Benzene Prediction: A Comparative Study of ANFIS, LSTM and MLR

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Abstract: It is generally recognized that road traffic emissions are a major health risk and responsible for a substantial share of death and disease in Europe. Although artificial intelligence methods have been used extensively for air pollution forecasting, there is little research on benzene prediction and the use of long short-term memory networks. Benzene is considered one of the pollutants of greatest concern in urban areas and has been linked to leukemia. This paper investigates the predictive power of adaptive neuro-fuzzy inference systems, long short-term memory networks and multiple linear regression models for one hour ahead benzene prediction in the city of Augsburg, Germany. The results of the analysis indicate that adaptive neuro-fuzzy inference systems have the best in sample performance for benzene prediction, whereas long short-term memory networks and multiple linear regressions show similar predictive power. However, long short-term memory models have the best out of sample performance for one hour ahead benzene prediction. This supports the use of long short-term memory networks for benzene prediction in real emission forecasting applications.

1 INTRODUCTION

Recently, the European Environment Agency (EEA, 2020) announced that the single largest environmental health risk and a major cause of premature death and disease in Europe is air pollution. In urban areas, road transport is the main contributor to emissions of nitrogen dioxide (NO_2) and benzene (C_6H_6) (for a discussion see Krzyzanowski et al., 2005). Other traffic related air pollutants include e.g. carbon monoxide (CO), nitrogen monoxide (NO), ozone (O_3) and particu-late matter (PM10, PM2.5). Thus, traffic induced air pollution is still a serious issue in many large cities.

Heart disease, stroke, lung diseases and lung cancer are the most common reasons for premature death attributable to air pollution (European Environment Agency, 2020). According to Künzli et al. (2000) air pollution is responsible for more than 5% of deaths in Europe and half of this can be attributed to motor vehicles. Overall, European air quality has improved in recent years, but is still too high (The Lancet Commission, 2017). Consequently, there is a need for air quality management and for tools to quantify the effects of proposed and implemented measures (European Environment Agency, 2019).

Benzene is considered one of the pollutants of most concern in urban areas that is associated with various diseases (De Donno et al., 2018 and Smith, 2010). Benzene is included in the gasoline for motor vehicles. For instance, when a car is refuelled, benzene evaporates from the tank of the car and an aromatic odour can be perceived. However, the escape of benzene during refuelling has been solved in recent years by "gas displacement". Nevertheless, the main part of the pollution is due to road traffic. Benzene is a component of the escaping exhaust gases from the tailpipe (German Federal Environment Agency, 2021).

In June 2021 the Court of Justice of the European Union ruled that Germany has breached EU laws by failing to limit poor air quality. The European Commission accused German authorities of not taking enough action to comply with EU air pollution limits

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and the Court of Justice of the European Union now confirmed this appraisal (Court of Justice of the European Union, 2021). In order to limit traffic induced air pollution, it is necessary to implement good forecasting tools. With the ability to predict air pollution in advance, traffic management systems can limit exhausts by limiting access of motor vehicles to city centres. For this reason, the present research work investigates which machine learning algorithms are particularly well suited for the prediction of benzene, as one of the most toxic exhaust gases in road traffic. The results here should be of interest to academic and traffic management authority alike who are concerned with reducing air pollution by traffic control based on accurate forecasting.

Artificial intelligence (AI) has been one of the advanced tools for modelling and forecasting air quality. For instance, Kaur et al. (2020) applied four different artificial neural networks (ANN) to predict PM2.5 concentration at hotspots in the city of Delhi. The authors conclude that ANNs are well suited for PM2.5 prediction and that the non-linear autoregressive network with exogenous input (NARX) outperforms other ANNs in step ahead prediction. Similarly, Sayeed et al. (2020) makes use of a deep convolutional neural network (CNN) to predict ozone concentration. The model predicts ozone concentration 24 hours in advance with great accuracy and according to the authors, might be used as an early warning system for individuals susceptible to ozone. Further examples of successful ANNs applications for air quality forecasting include Molina-Cabello (2019) and Pawlak (2019).

In contrast, Ly et al. (2019) apply an adaptive neuro-fuzzy inference system to predict NO_2 and CO from multisensor and weather data in an unnamed Italian city. They show that combining multioutput sensor data with ANFIS techniques offers a powerful way to model nonlinear processes such as air quality. Others that have concluded that ANFIS models are well suited for air pollution prediction include Ausati et al. (2016), Mihalache et al. (2016), Oprea et al. (2017) and Humpe et al. (2021).

