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Article

Comparison of Selected Ensemble Supervised Learning Algorithms Used for Meteorological Normalisation of Particulate Matter (PM₁₀)

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Abstract: Air pollution, particularly PM₁₀ particulate matter, poses significant health risks including respiratory and cardiovascular diseases as well as cancer. Accurate identification of PM₁₀ reduction factors is therefore essential for developing effective sustainable development strategies. This study evaluated the performance of three machine learning algorithms - Decision Trees (CART), Random Forest, and Cubist Rule - in predicting PM₁₀ concentrations and estimating long-term trends following meteorological normalisation. The research focused on Tarnów, Poland (2010-2022), with comprehensive consideration of meteorological variability. Results demonstrated superior accuracy for the Random Forest and Cubist models ($R^2 \sim 0.88-0.89$, RMSE $\sim 14 \mu\text{g}/\text{m}^3$) compared to CART (RMSE $19.96 \mu\text{g}/\text{m}^3$). Air temperature and boundary layer height emerged as the most significant predictive variables across all algorithms. The Cubist algorithm proved particularly effective in detecting the impact of policy interventions, making it valuable for air quality trend analysis. While the study confirmed a statistically significant annual PM₁₀ decrease ($0.83-1.03 \mu\text{g}/\text{m}^3$), concentrations persistently exceeded both updated EU air quality standards (2024) and WHO guidelines (2021).

Keywords: PM₁₀ particulate matter; meteorological normalisation; machine learning; air quality; air pollution trends

1. Introduction

PM₁₀ contamination in the air has a strong impact on human health. According to the International Agency for Research on Cancer (IARC), air pollution is considered a mixture of potentially carcinogenic substances. PM₁₀ particles can penetrate deep into the lungs, contributing to respiratory and cardiovascular problems. This impact is comparable to other significant health risks, such as tobacco smoking or an unhealthy diet. Long-term exposure is associated with reduced lung function, worsened asthma symptoms, and respiratory infections, especially in children. Among adults, the risk of ischemic heart disease and stroke increases—both of which are major causes of premature death linked to air pollution. In Poland, the number of premature deaths caused by particulate pollution was approximately 44,000 in 2012 and 43,000 in 2019.

An effective assessment of air pollution concentration trends is possible through the application of meteorological normalisation. This method was developed by Stuart K. Grange and David C. Carslaw [1,2]. This method makes it possible to eliminate the influence of meteorological conditions from the time series of air pollution concentrations. Meteorological normalisation (also known as deweathering) involves generating multiple concentration forecasts for random meteorological scenarios using developed supervised learning models, with the resulting values being averaged. As a result, it becomes possible to estimate non-parametric trend values of air pollution concentrations corresponding to averaged meteorological conditions. Meteorological normalisation is a relatively new method that has been used by many researchers for various scientific purposes in different regions of the world [1–17].

The Random Forest (RF) algorithm is commonly used in meteorological normalisation due to its robustness to missing data, multicollinearity among explanatory variables, and the relative simplicity of hyperparameter tuning [2,3,8]. Besides RF, the Gradient Boosted Regression Model (GBM) algorithm has also often been used for meteorological normalisation. [4,6]. These two algorithms are most often compared to each other because both are characterised by high prediction accuracy and low bias [1,5,9,16]. Mallet (2021) [16] tested the above methods. The GBM was able to explain 46% of the predicted variable (PM_{10}). In the case of the Random Forest model, the coefficient of determination (R^2) was 0.59, indicating that this model explained 59% of the variance in the predicted variable. Comparing the RF and GBM models in terms of NO_x predictions, the values of the coefficient of determination were 0.73 and 0.76, respectively [9]. Moreover, it was shown that the Random Forest algorithm is characterised by lower systematic errors. Lovric et al. (2022) [5] compared the Random Forest algorithm (RF) and the Gradient Boosting Method (LightGBM) for predicting concentrations of particulate matters. In this case, they obtained similar results from the above models. RF achieved an R^2 value of 0.78 and LightGBM a value of 0.77. The study conducted in London showed that the Random Forest algorithm has varying accuracy depending on the predicted substance (SO_2 , NO_2 and NO_x). For NO_x and NO_2 on Marylebone Road, R^2 values of 0.82 and 0.83 were achieved, respectively. However for SO_2 , the R^2 results were significantly lower, ranging from 0.63 to 0.67 [1]. This means that the methods under consideration have varying accuracy depending on the location of the study and the predicted substance. This is also confirmed by the studies carried out for 3 Chinese mega cities, where for many substances ($PM_{2.5}$, PM_{10} , NO_2 , SO_2 , CO , O_3) R^2 values ranging from 0.7 to 0.86 were obtained using the Random Forest algorithm [8].

