i} \right) 100 \quad (1)$$

where:

a_i = the value of R² after a leave-one-out parameter for each model

b_i = the reference value of R² from ANN-CO-AP

z_i = the sum value of difference R²

SA has been used in various fields of environmental studies. For instance, it has been used by (Latif et al., 2014) in their study to investigate the important level of each inputs (CO, NO, NO₂, NO_x, O₃, PM₁₀, SO₂, THC, CH₄ and NmHC) on the output (vehicles). Meanwhile, (Asadollahfardi et al., 2016) applied SA to determine which of the input variables have a great role in predicting ground layer of O₃ where in their study, the maximum and minimum roles for ground-level O₃ concentration prediction are PM_{2.5} and benzene, respectively. On top of that, research done by (Rahimi, 2017) also applied SA in prediction of NO₂ and NO_x by calculating important level of input variables in prediction.

Table 1

Parameter	Model equipment
3DUWLFXODW6DWWU30	%0%WD0W0DWRQ
:LQ6S6:6NPKU	0W20
:LQLUFWLR0	0W20
5U7F5HDWXU0	0W20
50DWLWPLGLW5+	0W20
2LGMR11LWUR025SP	70000R0000
1LWUR0R0LGH2SSP	70000R0000
80WUDKROWE00 KU	
0WK00 SSP	70000
10WK00URFDUERQ	70000
1P00SP	
7RWDO0URFDUERQ0SP	70000
6XOSKXULR0GH2 SSP	70000R0000
1LWUR0R0LGH2 SSP	70000R0000
2R0 SSP	70000R0000
0UER0R0LGH0SP	70000R0000

Data pre-processing

Analysis, filtration and transformation were implemented to organize the obtained data set for the model development. There were a few missing data and outliers observed which might be resulted due to technical failure (Zakaria & Noor, 2018) and incorrect recorded results during the data collections. The outliers should not be deleted because they might give true measurements (Burke, 1999). Moreover, in air pollution modelling, it was important to use whole year data by considering the full coverage variation of the seasonal pollutant levels and meteorological parameters (Arhami et al., 2013).

In this study, the missing data was replaced by using the EMB (expectation-maximization with bootstrapping) algorithm. Likelihood observed data was represented as shown in Equation 2:

$$p(D^{obs}, M|\theta) = p(M|D^{obs})p(D^{obs}|\theta) \quad (2)$$

With D^{obs} and M were known as observed data and missingness matrix, respectively. While, likelihood was written as Equation 3 if only complete data parameters were concerned:

$$L = (\theta|D^{obs}) \propto p(D^{obs}|\theta) \quad (3)$$

While, equation could be rewrite as Equation 4 based on the iterated expectations law:

$$p(D^{obs}|\theta) = \int p(D|\theta) dD^{mis} \tag{4}$$

The posterior with this likelihood and a flat prior on θ as shown in Equation 5:

$$p(\theta|D^{obs}) \propto p(D^{obs}|\theta) = \int p(D|\theta) dD^{mis} \tag{5}$$

Table 2 illustrates the statistical measurements for selected meteorological and air pollutant variables (after SA) for the modelling of CO missing data using ANN.

Table 2 MFULSWLMRUPDWLRUVBFWBULDEOMIRUPRGEOLB 2PLVVLQDWD

Variables	Min	Max	Mean
2 SSP			
30 $\mu\text{g}/\text{m}^3$			

The best input variables were used in prediction, evaluation and validation processes of the ANN technique. However, prior to these processes, the data variables were normalized by employing scaling range of (-1,1) to increase training speed, minimize variable values differences and reduce computational problems (Srinivasan et al., 1994). The hyperbolic tangent function was used to transform value to be between -1 and 1, for normalization (JMP, 2012) with the formula of the hyperbolic tangent function as shown in equation 6:

$$\text{Hyperbolic tangent function} = \frac{e^{2x}-1}{e^{2x}+1} \tag{6}$$

In addition, data normalization within range output of activation function of ANN output layer was necessary when using non-linear activation function (Zhang et al., 1998). Studies revealed that only small errors of prediction were produced when applying the hyperbolic tangent function as compared to the sigmoid (logistic) transfer function (Chaloulakou et al., 2003).

It was crucial to select the optimum number of nodes in hidden layer since high number of nodes might result in overfitting (He et al., 2014) while less number of nodes might not adequately capture the information. The proposed equation was to determine the appropriate number of nodes ranges (Fletcher & Goss, 1993) as shown Equation 7:

$$\text{Number of nodes ranges} = 2S^{\frac{1}{2}} - O \text{ to } 2S - 1 \tag{7}$$

where, S is the number of input nodes and O is the number of output nodes.

Prediction, evaluation and validation of ANN model

The system predicted missing data of CO with the input selection used in ANN was based on the results of SA. To determine the error in predicting the concentration of CO and models performance evaluation, a Root Mean Squared Error (RMSE) which indicated in Equation 8 was applied:

$$\text{RMSE} = \sqrt{\frac{1}{n} \sum_{t=1}^n (O_t - P_t)^2} \tag{8}$$

Meanwhile, model validity was illustrated by applying coefficient of determination (R^2) between observations and predicted as shown in Equation 9:

$$R^2 = 1 - \left(\sum_{t=1}^n \frac{(O_t - P_t)^2}{(O_t - \bar{O})^2} \right) \tag{9}$$

where, O_t , P_t and \bar{O} represent observed value, predicted value and observed mean value of CO concentrations at time, t respectively, a n is the number of data (Ahmat et al., 2015).