Furthermore, decision tree methods have been used to forecast air pollution by inter alias Loya et al. (2012) or Lee et al. (2019). Overall, it has been concluded that decision trees are quite helpful to illustrate dependencies, but not particularly accurate in forecasting compared to other methods.

More recently, long short-term memory networks (LSTM) have been applied to pollution forecasting. For instance, Bai et al. (2019) has used LSTM for hourly PM2.5 concentration forecasting. Similarly, Chang et al. (2020) apply LSTM models for forecasting various air pollutants. Generally, the literature on the use of LSTM models for forecasting road traffic emissions is rather limited. In contrast to standard recurrent neural networks (RNN) the long short-term memory network (LSTM) considers both, the short-term as well as long-term dependency of a time series. Thus it has the advantage that it exhibits temporal dynamic behaviour for a time sequences (Greff et al., 2016). As emissions are characterised by dynamic behaviour, LSTM networks might be particularly useful in emission forecasting.

Furthermore, benzene forecasting research is also underrepresented although benzene is considered one of the pollutants of most concern in urban areas and can be associated with acute myeloid leukemia, myelodysplastic syndromes and lymphoma and childhood leukemia (De Donno et al., 2018 and Smith, 2010). An exception to this is Karakitsios et al. (2006) who predicted benzene concentration in a street canyon using artificial neural networks. This paper adds to the literature by analysing benzene concentration in the German city Augsburg and applying LSTM networks. The results are expected to contribute to a better understanding of benzene air pollution in the future. This in turn might be used in traffic regulation to improve air quality in cities and towns.

In a related article, Humpe et al. (2021) investigate air pollution in Munich with a similar data set and methodology. However, benzene as one of the most worrisome pollutants is not measured and recorded for the city of Munich. This article therefore extends the study by analysing another hazardous traffic pollutant that has been recorded for the city of Augsburg. Furthermore, in comparison to the earlier study this article includes LSTM networks that might be particularly suited to forecast out of sample benzene concentration due to their ability to forget part of its previously stored memory and at the same time also add a part of new information.

2 MATERIAL

This research used hourly data of benzene, road traffic, and meteorological data from Augsburg, Germany. The city of Augsburg is located in the southwest of Bavaria and is the third largest city in Bavaria (after Munich and Nuremberg) with almost 300.000 inhabitants.

The overall dataset for our study covers the period between 01.01.2014 and 31.12.2018 with a total of 43,824 hours of data. Traffic data for two major access roads to the city of Augsburg was provided by the German Federal Roads Agency (Bundesanstalt für

Straßenwesen)[1]. These motorways (A8 – Augsburg Ost and A8 – Augsburg West) use automatic traffic counting systems to register all vehicles. The benzene (C_6H_6) concentration in the city of Augsburg was collected from the Bavarian State Office for the Environment (Bayerisches Landesamt für Umwelt)[2] and is reported in µg/m^3. Finally, temperature, precipitation, relative humidity, sunshine duration, wind speed and wind direction were available from the German Meteorological Service (Deutscher Wetterdienst)[3]. As road traffic variable we add up the vehicles from both roads to get a single traffic indicator on an hourly basis. Benzene concentration in Augsburg is used as dependent variable in the analysis. Figure 1 shows the hourly benzene concentration in Augsburg between 2014 and 2018.

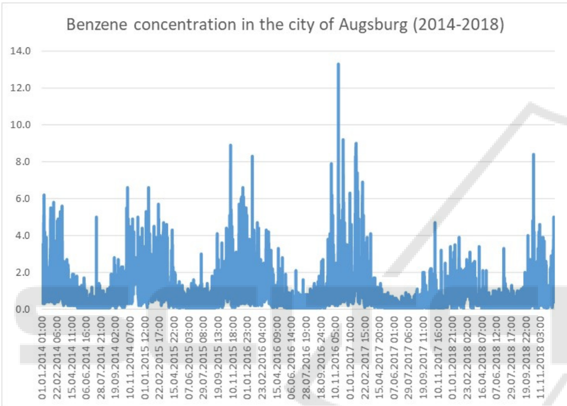

Figure 1: Hourly benzene concentration in Augsburg, Germany.

3 METHODS

To assess the forecasting performance for one hour ahead benzene, multi linear regression, adaptive neuro-fuzzy inference system and long short-term memory network are applied and compared. Standard goodness of fit measures help to evaluate the different methods and select the best model.