The aim of this study was to compare the effectiveness of three machine learning models (decision trees, random forests, and Cubist Rules) in forecasting and estimating trends in PM_{10} concentrations based on normalised data. This task was undertaken due to the lack of comprehensive comparative analyses of various supervised learning algorithms regarding their impact on nonparametric estimation of pollution trends. In the study, boosted methods (GBM, LightGBM) were intentionally omitted, as the literature [1,5,16] indicates that they demonstrate comparable or lower accuracy compared to the Random Forest. Only Gagliardi and Andenna (2021) [9] observed slightly higher R^2 (0.76 vs 0.73) for GBM; however, other metrics did not confirm its superiority. It was decided to use the Cubist Rules algorithm [18,19], which—unlike other ensemble methods—has not yet been used in meteorological normalisation. Its advantage is the better interpretability of the results and the ability to generate transparent decision rules while maintaining high accuracy. It is an ensemble algorithm that combines a tree-based approach with rule generation. The conducted analyses enabled the identification of the most effective algorithms for modelling normalised PM_{10} concentrations, which in turn allows for reliable trend estimation and assessment of the effectiveness of remedial actions.

2. Materials and Methods

2.1. Research Area

The location of the research area, along with the air quality monitoring station and the meteorological station, is shown in Figure 1. The city of Tarnów is located in the eastern part of the Małopolska voivodeship in Poland. It is located on the Tarnów Plateau at the boundary between the Sandomierz Basin and the Carpathian Foothills. The city is inhabited by 103,130 people (data for the year 2023). The area of the city is 72.38 km².



Figure 1. Graphical representation of the location of measurement stations.

The analysed period covered the years 2010–2022. During this time, a significant improvement in air quality was observed in terms of PM_{10} concentrations. The current allowable average annual level of PM_{10} concentration is $40 \mu\text{g}/\text{m}^3$. This limit was exceeded in the first three analysed years. The year 2013 was omitted due to data completeness being less than 50%. A decrease in PM_{10} concentrations was observed from $41.9 \mu\text{g}/\text{m}^3$ (2010) to $23.7 \mu\text{g}/\text{m}^3$ (2022) (Figure 2). Despite the 43.4% reduction through the years, average annual PM_{10} concentrations are still higher than the values set out in the recommendations issued by the WHO in 2021 ($15 \mu\text{g}/\text{m}^3$) and the new guidelines adopted by the Council of the European Union in November 2024 ($20 \mu\text{g}/\text{m}^3$). It was also found that the daily average standard was not met during the years 2010–2021 (Figure 3). Currently, it is permissible for air quality standards to be exceeded on 35 days per year, but the revised EU regulations [18] reduce this number to 18. Over these 12 years, two of them (2010 and 2012) exceeded the annual limit and only four (2015, 2019, 2020 and 2020) had fewer than thirty-five days per year on which the daily limit was exceeded.



Figure 2. Distribution of average annual PM₁₀ concentrations.