RESULTS AND DISCUSSION

Table 3 shows the SA results for the prediction of CO. From the result, different values R^2 exhibited different parameter values that affected the prediction of CO. The % contribution > 10% indicated strong contribution towards the CO presence (Azid et al., 2016). The highest and lowest influences of input variable were PM_{10} and WD with % contribution of 35.95% and 0.92%, respectively.

Based on the R^2 and % contribution in Table 3, the most important input variables were ranked as $PM_{10} > O_3 > NO_2 > SO_2 > NO_x > CH_4 > \text{Temp} > NO > \text{Humidity} > \text{THC} > \text{WS} > \text{UVB} > \text{NmHC} > \text{WD}$ with PM_{10} and O_3 became the main contributors to the CO presence in this study.

Studies on SA shown that air pollutants rendered a strong influence on the climate daily variability (Ababneh et al., 2014). This finding was supported by SA study on the air pollution index (API) which was found that PM_{10} and CO were the main contributors to the air pollutants (Azid et al., 2016). In the Southeast Asia including Malaysia, these pollutants have been acknowledged as significant atmospheric pollutants in major cities and were produced by complete combustion of motor vehicles as well as various industrial practices (Latif et al., 2011; Mustafa et al., 2012). Beside of PM_{10} , O_3 was also correlated to CO since the letter was originated from diesel fuel (Rani et al., 2017) and mobile sources, causing it to become secondary contributor to ozone depletion (Kumar et al., 2017).

Table 3 MLWLKWDQOVLVIRUVBFWBLSXWULDEOMIRU& SUBLFWBPRGE

Model	R^2	Difference, R^2	% Contribution
\$12\$	0.7639		
\$1/30	0.6618	0.1021	35.95
\$1/2	0.6784	0.0855	30.11
\$1/12			
\$1/62			
\$1/12			
\$1/&			
\$1/703			
\$1/12			
\$15+			
\$1/7&			
\$1/6			
\$1/89%			
\$1/10&			
\$1/:'			
7RWDO	0.2839		100.00

Table 4 shows the R^2 and RMSE values for ANN with a hidden layer and different number of hidden nodes. Based on two main input variables obtained from SA, the most appropriate number of hidden nodes was between 1 to 3. Among these hidden nodes, three hidden nodes exhibited the highest R^2 and the lowest RMSE. Higher value of R^2 indicated a closer relation between predicted output value and the exact output value. Moreover, the three hidden nodes have lower RMSE value compared to other hidden nodes where the nearest RMSE value to 0 was indicated to the best ANN model performance (Ababneh et al., 2014). Thus, three hidden nodes were considered as the optimum number for the ANN model.

Post ANN-model prediction step, model evaluation and validation were carried out to evaluate the ability of ANN in the prediction process. In Table 5, ANN-CO-AP (14 variables) and ANN-CO-LO (using PM₁₀ and O₃) prediction models showed RMSE (0.2482 and 0.3506) and R² (0.7639 and 0.5311) respectively. The nearest RMSE value to 0 and R² to 1 were indicated to the best ANN model performance and model robustness (Zali et al., 2011), as well as provided the highest accuracy between predicted and actual output values (Ababneh et al., 2014). ANN-CO-LO was considered as the optimum model as it used fewer input variables (PM₁₀ and O₃) although the model exhibited lower R² (0.5311) and higher RMSE (0.3506). Moreover, more input data would lead to better predictions (Esfandani & Nematzadeh, 2016). Thus, by reducing the input variables, R² value would become lower.

Table 4 RMSE and R² values for ANN models with different numbers of hidden nodes

No. of hidden nodes	R ²	RMSE
3	0.5311	0.3506
4	0.7639	0.2482
5	0.7639	0.2482
6	0.7639	0.2482
7	0.7639	0.2482
8	0.7639	0.2482
9	0.7639	0.2482
10	0.7639	0.2482
11	0.7639	0.2482
12	0.7639	0.2482
13	0.7639	0.2482
14	0.7639	0.2482

Table 5 RMSE and R² values for ANN models with different numbers of hidden nodes and input variables

Models	Model evaluation	Model validation
	RMSE	R ²
ANN-CO-AP (14 variables)	0.2482	0.7639
ANN-CO-LO (PM ₁₀ and O ₃)	0.3506	0.5311

¹All input variables were employed in ANN model.
²PM₁₀ and O₃ input variables were employed in ANN model.
From the developed model, the ANN-CO-LO model equation could be interpreted as in Equation 10:

$$\text{Predicted CO} = -0.23 + (-1.85 \times H1) + (-0.43 \times H2) + (9.19 \times H3) \quad (10)$$



CONCLUSION

In conclusion, only selected input variables were used to generate a model for missing CO data. By using SA, the number of input variables could be reduced based on their significant values to the presence of CO. In this study, the most significant input variables were PM₁₀ and O₃. In addition to the selection of input variables, the selection number of hidden nodes was also vital to ensure the obtained results were not over fitting and only captured sufficient information. The optimum number of hidden nodes for this study was three, which exhibited had the highest R² (0.5311) and the lowest RMSE (0.3506) values as compared to other hidden nodes. Research done by Esfandani & Nematzadeh (2016) showed that greater input number would give better prediction. Thus, by decreasing the input number by using less number of input variables, ANN-CO-LO model (used input variables PM₁₀ and O₃) gave lower R² value compared to ANN-CO-AP which used all input variables (14 parameters). Although ANN-CO-LO model gave lower R² value compared to ANN-CO-AP R² value, ANN-CO-LO

model still possessed better performance with good R² value (R² = 0.5311). On top of that, the reductions of air quality parameters was much applicable for air resource management because of its time and cost of operation. Hence, the ANN-CO-LO model could be utilized in predicting missing CO data.

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