3.1 Multiple Linear Regression

In order to compare the different methods, a multiple linear regression model (MLR) was estimated as a base model first. The standard linear regression model can be described by:

[1] https://www.bast.de/BASt_2017/DE/Verkehrstechnik/Fachthemen/v2-verkehrszaehlung/zaehl_node.html

[2] https://www.lfu.bayern.de/luft/immissionsmessungen/messwertarchiv/index.htm

$$Y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \cdots + \beta_k X_k + u \quad (1)$$

In that equation Y represents the dependent variable, β_0 represents the intercept and β_1 is the parameter related with the first independent variable X_1. Further, β_2 is the parameter associated with X_2 and β_k is the parameter linked with X_k. The error term is labelled u (Wooldridge 2003). The standard multiple linear regression model implies a linear relationship among the dependent and the independent variables.

3.2 Adaptive Neuro-Fuzzy Inference System

The adaptive neuro-fuzzy inference system (ANFIS) was developed by Jang (1993) and is a combined model that incorporates a fuzzy system with an artificial neural network (ANN). The idea here is to combine the advantages of both methods. The ANFIS model is defined as a fuzzy inference system (FIS) with distributed parameters (Quej et al., 2017). In our analysis a Sugeno first-order fuzzy model is used (for a discussion see Sugeno, 1985 and Takagi et al., 1983). In a first-order Sugeno system, a typical rule has the form:

If input 1 is x and input 2 is y, then output is given by $z = ax + by + c$

For a fuzzy inference system with two inputs x and y as well as one output variable z, with two Sugeno type fuzzy if-then rules, according to Sugeno (1985) and Takagi et al. (1983) we get:

Rule 1:

$$\text{If } x \text{ is } A_1 \text{ and } y \text{ is } B_1, \text{ then } f_1 = p_1 x + q_1 y + r_1 \quad (2)$$

Rule 2:

$$\text{If } x \text{ is } A_2 \text{ and } y \text{ is } B_2, \text{ then } f_2 = p_2 x + q_2 y + r_2 \quad (3)$$

In the equations, the parameters in the then-part of the first-order Sugeno fuzzy model are labelled p_1, q_1, r_1 and p_2, q_2, r_2 respectively (Jang 1993).

Following Jang (1993) the ANFIS system contains five-layers. The first layer is related to a fuzzy model (Ausati et al. 2016). Each node i in the first layer is a node function:

$$O_i^1 = \mu_{Ai}(x) \quad (4)$$

where the parameter x is the input node i, and A_i is the fuzzy set (linguistic label) associated with this

[3] https://opendata.dwd.de/climate_environment/CDC/observations_germany/climate/hourly/

node function. Thus, O_i^1 is defined by the shape of the membership function of A_i and identifies the degree to which a given value of x fulfils the linguistic label (Jang, 1993). Typical shapes of membership functions are triangular, trapezoidal, gaussian or bell-shaped. They are all bounded between zero and one.

The second layer (product layer) multiplies the incoming signals and sends out the result.

$$w_i = \mu_{Ai}(x) * \mu_{Bi}(y), \quad i = 1, 2 \qquad (5)$$

The third layer (normalized layer) calculates the ratio of the i_{th} rule's strength compared to the sum of strength of all rules (Jang, 1993 and Quej et al., 2017):

$$\overline{w}_i = \frac{w_i}{w_1 + w_2}, \quad i = 1, 2 \qquad (6)$$

In the fourth layer (de-fuzzy layer), the weighted output of each linear function is derived by:

$$O_i^4 = \overline{w}_i f_i = \overline{w}_i (p_i x + q_i y + r_i \qquad (7)$$

where $\overline{w}_i$ is the output of the third layer and the parameter set is given by p_i, q_i and r_i. These parameters are called consequent parameters (Jang, 1993).

In the fifth layer (total output layer) the overall output of all incoming signals is calculated as the sum of all input signals:

$$O_i^5 = \sum_i \overline{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i} \qquad (8)$$

The figure below shows the ANFIS structure:

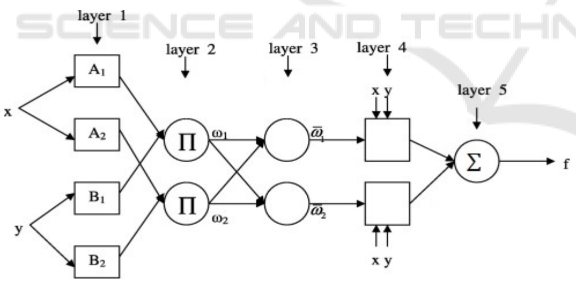

Figure 2: ANFIS structure (Guneri et al., 2011).

