Forecasting Air Pollution in Munich: A Comparison of MLR, ANFIS, and SVM

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Abstract: As motor vehicle air pollution is a serious health threat, there is a need for air quality forecasting to fulfil policy requirements, and lower traffic induced air pollution. This article compares the performance of multiple linear regressions, adaptive neuro-fuzzy inference systems, and support vector machines in predicting one-hour ahead particulate matter, nitrogen oxides and ozone concentration in the City of Munich between 2014 and 2018. The models are evaluated with different performance measures in-sample and out-of-sample. The results generally support earlier studies on forecasting air pollution and indicate that adaptive neuro-fuzzy inference systems have the highest predictive power in terms of R-square for all pollutants. Furthermore, ozone can be predicted best, whereas nitrogen oxides are the least predictive pollutants. One reason for the different predictability might be rooted in the short lifetime of nitrogen oxides compared to ozone. The results here should be of interest to regulators and municipal traffic managements alike who are interested in predicting air pollution and improve urban air quality.

1 INTRODUCTION

It is generally recognized that motor vehicle air pollution is a serious health threat. Motor vehicle emissions include e.g. carbon monoxide (CO), nitrogen oxides like NO or NO_2, ozone (O_3) or particulate matter (PM10, PM2.5) (for a discussion see inter alia Klæboe et al., 2000, Crüts et al., 2008, Künzli et al., 2000 and Gössling et al., 2019).

Resulting health risks might be bronchitis, asthma, lung cancer, cardiopulmonary diseases and cardiopulmonary mortality (for a discussion see inter alia Hoek et al., 2002, Pope et al. 2002 and Zhang et al., 2013). Künzli et al., (2000) suggest that air pollution is responsible for 6% of total deaths in Europe and half of this can be attributed to motor vehicle transport.

Although air quality has improved over the last decades, there is scientific evidence that current levels of air pollution are still too high (Lancet Commission, 2017). As a result, there is a need for air quality monitoring to fulfil legislative and policy requirements in order to lower traffic-induced air pollution by traffic control (Molina-Cabello et al., 2019). In recent years, artificial intelligence (AI) methods like artificial neural networks (ANN) or decision trees (DT) have been applied to air quality modelling and forecasting.

For instance, Pawlak et al., (2019) used ANNs to forecast surface ozone concentration in central Poland for the following day. They concluded that ANNs can be used as a significant, effective tool to predict extreme levels of ozone. Similarly, Molina-Cabello et al., (2019) successfully applied transferable neural networks to infer NO_2 and PM10 emissions in the city of Leicester, UK.

In addition, adaptive neuro-fuzzy inference systems (ANFIS) models have been used to forecast pollutants like nitrogen oxides (NOx), carbon dioxide CO_2 or PM2.5 and PM10 by e.g. Ausati et al., (2016), Mihalache et al., (2016) or Oprea et al., (2017). Authors concluded that the ANFIS models perform

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well, also in comparison to other statistical or AI models.

With the emergence of support vector machines (SVM), researchers have applied SVMs to emission forecasting as well. Lu et al., (2002) investigate air pollutant parameter forecasting using support vector machines and found them superior to ANNs in predicting air quality parameters. In contrast, Luna et al., (2014) compared ANNs and SVMs to predict ozone concentration in Rio de Janeiro and found both methods equally well suited for ozone forecasting.

Finally, Opera et al., (2017) used decision trees (DT) to predict particulate matter and compared the technique to ANNs. The results clearly showed that ANNs are superior to DTs in predicting PM.

In summary, there are many studies investigating the performance of different AI methods in forecasting a variety of pollutants. However, most studies have only used a short time-frame of e.g. one year and focused on one or two pollutants exclusively. Furthermore, in literature mixed evidence exists on the performance of SVMs in comparison to ANN or ANFIS methods. Most studies have not evaluated the out-of-sample performance and only relied on in-sample performance measures. We therefore add to the literature by using an extended time span of 5 years of hourly data and comparing the one-hour forecast performance of multiple linear regressions (MLR), adaptive neuro-fuzzy inference systems (ANFIS) and support vector machines (SVM) for five pollutants. The selection of methods was thus based on literature. We also make use of an extended time frame of four years in-sample training (80%) and one year out-of-sample testing (20%).

