Performance Evaluation of Various Regression Models and Features for Prediction of Ozone Concentration

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Abstract

Air pollution caused by ozone is a problem which threaten human health. Therefore, prediction of O₃ concentration is important. In this work, O₃ concentration level for Adana, Turkey is predicted with support vector regression (SVR), multi-layer perceptron (MLP), gradient boosting decision trees (GBDT), K nearest neighbors (KNN), elastic net machine learning methods. Parameters utilized for this prediction are hourly measurement of pollutants like particular matter (PM10), sulfur dioxide (SO₂), nitrogen dioxide (NO₂), nitrogen oxides (NOₓ), nitric oxide (NO) concentrations and also meteorological parameters like air temperature, wind speed, relative humidity, air pressure, wind direction. Additionally, hour, day and season information are used as features. It has been shown that SVR method achieves the best result with R² value of 0.9697. Furthermore, backward elimination method is implemented for feature selection process and according to the results, current O₃ concentration has the highest importance to predict the concentration for the next hour.

Keywords: Air quality, Ozone concentration, Machine learning, Regression

Ozon Konsantrasyonu Tahmininde Çeşitli Regresyon Modelleri ve Özünteliklerin Performans Değerlendirmesi

Öz

Ozonun hava kirliliği, insan sağlığı tehdit eden bir problemidir. Bu nedenle, O₃ konsantrasyonunun tahmini önemlidir. Çalışmada, Türkiye’nin Adana il için O₃ konsantrasyon seviyesi, destek vektör regression (DVR), multi-layer perceptron (ÇKA), gradyan artırma karar ağaçları (ÇAKA), K en yakın komşu (KEK) ve elastik net makinesi öğrenme yöntemleri kullanılarak tahmin edilmiştir. Bu tahmin için kullanılan parametreler, partiküler madde (PM10), sülfür dioksit (SO₂), azot dioksit (NO₂), azot oksitler (NOₓ), azot monoksit (NO) gibi meteorolojik parametrelerin saatlik ölçümleridir. Ek olarak saat, gün ve sezon bilgileri de parametre olarak kullanılarak tahmin yapmıştır. DVR yöntemi ile elde edilen R² değeri 0,9697 olup diğer yöntemlerle elde edilen değerlerden yüksektir. Ayrıca öznitelik seçimi için genelde doğru eleme yöntemi uygunluğunu ve sonuçlara göre bir sonraki saatin O₃ konsantrasyonunu tahmin etmek için şimdiki O₃ konsantrasyonunun en önemli öznitelik olduğu görülmüştür.

Anahtar Kelimeler: Hava kalitesi, Ozon konsantrasyonu, Makine öğrenmesi, Regresyon

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1. INTRODUCTION

Tropospheric ozone ($O_3$) is an air pollutant that has negative effects on human health and climate change [1,2]. Since $O_3$ is not released directly into the air, it is considered as a secondary pollutant. With industrialization without emissions controls, the release of precursors to $O_3$, such as nitrogen oxides ($NO_x$) and volatile organic compounds (VOCs), are gradually increasing [3]. In addition, $O_3$ formation is related with some meteorological parameters like temperature, wind speed, wind direction and rainfall. [4].

Negative effects of $O_3$ and the other air pollutants are admitted worldwide. Thus, limits for hazardous levels of these air pollutants are officially determined by the governments. In Turkey, these limits are set as 500 µg/m³ for sulfur dioxide (SO₂), 400 µg/m³ for nitrogen dioxide (NO₂), 240 µg/m³ for $O_3$ [5]. Besides, having high concentration of these gases in the air is dangerous for those people having health conditions like asthma or chronic obstructive pulmonary disease (COPD). Considering this information, determination of $O_3$ concentration in the atmosphere is an important problem not only for air pollution analysis, but also for medical purposes.

Various machine learning methods have been utilized in the literature for estimation of pollutant gas concentrations. For instance, in some of the previous works, threshold values or concentration ranges have been determined for air pollutants and air pollution estimation have been done with classification methods such as decision trees, random forest classification, and artificial neural networks (ANN) [6-8]. In addition, various regression methods were used for concentration estimates [9-13]. For instance, root mean square error (RMSE) values obtained through support vector regression (SVR), ANN and decision tree methods were compared in estimation of $O_3$, SO₂ and NO₂ concentration levels [9]. It was shown that SVR produces the lowest RMSE value. In another study, regression models such as linear regression, ridge regression, multilayer perceptron (MLP), Elman neural network were used for prediction of $O_3$ level [10]. Among these methods, the best RMSE result was obtained with the MLP method. Besides, the results of a study handled in Canada shown that extreme learning machine (ELM) method outperformed ANN and multiple linear regression (MLR) to predict $O_3$, particular matter 2.5 micrometers or less in diameter (PM2.5) and NO₂ concentration levels [11]. In another comparative study, ANN was shown to be giving better results than MLR method in predicting the maximum hourly $O_3$ concentration for the next day [12]. On the other hand, algorithms utilizing deep learning methods are mentioned in more recent studies. For example, a new deep learning model to forecasting of $O_3$ concentration was proposed by researchers in Aarhus, Denmark [13]. According to the results of the study, this new method outperformed SVR, ANN and MLR methods.