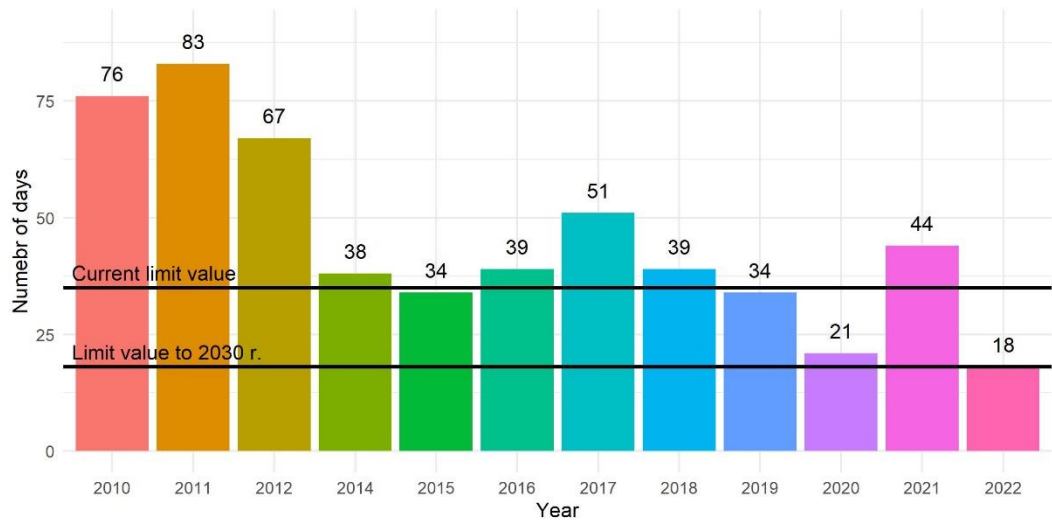


Figure 3. Distribution of days in year when the daily average air quality standard for PM₁₀ was exceeded.

2.2. Data Sources and Computational Methods

The data of hourly PM₁₀ concentration for the period 2010 – 2022 were obtained from the database of the Chief Inspectorate of Environmental Protection [19], while meteorological data such as wind speed (ws), wind direction (wd), relative humidity (rh), air temperature (tt) and atmospheric pressure (pres) were obtained from the archives of the Institute of Meteorology and Water Management [20]. Boundary layer height (blh), Cloud base height (cbh) and surface net solar radiation (ssr) was obtained from reanalysis for the global climate and weather ERA5 [21].

The study compared three supervised learning algorithms classified as ensemble methods: Decision Tree (cart) [22], Random Forest (ranger) [23,24], and Cubist Rules (cubist) [25]. Based on the date, auxiliary variables were created, such as Julian day (jday), day of the week (wday), and hour of the day (hour), representing typical periods of changes in air pollution emissions due to anthropogenic activities. The date variable was converted into a numerical format of the date to reflect the trend. The dataset was divided into a training (80% of samples used to adjust the model parameters) set, and test (20% of samples used to evaluate the model performance) set. From the training set, a validation set was created for the purpose of applying the resampling method (10-fold cross-validation). The use of this method provides a reasonable estimation of model accuracy

assessment parameters at a level similar to the test set during the hyperparameter tuning stage of individual algorithms. For hyperparameter optimisation, a racing method was applied based on the statistical significance of the configurations of individual algorithms from the ANOVA model [26]. The application of this method allowed for a reduction in computation time by approximately 20%. The best-performing algorithms were evaluated on the test set. The evaluation of the model was carried out using basic statistical metrics, i.e., FAC2 (fraction of predictions within a factor of two), MB (mean bias), MGE (mean gross error), NMB (normalised mean bias), NMGE (normalised mean gross error), RMSE (root mean squared error), r (Pearson correlation coefficient), COE (Coefficient of Efficiency), and IOA (Index of Agreement based on Willmott) [27].

In order to determine the importance of predicted variables, EMA (Exploratory Model Analysis) was conducted. The identification aimed to determine which meteorological data has the greatest impact on PM₁₀ concentration. This method demonstrated how the model's performance would change when one of the variables was removed. The significance was presented as RMSE values. The higher the metric, the greater the importance of the explanatory variable. The use of RMSE as a consistent metric enabled uniform comparisons of the applied supervised learning algorithms [28].

The developed models were used to carry out meteorological normalisation of particulate matter (PM₁₀). For this purpose, we used bootstrap [29] with the number of repetitions equal to 200 for each data record. Based on normalised data determined using three models (cart, ranger, cubist), the PM₁₀ trend was identified using the Theil-Sen robust linear regression estimator [30].

