MJFAS MALAYSIAN JOURNAL OF FUNDAMENTAL AND APPLIED SCIENCES
PRINT ISSN: 2289-5981 | ONLINE ISSN: 2289-599X

RESEARCH ARTICLE

Development of missing data prediction model for carbon monoxide

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Article history
Received 17 January 2018
Revised 22 March 2018
Accepted 20 May 2018
Published Online 4 February 2018

Abstract

Carbon monoxide (CO) is one of the most important pollutants since it is selected for API calculation. Therefore, it is paramount to ensure that there is no missing data of CO during the analysis. There are numbers of occurrences that may contribute to the missing data problems such as inability of the instrument to record certain parameters. In view of this fact, a CO prediction model needs to be developed to address this problem. A dataset of meteorological and air pollutants value was obtained from the Air Quality Division, Department of Environment Malaysia (DOE). A total of 113112 datasets were used to develop the model using sensitivity analysis (SA) through artificial neural network (ANN). SA showed particulate matter (PM_{10}) and ozone (O_3) were the most significant input variables for missing data prediction model of CO. Three hidden nodes were the optimum number to develop the ANN model with the value of R^2 equal to 0.5311. Both models (artificial neural network-carbon monoxide-all parameters (ANN-CO-AP) and artificial neural network-carbon monoxide-leave out (ANN-CO-LO)) showed high value of R^2 (0.7639 and 0.5311) and low value of RMSE (0.2482 and 0.3506), respectively. These values indicated that the models might only employ the most significant input variables to represent the CO rather than using all input variables.

***Keywords*:** Prediction model, carbon monoxide, Malaysia, sensitivity analysis, missing data model

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 PM_{10}, 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) PM_{10} and CO are being grouped into the same component, indicating that CO is as important as PM_{10} and may come from the same sources since it is being grouped together with PM_{10}.

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.

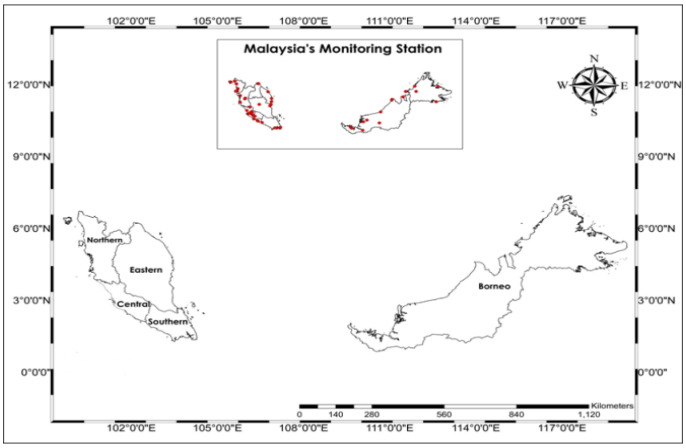
In general, single and multiple imputation methods are the acceptable approaches to generate complete information matrices (Little & Rubin, 1987). One value for each missing one is specifically filled in the former method. For the multiple-imputation, simulated values for each missing data are generated to appropriately determine the uncertainty of the missing data (Junninen *et al*., 2004) using expectation maximization based (EMB) algorithm. Other algorithms are also applicable; however, EMB 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 Continuous ambient air quality monitoring stations in Malaysia.

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 (PM_{10}, NO_2, CO, O_3, NO, NO_x, THC, CH_4, NmHC, SO_2) 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 continuousl~~y~~ 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 R^2 values of each leave one out parameters were applied to show the differences of R^2. The percentage (%) contribution of the parameters was determined by applying Equation 1:

$$\%\, \boldsymbol{contribution} = \left(\frac{b_i - a_i}{z_i}\right) \mathbf{100} \tag{1}$$

where:
ai = the value of R^2 after a leave-one-out parameter for each model
bi = the reference value of R^2 from ANN-CO-AP
zi = the sum value of difference R^2

SA has been used in various fields of environmental studies. For instance, it has been used by (Latif *et a*l., 2014) in their study to investigate the important level of each inputs (CO, NO, NO_2, NO_x, O_3, PM_{10}, SO_2, THC, CH_4 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 O_3 where in their study, the maximum and minimum roles for ground-level O_3 concentration prediction are $PM_{2.5}$ and benzene, respectively. On top of that, research done by (Rahimi, 2017) also applied SA in prediction of NO_2 and NO_X by calculating important level of input variables in prediction.

Table 1 The CAQM model equipment for each parameter.