Therefore, the objective of this study is to develop a one-hour forecasting model for different air pollutants in the city of Munich between 2014 and 2018. Before the introduction of the pre-stage of the low emission zone (LEZ) in 2008, many heavy-duty trucks drove through the city centre of Munich (Qadir et al., 2013). Following the pre-stage, the LEZ was extended in the following months and only allowed vehicles with emission requirement of Euro2, Euro3 and Euro4 to enter the inner city. In October 2010, regulations were tightened further to only allow vehicles with emission requirement Euro3, Euro4 and higher to go through the LEZ area. The final stage was introduced in October 2012 and merely allows vehicles with Euro4 emission requirements to access the LEZ area[4]. Research that analysed air quality modelling and forecasting in Munich before or during the introduction of the LEZ includes Hülsmann et al., (2014) and Fensterer (2014). They reported a significant reduction in air pollution after the introduction of the LEZ in the city of Munich.

We therefore analyse the predictability of air pollution in Munich after the introduction of the final stage of the LEZ. However, since 2019 there has been an ongoing discussion regarding a diesel-driving ban in Munich due to high particulate matter emissions exceeding EU limits[5]. Our analysis will help to better understand the current emotional discussion and underpin it with facts.

2 MATERIAL AND METHODS

A short description of the material and methods that were used in our analysis is given in the following section.

2.1 Material

This study used hourly data of vehicle traffic, air quality measurements, and meteorological data from Munich, Germany. The dataset spans from 01.01.2014 to 31.12.2018 and therefore consists of 43,824 hours of traffic, air quality, and meteorological data.

The traffic data was collected by the German Federal Roads Agency (Bundesanstalt für Straßenwesen)[6] for five major access roads to the city of Munich. These motorways (A8 – München West, A9 - Schwabing, A94 – München Riem, A96 – München Laim, A995 – München Giesing) are equipped with automatic traffic counting systems and register all vehicles going to or leaving Munich.

The Bavarian State Office for the Environment (Bayerisches Landesamt für Umwelt)[7] provided hourly data for particulate matter (PM10 and PM2.5), nitrogen monoxide (NO), ozone (O_3) and nitrogen dioxide (NO_2) from five air measurement stations located in Munich (Allach, Johanneskirchen,

[4] https://www.muenchen.de/rathaus/home_en/Environment-and-Health/Low_emission_zone.html

[5] https://www.right-to-clean-air.eu/fileadmin/Redaktion/Downloads/Laymans_report_ENG_Right_to_clean_Air.pdf

[6] https://www.bast.de/BASt_2017/DE/Verkehrstechnik/Fachthemen/v2-verkehrszaehlung/Aktuell/zaehl_aktuell_node.html

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

Landshuter Allee, Lothstraße, Stachus). All five pollutants are reported in µg/m^3.

Precipitation, relative humidity, sunshine duration, temperature, wind speed and wind direction were available from the German Meteorological Service (Deutscher Wetterdienst)[8].

Furthermore, we include dummy variables for New Year's Eve and working days because both show variations in emissions. In particular, particulate matter levels are ten times higher during New Year’s Eve compared to average levels. The working day dummy variables reflect different driving patterns during public holidays and weekends. Figure 1 shows the hourly PM10 concentration between 2014 and 2018 with extreme spikes of the pollutant during New Year’s Eve.

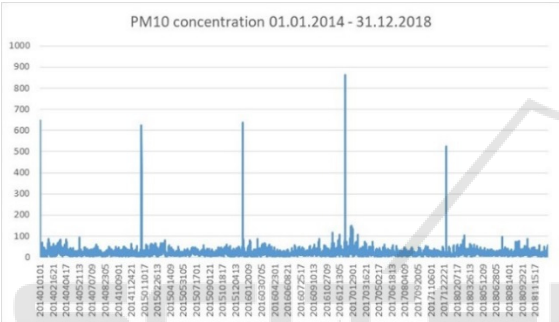

Figure 1: Hourly PM10 concentration in µg/m3 between 01.01.2014 and 31.12.2018.

As traffic variable, we add all vehicles that are going to or leaving Munich as recorded by the automatic traffic counting system. For the five pollutants, we calculate the average value of each pollutant from the air measurement stations.

2.2 Methods

To evaluate the air forecasting performance of artificial intelligence methods we compare adaptive neuro-fuzzy inference systems (ANFIS) and support vector machines (SVM) to multiple linear regressions (MLR). The MLR as standard statistical method serves as a benchmark for comparison. The selection of ANFIS and SVM was based on recent literature in atmospheric environmental sciences and artificial intelligence (see inter alia Oprea et al., 2017; Ausati et al., 2016; Quej et al., 2017; Pawlak et al., 2019 and Mehrotra et al., 2020).