3. Result and Discussion

3.1. Evaluating the Accuracy of Machine Learning Algorithms

Figure 4 shows a comparison of observations with modelling results based on the applied algorithm. Three reference lines were added to the plot. One of them represents perfect mapping, while the other two indicate the error margin corresponding to a twofold overestimation or underestimation. All models accurately predict PM₁₀ concentrations below 100 µg/m³, as evidenced by the high density of observations along the ideal model line. Nonetheless, regardless of the applied algorithm, there are instances of twofold overestimations and underestimations of PM₁₀ concentrations. According to FAC2 values (shown in Table 1), the frequency did not exceed 10% when using the Random Forest (ranger) and Cubist Rules (cubist). In the case of the decision tree algorithm (cart), the frequency was almost twice as high. It is worth noting that the obtained FAC2 values for the Random Forest and Cubist Rules are comparable to those reported in other studies. Lv et al. (2022) [8], using the Random Forest model for PM₁₀, achieved a FAC2 value of 0.91.

Table 1 summarises the statistical metrics used to assess the accuracy of models based on the machine learning algorithm. For the Ranger and Cubist algorithms, similar accuracy metric values were obtained. The values of the normalised mean gross error (NMGE), the coefficient of efficiency (COE), and the Index of Agreement (IOA) are the same. Ranger reached the highest value of correlation coefficient (r): 0.89, Cubist had a slightly lower score: 0.88. The models differed by RMSE by 0.03 µg/m³. The models had opposite values of mean bias (MB). For Ranger, the parameter assumed a positive value, which indicates a tendency to overestimate the results. The negative result obtained for CART and Cubist indicates a tendency to underestimate the results. For all three models, the normalised mean bias (NMB) value hovered around zero, indicating that no model had a significant tendency to overestimate or underestimate. The statistics for the CART algorithm significantly deviate from those of the other two models. RMSE reached its highest value of 19.96 µg/m³. NMGE indicated that the uncertainty of the Ranger algorithm's forecasts occurs at a level of 39% of the mean value.

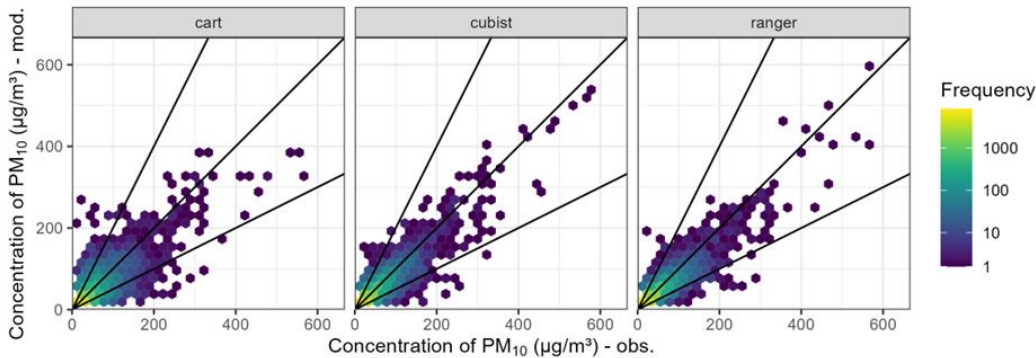


Figure 4. Scatterplot of the comparison of PM₁₀ observations with modelling results on the test dataset for three machine learning algorithms.

Compared to other studies, the machine learning models applied in this analysis exhibit varied effectiveness. Lv et al. (2022) [8] achieved a higher mean systematic error (MB ~0.11) with lower NMB and NMGE values, while the Random Forest model developed by Lovrića et al. (2022) [5] demonstrated a lower RMSE (10.47) compared to Mallet’s (2021) [16] result of 19.5. The best accuracy in terms of RMSE (5.39 µg/m³) was demonstrated by Gagliardi and Andenna (2021) [9], which maintained the same IOA value (0.76) and slightly lower R² (0.73). However, it pertained to nitrogen oxides (NO_x) concentrations. In terms of the coefficient of determination R², the presented Random Forest (RF) model outperforms Mallet (2021) [16] (0.49-0.59), Grange and Carslaw (2019) [1] (0.54-0.71), and Gagliardi and Andenna (2021) [9], approaching to results achieved by Lv et al. (0.81-0.94) and Wu et al. (2022) [17] (0.52-0.94). These findings confirm that the effectiveness of models depends both on the applied algorithm and the specificity of the analysed environmental data. Additionally, the appropriate selection of parameters and consideration of the local context are crucial for accurate air quality modelling.