Instead of predicting the parameters related with air pollution, it is also possible to analyze the correlation between the pollutant gases. For example, relationship of $O_3$ concentration with other gas concentrations and meteorological parameters are analyzed using ANN and support vector machines (SVM) methods [14]. It has been verified that the $O_3$ concentration was negatively correlated with carbon monoxide (CO), nitric oxide (NO) and NOₓ as these pollutants are known precursors of $O_3$.

In this study, $O_3$ concentration for Adana, Turkey is estimated using five different machine learning methods. These methods are SVR, MLP, gradient boosting decision tree (GBDT), K nearest neighbors (KNN), and elastic net. Measurements for various gases (particular matter 10 micrometers or less in diameter (PM10), SO₂, NO₂, NOₓ, NO, $O_3$) and meteorological parameters together with temporal data are used as features. Additionally, backward feature elimination method is used for determining the most appropriate predictors for $O_3$ estimation and select a subset of features that are more useful in modeling $O_3$ level.
2. MATERIALS AND METHODS

2.1. Machine Learning Methods

SVM is a supervised learning method used for binary classification problems [15]. In this method, a given dataset is non-linearly mapped to a higher dimensional feature space. For classification problems, in this feature space, data is separated by hyperplanes with the maximum margin between class boundary. SVM can also be used for regression (SVR) or multi-label classification problems.

The performance of an SVR model highly depends on choice of kernel function for mapping and parameters C and ε. In this work Gaussian kernel function is used. This kernel has only one parameter, γ, which is associated with the width of the Gaussian function. On the other hand, C and ε parameters control the tradeoff between the variance and bias in the training process. Therefore, careful selection of these parameters is important. For this purpose, best combination of these parameters is searched in a grid space. As a result, optimum parameters are found as 100 for C, 0.01 for γ and 0.1 for ε.

MLP is a feed-forward ANN [16]. MLP network consists of the input, hidden, and output layers with their nodes called neurons [17]. There can be multiple hidden layers between the input layer and the output layer. The inputs of each neuron are multiplied by a value called weight and all of them are summed up and passed through the activation function. Widely used activation functions are sigmoid, step, linear, hyperbolic tangent and rectified linear unit (ReLU). The output of this activation function is transferred to the next layer in the same way. Each node in one layer is connected to each node in the next layer. Also, back-propagation method is used for updating the weights and reduce the error. In this method, number of neurons in hidden layer can affect the performance of model. The network structure used in this work consist of one hidden layer containing 50 neurons.

Elastic net is a regularization and variable selection method. Elastic net regression is mixture of lasso and ridge regression models. This method is particularly useful when the number of features is much bigger than the number of data samples and when there are correlated features [18]. The formulation of the elastic net regression model is as where λ₁ and λ₂ are regularization parameters, X is sample matrix, y is response vector, β is weight vector (Equation 1).

$$\hat{\beta} = \arg\min_{\beta} |y-X\beta|^2 + \lambda_2|\beta|^2 + \lambda_1|\beta|$$  (1)

For this method, parameter selection is applied to choose the best λ₁ and λ₂ parameters and optimum values of these parameters are found as 0.009 for λ₁ and 0.0005 for λ₂.

GBDT is a machine learning method for regression and classification problems [19]. Considering decision trees as weak learners, GBDT algorithm is a strong learner created by combining many decision trees. A single decision tree tends to overfitting, while a GBDT reduces the risk of overfitting [20]. Each new decision tree in the gradient boosting algorithm is created using the residuals from the previous step.

Number of weak learners is the key parameter that affects the performance of the GBDT method. This parameter should be well adjusted in order to prevent overfitting. After trying several values, it has been determined that 200 is appropriate for this parameter.