For the analysis, we apply two triangular membership functions for every input variable in the fuzzy inference system. The triangular membership function can be formulated as follows:

$$\mu_{Ai}(x) = max\left\{min\left(\frac{x-a}{b-a}, \frac{c-x}{c-b}\right), 0\right\} \qquad (9)$$

In this equation the parameters a, b and c change the shape of the triangular membership function. Furthermore, the triangular membership function is bounded between a maximum value of 1 and minimum value of 0.

3.3 Long Short-Term Memory Network

The long short-term memory network (LSTM) was originally introduced by Hochreiter and Schmidhuber (1997). In contrast to standard recurrent neural networks (RNN) the LSTM considers both, the short-term as well as long-term dependency of a time series. Thus it exhibits temporal dynamic behaviour for a time sequences (Greff, 2016). The LSTM that is used in this paper can be found in Fig. 3 and is composed of cell, input gate, output gate, and forget gate.

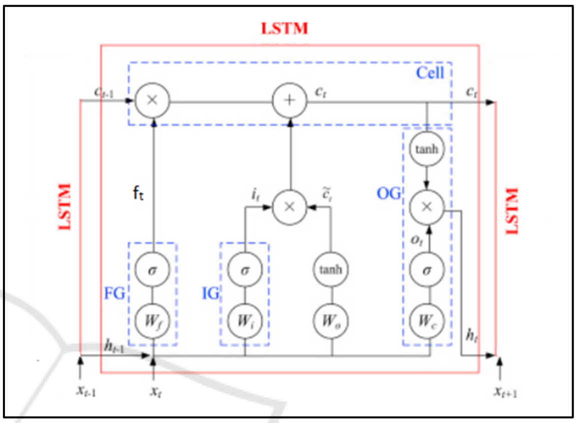

Figure 3: LSTM structure (Bai et al., 2019).

The forget gate (FG) determines what information is removed from the cell state.

$$f_t = \sigma(W_f \cdot [h_{t-1}, x_t] + b_f) \qquad (10)$$

With h_{t-1} as the output of the previous cell state and x_t as the input of the current cell state. The expressions W_f and b_f represent the weights and the bias of the forget gate respectively, whereas σ refers to the sigmoid function (Le et al. 2019). The value f_t is bounded between 0 (full fail) and 1 (full pass) to denote the degree of information withholding (Bai, 2019).

The input gate (IG) determines what new information will be added to the cell state.

$$i_t = \sigma(W_i \cdot [h_{t-1}, x_t] + b_i, \qquad (11)$$

$$\tilde{c}_t = \tanh(W_c \cdot [h_{t-1}, x_t] + b_c \qquad (12)$$

and

$$c_t = f_t \times c_{t-1} + i_t \times \tilde{c}_t \qquad (13)$$

With W_i and b_i as weights and bias for the input gate, whereas W_c and b_c are the weights and the bias of the cell state (Le at al. 2019). The operator × stands for point-wise multiplication. Equations 15 and 16 calculate the information to be updated, whereas equation 17 realizes the cell state update (Bai, 2019).

The output gate (OG) controls the current information in the cell state to flow into the outputs.

$$o_t = \sigma(W_o \cdot [h_{t-1}, x_t] + b_o \quad (14)$$

and

$$h_t = o_t \times \tanh(c_t) \quad (15)$$

With W_o and b_o as weights and bias of the output gate. The term o_t evaluates which part of the cell state is exported. The expression h_t calculates the final output (Bai, 2017).

3.4 Model Evaluation

In order to achieve the goal of the article, the in- and out-of-sample forecasting performance of the different models must be evaluated. To do so, we apply the means squared error (MSE), the root mean squared error (RMSE), r-squared (R2) and the mean absolute error (MAE).

The mean squared error (MSE) is calculated as the average squared difference between the forecasted output y and the actual value $\hat{y}$ (Ciaburro, 2017):

$$MSE = \frac{1}{n}\left(\sum_{i=1}^{n}(\hat{y}_i - y_i)^2\right) \quad (16)$$

Lower values of MSE indicate a better performance of the model. The square root of the MSE yields the root mean squared error (RMSE). In contrast to the MSE, the RMSE measure has the same units as the forecasted variable. The RMSE is calculated as:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}} \quad (17)$$

The mean solute error (MAE) can be calculated by:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i| \quad (18)$$

The MAE penalizes large and small differences from the actual by the same amount as the size of the error, whereas MSE penalizes bigger errors more (Fenner, 2020).