Table 1. Summary of model accuracy metrics depending on the supervised learning algorithm used.

Model	FAC2	MB	MGE	NMB	NMGE	RMSE	r	COE	IOA
Cart	0.82	-0.14	11.94	-0.001	0.39	19.96	0.75	0.33	0.66
Cubist	0.90	-0.11	8.52	-0.040	0.28	14.06	0.88	0.52	0.76
Ranger	0.91	0.11	8.46	0.004	0.28	14.09	0.89	0.52	0.76

3.2. Importance Variable

The plot of the evaluation of the importance of an explanatory variable is shown in Figure 5. Boxplots demonstrate the change of RMSE value after deleting individual variables [31,32]. The line inside the box indicates the median for the series of permutations, while the grey dots represent outlier values. The dashed vertical lines denote the loss function values for each model. The value of the loss function is constant and depends on model structure. It reflects error in the absence of predictive variables. For CART, the value is 16.69 µg/m³, for Ranger 10.03 µg/m³, and for Cubist 9.29 µg/m³. The value of the loss function were similar for Ranger and Cubist. In all the applied algorithms, air temperature (tt) turned out to be the variable with the greatest impact on PM₁₀ concentrations. The median error after removing this variable was 23.9 µg/m³ (ranger), 21.5 µg/m³ (cubist) and 31.6 µg/m³ (cart). The significant impact of temperature likely stems from its association with the seasonal variability of emissions in the municipal and residential sector [33] and the deterioration of the conditions of dispersion of pollutants in winter, associated with the frequent occurrence of stable atmospheric layers [34]. It is worth noting that the decision tree algorithm (cart) showed a particularly strong dependence on the variable temperature compared to other models.

This is a consequence of the collinearity of explanatory variables. In this case, the tuning process focused on one variable (tt), which is highly correlated with the dependent variable (PM_{10}).