KNN algorithm is another machine learning method used in this study. Due to its simplicity and straightforward idea, it is a very common method [21]. In this method, the distance values between a test sample and all training samples are calculated. The K nearest samples to the test sample is used for classification or regression. The key part in this algorithm is to choose the optimum value of K. For this study, models have been trained with K values between 1 and 5 and optimum K value is found as 4.
2.2. The Dataset

The dataset was obtained from the air monitoring database of the Republic of Turkey Ministry of Environment and Urbanization [22]. The download settings were adjusted to include hourly data for gas concentrations such as PM10, SO2, NO2, NOx, NO, O3 and meteorological parameters such as air temperature, wind speed, relative humidity, air pressure and wind direction. All data between the years 2016 and 2020 were downloaded. However, the proportion of missing data was very high. After removing the samples containing missing data, total of 11 weeks of data was obtained which is used for prediction of O3 concentration. Hourly change of the gas concentrations for one week for duration of the data is shown in Figure 1.

![Figure 1. Hourly change of gas concentrations for one week of data](image)

Since the pollutant gas concentrations vary with time, the involvement of temporal features to the dataset may have positive effect on the prediction performance. Therefore, three temporal information (day, hour and season information) were added as new features by using one hot encoding method. In one-hot encoding method, categorical variables are represented as vectors. The related element in the set of categorical variables is represented by 1 and other elements by 0. Hence, in this study, 24 new columns were added to represent “hour of day” information, 7 new columns were added to represent “day of week” information and 4 new columns were added to represent “season of year” information. Using the timestamp of each row, the related hour, day and season column was set as 1 while other columns were assigned 0.

In addition to the temporal features, O3 concentrations belonging to five different previous measurements were added as new features. These previous data are O3 values for one week ago, one day ago, three hours ago, two hours ago and one hour ago of the O3 concentration to be predicted. Eventually, a dataset containing 1848 rows and 51 columns was obtained.

2.3. Experiments

70% of the dataset was randomly selected as training set and the remaining part was left as test set. Since the continuous features in the dataset had been on different scales, these features were scaled through z-score normalization given by

$$Z = \frac{X - \mu}{\sigma}$$

where $\mu$, $\sigma$ are mean and standard deviation of the feature vector $X$, respectively (Equation 2).

In order to estimate O3 concentration for the next hour, SVR, MLP, GBDT, KNN, elastic net models were trained with the optimum parameters given in section 0. In addition, $R^2$, RMSE, mean absolute error (MAE), mean absolute percentage error (MAPE) metrics were used for performance evaluation of the models.

In addition to estimation of O3 concentration using all 50 features, a subset of features giving higher test performance was searched through backward feature elimination method. This method is a feature selection process where one feature is removed at every step [23]. The difference in test performance caused by individual removal of every single feature is observed and the feature whose removal generates the higher performance is discarded. These steps are then repeated for the remaining features until the desired number of
3. RESULTS AND DISCUSSION

Prediction performances of the machine learning methods trained using all the features are given in Table 1. As can be seen in Table 1, the highest $R^2$ value is achieved by the SVR method followed by elastic net and GBDT methods, respectively (Figure 2). Additionally, the lowest RMSE, MAE and MAPE values are obtained by SVR as well. KNN and MLP methods have poor performance compared with the others for the problem in this study. While MLP has better performance than KNN in RMSE and $R^2$ metrics, KNN has better performance than MLP in MAE and MAPE metrics.

### Table 1. Prediction results of the methods when all features are used

|       | RMSE | MAE  | MAPE | $R^2$ |
|-------|------|------|------|-------|
| SVR   | 4.8119 | 2.9961 | 7.8820 | 0.9697 |
| GBDT  | 5.0216 | 3.2637 | 8.8934 | 0.9670 |
| MLP   | 5.2853 | 3.6139 | 9.9880 | 0.9635 |
| KNN   | 5.5198 | 3.5452 | 9.5762 | 0.9601 |
| Elastic net | 5.0178 | 3.2144 | 8.5179 | 0.9671 |

Figure 2. Predictions versus actual $O_3$ concentrations for SVR method

The $R^2$ values at every step of backward elimination for all of the methods are given in Table 2. For SVR method, removal of PM10 and relative humidity features does not affect the performance so these two features are considered to be redundant. Besides, removal of a feature does not necessarily cause a decrement in the performance. This is true when a feature does not represent the target value well. In other words, presence of such features makes it more complicated to model the data, hence causes low performance. Some examples of this situation can be seen in Table 2. For instance, performance of MLP method is increased when PM10 feature is removed. Similarly, for the same feature, higher $R^2$ values are obtained in GBDT and KNN methods. Furthermore, the same single feature, which is current $O_3$ concentration, has remained at the final step of the backward elimination in all of the methods. This means that the current $O_3$ concentration has the highest importance on prediction of the $O_3$ concentration for the next hour.