The coefficient of determination (R^2) is the ratio of the explained sum of squares to the total sum of squares (Studenmund, 2001). The R^2 is bounded between zero (the variation in the data cannot be explained at all by the model) and one (the model perfectly explains the variation in the data). The R^2 is calculated by:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \quad (19)$$

All four performance measures are used and compared in order to evaluate the different models.

4 RESULTS

The in-sample period comprises of four years (2014-2017) and the out-of-sample period of one year (2018). Therefore, we use 80% of the data as training set and the remaining 20% as testing set. The table 1 below shows the outcome of the in- and out-of-sample performance measures of MLR, ANFIS and LSTM in predicting benzene concentration. For the in-sample results, the ANFIS method has the highest predictive power, whereas MLR and LSTM have a very similar predictive power for one hour ahead benzene forecasting. However, the out of sample results indicate that the LSTM has the best forecasting performance in terms of RMSE, MAE and MSE, whereas the MLR and ANFIS show similar results. Only the R^2 is the highest for ANFIS in the out of sample period.

Table 1: Forecasting benzene one hour ahaead.

	MLR	ANFIS	LSTM
R^2 in sample	0.3767	0.5022	0.3806
RMSE in sample	0.6617	0.5913	0.6642
MAE in sample	0.4206	0.3627	0.3906
MSE in sample	0.4378	0.3496	0.4412
R^2 out of sample	0.3167	0.3875	0.2727
RMSE out of sample	0.5233	0.5272	0.4710
MAE out of sample	0.3907	0.3644	0.2814
MSE out of sample	0.2738	0.2779	0.2218

5 DISCUSSION

A major advantage of LSTM networks is the ability to forget part of its previously stored memory and also add a part of new information to its memory. The results in this paper support the usefulness of this unique ability in out of sample forecasting. However, at least in the used in-sample, LSTM networks could not outperform ANFIS. Future research should verify whether this result can be confirmed with other pollutants and different samples.

Generally, the different methods that were applied can only explain between 37% and 50% of the variance in sample and between 27% and 38% out of sample. Thus a large share of variance cannot be explained by the models. The inclusion of other lagged pollutants might help to improve the forecasting performance. Some authors have extended the independent variables by other pollutants and reported an improvement in the forecasting performance (see inter alias Oprea et al., 2017)). Moreover, the traffic data could not be collected in the city centre where the benzene concentration is measured. As a result, the traffic data from the highway crossing by the city of Augsburg was used and this can only serve as an indicator of vehicle traffic. A precise traffic measurement might therefore improve benzene predictability.

Furthermore, one hour ahead forecasting is a fairly short period for traffic emissions and for longer periods it must be expected that the models become less predictive. Thus, future research should also investigate the long term predictability of benzene by ANFIS, MLR and LSTM. Nonetheless, the results show that machine learning algorithms in general, and LSTM in particular might be helpful in predicting benzene concentration in advance. This can help traffic management systems to anticipate raising air pollution and reduce traffic by temporary restrictions.

Not least because of the decision of the European Court of Justice, it is necessary to immediately reduce air pollution in German cities. The automatic traffic counting stations already make it possible to forecast the development of air pollution. Therefore, the findings of this article should be used by local authorities to introduce a traffic control system promptly and to curb traffic in case of high predicted air pollution. In addition, it is necessary to install more traffic counting stations and also the number of air monitoring stations should be increased to achieve a more accurate forecast of air pollutants.

6 CONCLUSION

In this paper the predictive power of adaptive neuro-fuzzy inference systems, long short-term memory networks and multiple linear regression models for one hour ahead benzene prediction in the city of Augsburg is analysed. Artificial intelligence methods have been used for air pollution forecasting before, but we add to the literature in benzene prediction and in the use of long short-term memory networks. The results of the analysis indicate that adaptive neuro-fuzzy inference systems have the best in sample performance for benzene prediction, whereas long short-term memory networks and multiple linear regressions show similar predictive power. However, long short-term memory models have the best out of sample performance for one hour ahead benzene prediction. This supports the use of long short-term memory networks for benzene prediction in real world applications.

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