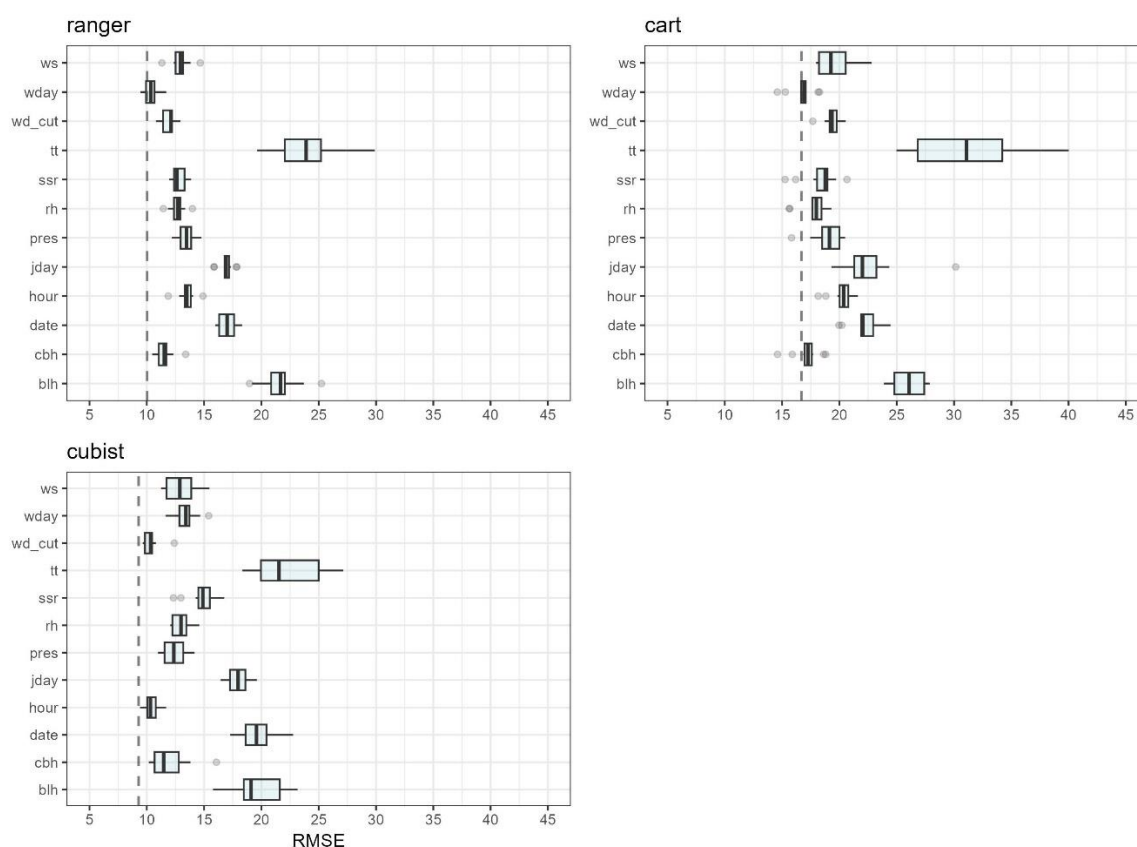


Figure 5. Measure of importance of predictor variables for three machine learning algorithms.

Other variables affecting the result were boundary layer height (blh), date (date), and the day of the year from Julian calendar (jday). In the case of the Ranger algorithm, removing the blh variable increased the median RMSE to $21.7 \mu\text{g}/\text{m}^3$, while for Cubist the median increased to $19.1 \mu\text{g}/\text{m}^3$, and for CART to $26.1 \mu\text{g}/\text{m}^3$. Boundary layer height is associated with surface temperature inversion. This phenomenon at low elevation negatively affects the dispersion of pollutants. During weak air mass movements, PM_{10} concentrations accumulate at ground level [35,36]. The variable numerically defining the date is significant because it reflects changes in pollutant emissions. After removing the "date" variable, RMSE increased to $16.9 \mu\text{g}/\text{m}^3$ in Ranger, in Cubist to $18.0 \mu\text{g}/\text{m}^3$, and in CART to $22.0 \mu\text{g}/\text{m}^3$. For decision trees, the least significant variable turned out to be the one representing the day of the week (wday). Its removal resulted in an RMSE increase of only $0.2 \mu\text{g}/\text{m}^3$ compared to the value of the loss function for this model. The second variable that slightly impacts the prediction quality is cloud base height (cbh). The increase in RMSE for this parameter was only $0.6 \mu\text{g}/\text{m}^3$ compared to the value of the loss function. Calculations performed on the cubist model indicated a low impact of the direction of wind (wd_cut) and the variable representing the hour of measurement during the day (hour). For both variables, RMSE increased by just $1 \mu\text{g}/\text{m}^3$ compared to the value of the loss function.

In each model, the temperature (tt) and the boundary layer height (blh) were the most important. The results obtained are not always consistent with earlier studies on other types of pollution and localisation. For example, studies conducted in the Alps focusing on nitrogen dioxide (NO_2) revealed that the most important explanatory variable was temperature, while the second most significant variable was the Julian day (jday) [10]. The high importance of jday resulted from the fact that studies conducted in the Alps did not consider the blh variable, focusing solely on the temperature gradient.

On the other hand, studies conducted in Australia on PM₁₀ revealed that the intensity of fires, trend, and temperature were more significant compared to wind speed and the boundary layer height. Other studies conducted in England on SO₂, NO₂ and NO_x provided evidence of the high significance of wind speed (ws) compared to temperature [1]. This stands in opposition to the obtained research findings, though it relates specifically to gaseous air pollutants. However, as in the present study, variables such as Julian day (jday), hour (hour) or wind direction (wd_cut) were of little importance. Research conducted in southern Italy on NO_x showed that the most significant variable was wind direction (wd_cut). This contrasts sharply with the findings of the presented studies, where this was typically a variable of little importance. It is essential to emphasise that the interpretation of the significance of explanatory variables depends on the type of substance and the location. The high importance of wind direction may be due to the location of the station, which is strongly influenced by emission sources located in a specific direction from the station. Caution should be exercised if results differ significantly from other studies. It is also important to consider the selection of an appropriate number of explanatory variables, as each of the aforementioned studies used non-standard quantities of explanatory variables.