2.2.1 Multiple Linear Regression

The multiple linear regression (MLR) was used as a benchmark model for comparison with the support vector machine (SVM) and the adaptive neuro-fuzzy inference system (ANFIS). The MLR model can be represented by:

$$Y_i = \beta_0 + \beta_1 X_{1i} + \beta_2 X_{2i} + \cdots + \beta_k X_{ki} + \varepsilon_i \qquad (1)$$

where Y_i is the i_{th} observation of the dependent variable Y, X_{ji} is the i_{th} observation of the j_{th} independent variable, β_0 is the intercept, β_j is the slope coefficient of the j_{th} independent variable and ε_i represents the error term. The MLR assumes a linear relationship between the dependent and the independent variables.

2.2.2 Support Vector Machine

A support vector machine (SVM) is a supervised learning algorithm from machine learning theory (Vapnik, 1995). SVMs were originally developed for classification problems, but can also be applied to regression applications. We therefore use a SVM for regression that is sometimes called a SVR model. The SVM structure is not determined a priori but through a model training process the input vectors are selected. The training dataset is represented by:

$$\{(x_i + d_i)\}_i^N \qquad (2)$$

Where x_i is the input vector, d_i is the desired value and N is the total number of data patterns (He et al. 2014). The regression function of the SVM is given by:

$$f(x) = w_i * \phi_i(x) + b \qquad (3)$$

where w_i is a weight vector, b is a bias, and ϕ denotes a nonlinear transfer function mapping the input vectors into a high-dimension feature space. A convex optimization problem with an e-insensitivity loss function to obtain a solution to the following equation was developed by Vapnik (1995):

$$Minimize: \frac{1}{2}\|w\|^2 + C\left(\sum_i^N \xi_i + \xi_i^*\right) \qquad (4)$$

Subject to:

$$\begin{cases} w_i * \phi(x_i) + b_i - d_i \leq \varepsilon + \xi_i^*, \ i = 1, 2, \ldots\ldots, N \\ d_i - w_i * \phi(x_i) - b_i \leq \varepsilon + \xi_i, \ i = 1, 2, \ldots\ldots, N \\ \xi_i, \xi_i^*, \ i = 1, 2, \ldots\ldots, N \end{cases} \qquad (5)$$

Where ξ_i and ξ_i^* are slack variables that penalize training errors by the loss function over the error

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

tolerance ξ (He et al., 2014). Furthermore, C is a positive trade-off parameter that determines the degree of the empirical error in the equation (4). The optimization problem in equation (4) is solved in a dual form by using Lagrangian multipliers and imposing the Karush-Kuhn-Tucker optimality condition (see He et al. 2014). Input vectors that have non-zero Lagrangian multipliers under the Karush-Kuhn-Tucker condition are called support vectors as they support the structure.

In our empirical analysis, we report the results of linear SVMs. We have also estimated quadratic, cubic and Gaussian SVMs and found very similar results to the linear version, but estimation time was very long. Hence, for practical reasons we make use of a linear kernel function in our SVMs.

2.2.3 Adaptive Neuro-fuzzy Inference System

An adaptive neuro-fuzzy inference system (ANFIS) was first introduced by Jang (1993) and is a hybrid model that combines a fuzzy with an artificial neural network (ANN). It is a fuzzy inference system (FIS) with distributed parameters (Quej et al., 2017). We use a Sugeno first-order fuzzy model comparable to Drake (2000). In a first-order Sugeno system, a typical rule set with two fuzzy IF/THEN rules with two inputs x and y and one output z is given by:

Rule 1:
If x is A_1 and y is B_1, then $f_1 = p_1x + q_1y + r_1$ (6)

Rule 2:
If x is A_2 and y is B_2, then $f_2 = p_2x + q_2y + r_2$ (7)

where p_1, q_1, r_1 and p_2, q_2, r_2 are the parameters in the then-part of the first-order Sugeno fuzzy model (He et al., 2014). The ANFIS consists of a five-layer network (Wei et al., 2007) and the initial layer is related to a fuzzy model (Ausati et al., 2016). Each node i in the first layer represents a node function:

$$O_i^1 = \mu_{Ai}(x) \tag{8}$$

where x is the crisp input to the node i, and A_i is the fuzzy set associated with this node, characterized by the shape of the membership functions (MFs). The MFs can be e.g. triangular, trapezoidal, gaussian or bell-shaped.

In the second layer (product layer) the rule operator AND/OR is applied (Quej et al., 2017). The outputs are obtained by multiplying ring layers with the input layers:

$$w_i = \mu_{Ai}(x) * \mu_{Bi}(y), \quad i = 1, 2 \tag{9}$$

In the third layer (normalized layer) the ratio of the i_{th} rule's strength compared to the sum of strength of all rules is calculated:

$$\bar{w}_i = \frac{w_i}{w_1 + w_2}, \quad i = 1, 2 \tag{10}$$

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

$$O_i^4 = \bar{w}_i f_i = \bar{w}_i (p_i x + q_i y + r)_i \tag{11}$$

where $\bar{w}_i$ is the output of the third layer and the final parameters are p_i, q_i and r_i.