4. CONCLUSION

Air pollution has harmful impact on human health and environment. Estimation of air pollutants concentration is a major significance for any country. In this work, different machine learning methods are used for prediction of hourly $O_3$ concentration in Adana, Turkey. Although, the performance measures of all methods used in this study are satisfactory and their results are close each other, SVR outperformed other machine learning methods.

Furthermore, feature selection is implemented to find the best feature subsets and analyze the effect of features on the performance of models. The results indicate that the current $O_3$ concentration has the highest importance for predicting the $O_3$ concentration of the next hour. It has been observed that using only the current $O_3$ concentration as a single feature can yield $R^2$ values above 0.95.
Table 2. Feature selection results. (RH: Relative humidity, AP: Air pressure, WS: Wind speed, WD: Wind direction, T: Temperature, 1wpO₃: One week previous O₃, 1dpO₃: One day previous O₃, 2hpO₃: Two hour previous O₃, 1hpO₃: One hour previous O₃, Date: All temporal features generated via one hot encoding)

| SVR    | Removed feature | R² after removed | Removed feature | R² after removed | Removed feature | R² after removed | Removed feature | R² after removed | Removed feature | R² after removed | Removed feature | R² after removed |
|--------|-----------------|------------------|-----------------|------------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| PM10   | 0.9697          | 1wpO₃            | 0.9690          | 1dpO₃            | 0.9678          | 1hpO₃           | 0.9604          | SO₂             | 0.9673          |                  |                 |                 |
| RH     | 0.9697          | PM10             | 0.9705          | NOₓ             | 0.9675          | PM10            | 0.9611          | 1wpO₃           | 0.9673          |                  |                 |                 |
| AP     | 0.9695          | RH               | 0.9712          | RH              | 0.9678          | SO₂             | 0.9626          | WS              | 0.9674          |                  |                 |                 |
| SO₂    | 0.9693          | AP               | 0.9717          | WD              | 0.9681          | 1dpO₃           | 0.9625          | RH              | 0.9674          |                  |                 |                 |
| NO     | 0.9691          | NO               | 0.9708          | NO              | 0.9681          | AP              | 0.9624          | NO              | 0.9674          |                  |                 |                 |
| NO₂    | 0.9690          | SO₂              | 0.9710          | AP              | 0.9674          | NO              | 0.9619          | T               | 0.9674          |                  |                 |                 |
| WS     | 0.9687          | 2hpO₃            | 0.9709          | 2hpO₃           | 0.9678          | T               | 0.9589          | PM10            | 0.9673          |                  |                 |                 |
| 1wpO₃  | 0.9686          | T                | 0.9724          | 1wpO₃           | 0.9675          | NOₓ             | 0.9583          | NO              | 0.9673          |                  |                 |                 |
| NO₂    | 0.9685          | Date             | 0.9694          | PM10            | 0.9681          | RH              | 0.9563          | AP              | 0.9671          |                  |                 |                 |
| T      | 0.9683          | WD               | 0.9680          | 1hpO₃           | 0.9677          | NOₓ             | 0.9515          | NO              | 0.9669          |                  |                 |                 |
| 1hpO₃  | 0.9677          | WS               | 0.9675          | WS              | 0.9658          | 2hpO₃           | 0.9477          | 2hpO₃           | 0.9667          |                  |                 |                 |
| WD     | 0.9670          | NOₓ              | 0.9677          | SO₂             | 0.9658          | WD              | 0.9406          | WD              | 0.9664          |                  |                 |                 |
| Date   | 0.9650          | NOₓ              | 0.9653          | NO₂             | 0.9650          | Date            | 0.9451          | Date            | 0.9651          |                  |                 |                 |
| 1dpO₃  | 0.9604          | 1dpO₃            | 0.9611          | T               | 0.9644          | WS              | 0.9459          | 1dpO₃           | 0.9608          |                  |                 |                 |
| 2hpO₃  | 0.9534          | 1hpO₃            | 0.9531          | Date            | 0.9448          | 1wpO₃           | 0.925           | 1hpO₃           | 0.9532          |                  |                 |                 |

Besides, PM10 and relative humidity are found to least important features as they are removed at initial steps of the backward elimination.

In addition, this work can be extended by using of parameters like solar radiation, rainfall, CO concentration and this may improve the performance of prediction models. Also, collection of more and clean data will definitely allow for deeper analysis.

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