3.3. Comparison of Particulate Matter Trends

The results of PM₁₀ concentration trends are presented in Figure 6. The solid red line shows the trend estimate and the dashed red lines show the 95% confidence intervals for the trend based on resampling methods. For CART, the trend is -0.83 (0.89 – 0.78) µg/m³, for Cubist -1.03 (1.11 – 0.94) µg/m³, and for Ranger -0.97 (1.04 – 0.9) µg/m³. The trend line for each model has a negative slope coefficient despite discrepancies in the accuracy assessment results (see Section 3.1). It should be noted that the 95% confidence intervals of the trend obtained from the Cubist and Ranger algorithms overlap. This indicates that they are not statistically significantly different at the 95% confidence level. Therefore, we can conclude that regardless of the applied algorithm (ranger or cubist), the differing importance of individual variables yields a similar trend value. Moving forward, when obtaining similar accuracy assessment results, a statistically comparable trend value is achieved. However, referring to the trend result obtained for the CART model, it was found to be statistically significantly different from the other algorithms. Furthermore, the mean value of the obtained trend was lower by approximately 0.14 – 0.20 µg/m³. This indicates that choosing the decision tree model, which is characterised by distinctly lower evaluation parameters, tends to underestimate the PM₁₀ trend level.

The variability of monthly average normalised concentrations, presented in Figure. 6, indicates that in the case of the CART model, it is not possible to detect interventions, thus limiting the application of the normalisation algorithm [1]. On the other hand, two distinct interventions were identified in the case of the other algorithms, where the cubist model proved to be more sensitive. This suggests that it may be significantly more useful for identifying the effects of remedial actions introduced. Mallet (2021) [16] also conducted an analysis of PM₁₀ concentration trends using the Random Forest and Gradient Boosted Regression models. The results obtained from both models were very close (the difference was only 0.1 µg/m³) and accurately reflected actual data. Similarly to our research, they did not show statistically significant differences as their confidence intervals overlapped. This indicates that models with similar accuracy, but not necessarily consistent structures (e.g., in terms of variable importance), can yield statistically similar results in trend analysis.