In the fifth layer (total output layer) a single node of total output with the sum of all inputs signals is computed:

$$O_i^5 = \sum_i \bar{w}_i f_i = \frac{\sum_i w_i f_i}{\sum_i w_i} \tag{12}$$

The figure below shows the ANFIS structure:

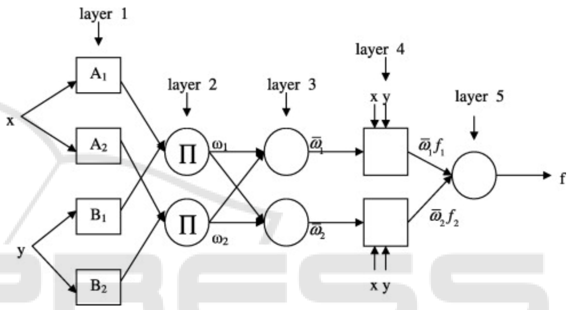

Figure 2: ANFIS structure (Guneri et al., 2011).

In our empirical analysis, we use two triangular membership functions for each input variable in the FIS. A triangular membership function is given by:

$$\mu_{Ai}(x) = max\left\{min\left(\frac{x-a}{b-a}, \frac{c-x}{c-b}\right)\right\} \tag{13}$$

where a, b and c are the parameters that change the shape of the triangular membership function with maximum 1 and minimum 0 (Quej et al., 2017).

2.2.4 Model Evaluation

To evaluate the in- and out-of-sample forecasting performance of the models, we use the means squared error (MSE), the root mean squared error (RMSE), r-squared (R2) and the mean absolute error (MAE).

The effect on MSE is more pronounced for large errors in the forecasted values than for smaller errors because the errors are squared. The MSE is calculated as follows:

$$MSE = \frac{1}{n}\left(\sum_{i=1}^{n}(\hat{y}_i - y_i)^2\right) \tag{14}$$

Where $\hat{y}$ is the actual value and y is the predicted output of the model.

The square root of MSE gives RAMSE, which has the same units as the forecasted values. The formula for RMSE is given by:

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}{n}} \tag{15}$$

The MAE is a directionless method for comparing forecasted values with realized outcomes in the data (Hipni et al., 2013). MAE can be calculated by:

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i| \tag{16}$$

The R^2 is the ratio of the explained variation that can be explained by the model and ranges between 0 (cannot explain any variation in the data) and 1 (can explain the data variation completely). The R^2 is given by:

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y}_i)^2} \tag{17}$$

To evaluate the model results, all four performance measures are used and compared.

3 RESULTS

Table 1 reports the results of the in- and out-of-sample performance measures of MLR, SVM and ANFIS in forecasting PM10, PM2.5, NO, O_3 and NO_2. For in-sample results, the ANFIS model has the highest R^2 and the lowest RAMSE/MSE for all pollutants. Only for MAE do we find the lowest value for PM10, PM2.5 and NO with the SVM, whereas for O_3 and NO_2 the ANFIS models shows the lowest MAE. Generally, the SVM[9] and MLR show similar in-sample performance results. However, the ANFIS tends to have the best performance in-sample for all five pollutants. Ozone has the best in-sample predictive power with a R^2 greater than 0.70 for all three methods. The R^2 of NO is the lowest with values below 0.40 for all models and is therefore the least predictive pollutant in-sample.

For the out-of-sample results, we get a similar picture as in-sample. The R^2 of the ANFIS is the highest for PM10, PM2.5, NO, O_3 and NO_2. ANFIS also shows the lowest RAMSE/MSE for PM10, PM2.5 and O_3 whereas the RAMSE/MSE for NO and NO_2 has the lowest value for the SVM model. The out-of-sample performance of MLR and SVM is again comparable, whereas the ANFIS model is generally superior to MLR and SVM. Ozone can be predicted best out-of-sample with a R^2 greater than 0.72 for all models. In contrast, PM10 and PM2.5 is least predictive with a R^2 of approximately 0.20.

[9] The number of support vectors are 11,968 for PM10; 10,085 for PM2.5; 17,649 for NO; 7,040 for O3 and 12,026 for NO2

Table 1: Forecasting pollutants one hour ahead.