Parameter	Model equipment
Particulate Matter (PM_{10}), μg/m^3	BAM-1020 Beta Attenuation
Wind Speed (WS), km/hr	Met One 010C
Wind Direction (WD), ˚	Met One 010C
Air Temperature (AT), ˚C	Met One 062
Relative Humidity (RH), %	Met One 083D
Oxides of Nitrogen (NOx), ppm	Teledyne API Model 200A/200E
Nitrogen Monoxide (NO), ppm	Teledyne API Model 200A/200E
Ultraviolet-b (UV_b), J/m^{2}hr	
Methane (CH_4), ppm	Teledyne API M4020
Non-methane Hydrocarbon (NmHC), ppm	Teledyne API M4020
Total Hydrocarbon (THC), ppm	Teledyne API M4020
Sulphur Dioxide (SO_2), ppm	Teledyne API Model 100A/100E
Nitrogen Dioxide (NO_2), ppm	Teledyne API Model 200A/200E
Ozone (O_3), ppm	Teledyne API Model 400/400E
Carbon Monoxide (CO), ppm	Teledyne API Model 300/300E

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:

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

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:

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

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

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

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

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

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 Descriptive information for selected variables for modelling of CO missing data.

Variables	Min	Max	Mean
O_3 (ppm)	0	0.2	0.03
PM_{10} (**μg/m³**)	0	763	49.68

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:

$$Hyperbolic\ tangent\ function = \frac{e^{2x}-1}{e^{2x}+1} \quad (6)$$

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:

$$Number\ of\ nodes\ ranges = 2S^{\frac{1}{2}} - O\ \ to\ \ 2S - 1 \quad (7)$$

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:

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

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

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

where, $\mathbf{O_t}$, $\mathbf{P_t}$ and ō 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 $PM_{10} > O_3 > NO_2 > SO_2 > NO_x > CH_4$ > Temp > NO > Humidity > THC > WS > UVB > NmHC > 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 Sensitivity analysis for selected input variables for CO predicted model.

Model	R^2	Difference, R^2	% Contribution
ANN-CO-AP	**0.7639**		
ANN-LPM$_{10}$	**0.6618**	**0.1021**	**35.95**
ANN-LO$_3$	**0.6784**	**0.0855**	**30.11**
ANN-LNO$_2$	0.7511	0.0128	4.50
ANN-LSO$_2$	0.7515	0.0124	4.36
ANN-LNO$_X$	0.7519	0.0120	4.21
ANN-LCH$_4$	0.7542	0.0097	3.41
ANN-LTEMP	0.7543	0.0096	3.37
ANN-LNO	0.7544	0.0095	3.35
ANN-RH	0.7545	0.0094	3.30
ANN-LTHC	0.7577	0.0061	2.17
ANN--LWS	0.7584	0.0054	1.92
ANN-LUVB	0.7601	0.0038	1.33
ANN-LNMHC	0.7607	0.0031	1.11
ANN-LWD	0.7613	0.0026	0.92
Total		**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 PM_{10} and O_3) prediction models showed RMSE (0.2482 and 0.3506) and R^2 (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 (PM_{10} and O_3) although the model exhibited lower R^2 (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, R^2 value would become lower.

Table 4 The coefficient of determination (R^2) and error value (RMSE) for the ANN with a hidden layer and different number of hidden nodes.

No. of hidden nodes	R^2	RMSE
1	0.4188227	0.3893862
2	0.5257966	0.3546468
3	0.5311124	0.3506089

Table 5 Model evaluation and model validation for the different CO. prediction models

	Models	Model evaluation	Model validation
		RMSE	R^2
1	ANN-CO-AP[1]	0.2482	0.7639
2	ANN-CO-LO[2]	0.3506	0.5311

[1]All input variables were employed in ANN model.
[2]PM_{10} and O_3 input variables were employed in ANN model.

From the developed model, the ANN-CO-LO model equation could be interpreted as in Equation 10:

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

Where;
H1= tanh [0.5 x ((-116.80 x O3) + (0.0075 x PM10) - 0.86)]
H2= tanh [0.5 x ((202.84 x O3) + (-0.026 x PM10) -1.81)]
H3 = tanh [0.5 x ((0.70 x O3) + (0.0016 x PM10) - 0.19)]

Based on this formula, the predicting CO missing data could be evaluated and validated efficiently.

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 PM_{10} and O_3. 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 h~~ad~~ the highest R^2 (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 PM_{10} and O_3) gave lower R^2 value compared to ANN-CO-AP which used all input variables (14 parameters). Although ANN-CO-LO model gave lower R^2 value compared to ANN-CO-AP R^2 value, ANN-CO-LO model still possessed better performance with good R^2 value (R^2 = 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.

ACKNOWLEDGEMENT

This manuscript has been funded through University Research Fund (Grant no.: UniSZA/2016/DPU/01) and Research Initiative Grant (RIGS16-363-0527) of International Islamic University Malaysia, Gombak, Selangor, Malaysia.

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