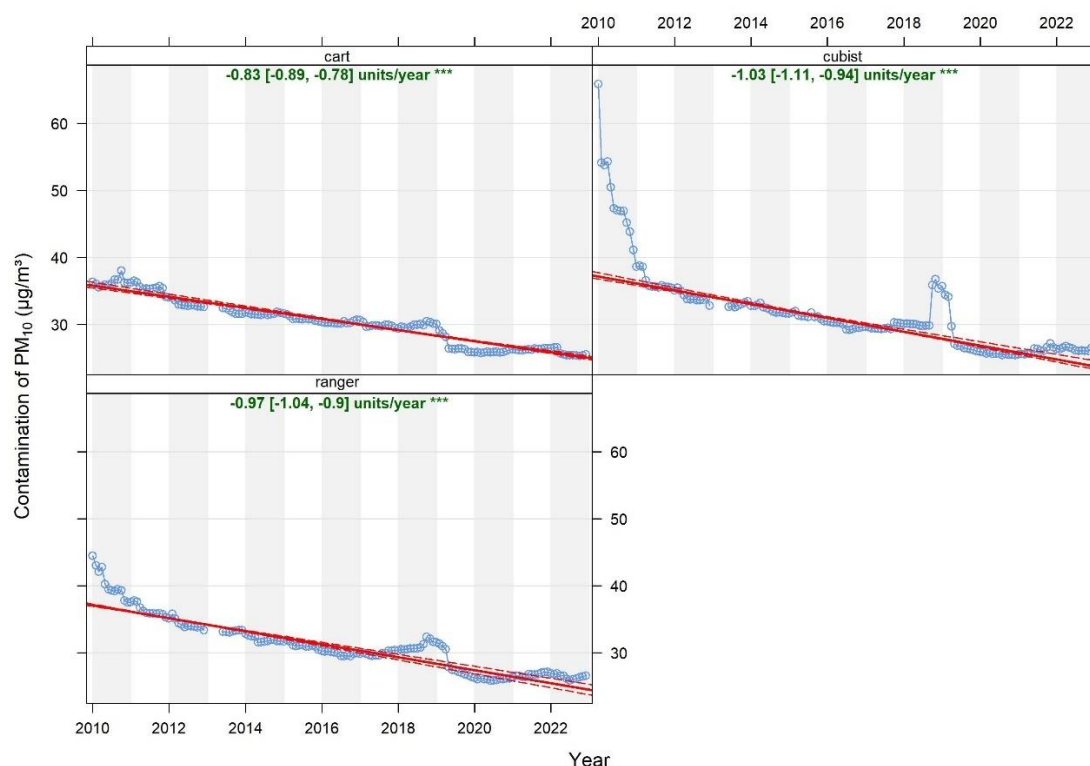


Figure 6. Graphical representation of the PM₁₀ concentration trend with 95% confidence intervals, determined using three machine learning algorithms.

4. Conclusions

The comparison of three algorithms reveals that the Random Forest (ranger) and Cubist Rules models achieved very similar accuracy in predicting PM₁₀ concentrations. Ranger demonstrated a slightly higher Pearson correlation coefficient (0.89 vs 0.88 for Cubist), while cubist had a marginally lower RMSE (14.06 vs 14.09 µg/m³). Both models had identical values for the coefficient of efficiency (0.52) and Willmott's index of agreement (0.76). The CART model exhibited noticeably worse results across all metrics (RMSE: 19.96 µg/m³, COE: 0.33).

The variable importance analysis demonstrated that air temperature (tt) and boundary layer height (blh) were the most significant predictors across all models. Removing the temperature variable led to an increase in RMSE to over 20 µg/m³ (median: 23.9 for Ranger, 21.5 for Cubist, and 31.6 for CART), while removing blh resulted in an RMSE exceeding 19 µg/m³. Temporal variables, such as date and day of the year, also had a significant impact, whereas parameters like the day of the week or cloud base height proved to be of little importance.

Meteorological normalisation results demonstrated statistically significant downward PM₁₀ trends across all models. The cubist model indicated the largest average annual decrease (-1.03 µg/m³), while the CART model showed the smallest (-0.83 µg/m³). It is important to note that the confidence intervals for cubist and ranger overlapped, signifying no significant difference between these models. The Cubist model proved particularly effective in identifying the impact of political interventions on air quality.

Despite the observed improvement in air quality (a 43.4% reduction in PM₁₀ concentrations between 2010 and 2022), the annual average concentrations in Tarnów still exceed both WHO guidelines (15 µg/m³) and the new EU standards (20 µg/m³). These results emphasise the need for further remedial actions in air protection. This demonstrates that municipal interventions, such as emission reduction programs aimed at achieving the required air quality standards, are yielding benefits. While air quality in Tarnów is improving, continued mobilisation by the local government

and residents is essential to strive for the achievement of the new, lower permissible PM₁₀ concentration levels and other air pollution standards established by the European Parliament and the Council of the European Union.

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Data Availability Statement: The datasets of this study are not publicly available. However, they may be made available upon reasonable request by the author.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

EU	European Union
WHO	World Health Organization
PM ₁₀	Particulate matter
NO _x	Nitrogen oxide
NO ₂	Nitrogen dioxide
SO ₂	Sulfur dioxide
CO	Carbon monoxide
O ₃	Ozone
RF	Random Forest
GBM	Gradient Boosted Regression Model
ws	Wind speed
wd_cut	Wind direction
rh	Relative humidity
tt	Air temperature
pres	Atmospheric pressure
blh	Boundary layer height
cbh	Cloud base height
ssr	Surface net solar radiation
cart	Decision Tree Model
ranger	Random Forest Model
cubist	Cubist Rules Model
jday	Julian day
wday	Day of the week
hour	Hour of the day
FAC2	Fraction of predictions within a factor of two
MB	The mean bias

MGE	The mean gross error
NMB	The normalised mean bias
NMGE	The normalised mean gross error
RMSE	The root mean square error
r	The Pearson correlation coefficient
COE	The Coefficient of Efficiency
IOA	The Index of Agreement based on Willmott
R2	The coefficient of determination
EMA	Exploratory Model Analysis

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