Pollutant/ model	In sample				Out of sample			
	R^2	RMSE	MAE	MSE	R^2	RMSE	MAE	MSE
PM10 MLR	0.497	14.72	8.49	216.74	0.191	13.24	7.88	175.41
PM10 SVM	0.485	15.24	8.13	232.32	0.168	13.33	7.48	177.74
PM10 ANFIS	0.502	14.69	8.90	215.85	0.235	11.83	8.32	139.84
PM2.5 MLR	0.566	11.21	6.00	125.58	0.196	10.94	5.88	119.69
PM2.5 SVM	0.520	11.80	5.67	139.05	0.162	11.32	5.71	128.12
PM2.5 ANFIS	0.596	10.83	5.84	117.28	0.279	9.25	5.75	85.47
NO MLR	0.375	30.07	20.63	904.40	0.353	25.74	20.01	662.78
NO SVM	0.352	31.82	19.33	1012.40	0.328	23.37	16.39	546.07
NO ANFIS	0.399	29.49	19.94	869.65	0.382	25.05	19.21	627.70
O_3 MLR	0.709	16.44	13.00	270.15	0.724	18.39	14.57	338.12
O_3 SVM	0.706	16.56	12.92	274.19	0.724	18.44	14.49	339.99
O_3 ANFIS	0.738	15.60	12.36	243.33	0.747	17.50	13.81	306.27
NO_2 MLR	0.429	14.33	11.01	205.26	0.391	14.57	11.96	212.34
NO_2 SVM	0.426	14.52	10.85	210.88	0.384	13.78	11.10	190.02
NO_2 ANFIS	0.510	13.29	10.10	176.61	0.466	13.91	11.25	193.36

4 DISCUSSION

In contrast to MLR and ANFIS, a major advantage of SVMs is that a relatively small sample might be sufficient to build an effective calibrated model (Balabin et al., 2011). However, in our case study of Munich, the dataset is quite large and the small sample advantage of SVMs cannot be exploited. This might explain why the MLR and SVM perform very similar in- and out-of-sample.

In recent years, particulate matter has been reported as one of the most harmful air pollutants that causes serious health problems especially to children and elderly people (Oprea et al., 2017). Although the R^2 indicates that only about 50% to 60% of the variance in PM10 and PM2.5 can be explained by our models, the ANFIS shows the highest R^2. A comparable R^2 between 50% and 60% has also been reported by earlier studies with artificial neural networks by e.g. Molina-Cabello (2019). Our results are therefore in line with literature on the predictability of particulate matter.

Ozone is a secondary pollutant, as it is not directly emitted by traffic, but produced through a chain of photochemical reactions involving NOx, CO and VOC (Volatile Organic Compounds). The concentration of surface ozone is determined by a combination of factors involved in its formation (photochemical reactions), destruction (dry deposition, chemical reactions) and transport (Pawlak et al., 2019). Therefore, ozone is primarily formed on warm summer days by solar radiation in combination with the above mentioned pollutants. The relatively long lifetime of ozone and its formation being dependent on sunshine, causes a clear seasonal pattern of ozone concentration over the year with a spike in summer and a low during winter (Austin et al., 2015). This might be the reason why ozone is more predictable than the other pollutants.

In contrast to ozone, nitrogen oxides (NO, NO_2) are short-lived pollutants with a lifetime of 1 to 12 hours (Lorente et al., 2019). Nitrogen oxides react by photochemical processing to form acid rain, ozone and particulate matter. This could be the reason why nitrogen oxides are the least predictable pollutants in our sample.

As ozone and particulate matter concentration depend on e.g. nitrogen oxides, some studies have included these pollutants to better predict PM10, PM2.5 and O_3 (see inter alia Ausati et al., 2016; Opera et al., 2017 and Arsic et al., 2020). Future research might therefore analyse the performance of our models to forecast emissions in Munich by incorporating NOx and CO as lagged predictors.

Future research in this area might include additional artificial intelligence methods like long short-term memory networks (LSTM). For instance, Lin et al., (2019) used LSTM for PM10 forecasting purposes.

5 CONCLUSIONS

This article compared the performance of multiple linear regressions, adaptive neuro-fuzzy inference systems and support vector machines in predicting one-hour ahead particulate matter, nitrogen oxides and ozone concentration in the City of Munich between 2014 and 2018. The models were evaluated with different performance measures in-sample and out-of-sample. The results show that adaptive neuro-fuzzy inference systems have the highest predictive power in terms of R-square for all pollutants. Furthermore, ozone can be predicted best, whereas nitrogen oxides are the least predictive pollutants. One reason for the different predictability might be rooted in the short lifetime of nitrogen oxides compared to ozone. As ozone and particulate matter depend on nitrogen oxides, some research studies have included these pollutants as lagged predictors. Future research might therefore review our models with lagged pollutants as predictor variables.

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