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Comparative study on total nitrogen prediction in wastewater treatment plant and effect of various feature selection methods on machine learning algorithms performance

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Abstract

Wastewater characteristics prediction in wastewater treatment plants (WWTPs) is valuable and can reduce the number of sampling, energy, and cost. Feature Selection (FS) methods are used in the pre-processing section for enhancing the model performance. This study aims to evaluate the effect of seven different FS methods (filter, wrapper, and embedded methods) on enhancing the prediction accuracy for total nitrogen (TN) in the WWTP influent flow. Four scenarios based on FS suggestions were defined and compared by three supervised Machine Learning (ML) algorithms, i.e. Artificial Neural Network (ANN), Random Forest (RF), and especially Gradient Boosting Machine (GBM). Input parameters, as daily time-series including pH, DO, COD, BOD, MLSS, MLVSS, NH_4-N, and TN concentration, were used. Data set divided into train and unseen test data-sets, and performance precision of all models was carried out based on Root Mean Square Error (RMSE), Mean Absolute Error (MAE), and correlation coefficient (R^2). Results reveal that scenario IV which was suggested by Mutual Information, including NH_4-N, COD, BOD, and DO had the best result rather than other FS methods. Furthermore, decision tree algorithms (RF and GBM) revealed better performance results in comparison to neural network algorithm (ANN). GBM generalized the dataset patterns very well and

produced the best performance on unseen data-set, which shows the effectiveness of this state-of-the-art ML algorithm for wastewater components prediction.

Keywords: *ANN; RF; GBM; Feature selection; total nitrogen*

1 Introduction

Nitrogen is one of the major wastewater pollutions, which should be reduced to the standard level before discharging wastewater to the environment [1, 2]. Total nitrogen (TN) is primarily presented in wastewater as ammonia, nitrite, nitrate, and organically bonded nitrogen [3]. Monitoring the TN from the influent of wastewater treatment plants (WWTPs) plays a significant role in the performance of nutrient removal systems, controlling sludge production, and operation of different parts of wastewater treatment processes [4].

Wastewater parameters especially nutrient compounds are really important for engineers to understand and calculate at the beginning and end of treatment [5]. To obtain the necessary information, the operator should determine the characteristics of the raw wastewater by receiving data from sensors or collecting samples and analyzing the influent/effluent flow of the plant. Insufficiently treated wastewater which is one of the nutrient sources can cause many health problems by entering into the water bodies like groundwater systems [6]. However, many facilities have been upgraded by WWTPs to progress in the removal of nutrient pollutants which resulting in a drastic decrease in the discharged nutrients from WWTPs [7, 8].

Artificial Intelligent (AI) technics, mostly used to predict natural or artificial processes in various disciplines. Machine learning (ML) as a subset of AI, is a process of recognizing a special pattern based on the given data for prediction or classification purposes [9]. Recently, modeling and prediction of environmental phenomena using AI technics are rapidly increased due to their high accuracy rather than mechanistic models [10]. These algorithms can learn sophisticated relations more efficiently than statistical methods [11-13].

A fully connected neural network known as ANN model acts as a universal function estimator, and each neuron in the network contains learnable parameters (weight and bias). A feed-forward ANN can be used for WWTPs influent and or effluent quality prediction [14, 15].

Many studies have been addressed to model the influent or effluent wastewater parameters. For instance, ANN models are employed to estimate the methane production in a biogas optimization scenario while having (R^2=0.87) [16]. Also, another similar modeling was conducted to follow the correlation of supplements membrane bioreactor of WWTP [17]. Ansari et al. integrated a hybrid genetic algorithm with fuzzy logic (GA-FIS) model to increase the prediction of missing value in the wastewater parameters record like COD, BOD, and NH_4-N and compared it with fuzzy logic (ANFIS) model. Results presented that integrated GA-FIS had lower errors in contrast to ANFIS prediction [18]. In another study, Abba et al. studied an extreme learning machine (ELM) model combined with kernel principal component analysis (KPCA) for prediction of pH, turbidity, total dissolved solids, and hardness, which had the highest accuracy for almost all predicted components (R^2> 0.95) [19]. Random forest (RF) and Gradient Boosting Machine (GBM) are other state-of-the-art and powerful ML methods [20-22]. An RF prediction model was found a useful and powerful method for the evaluation of reliability prediction of small WWTPs in the UK [23].

On the other hand, the feature selection (FS) process is utilized in the pre-processing section for increasing the speed of training and enhancing the prediction precision as well as simplifying the models [24]. Although there have been many different FS methods, most forecasting studies just use correlation models, like the Pearson correlation method. Hence, a comparative evaluation of the FS effect on enhancing the accuracy of simulation for WWTPs components is still required. Also, prediction of WWTP components with RF and GBM is less used in comparison to other ML techniques i.e. ANN, SVM, etc. [23, 25, 26].

This study aims to investigate the effect of various feature selection methods for enhancing the prediction performance of TN in the WWTPs. The specific objectives of this paper are: i) Defining scenarios according to the different FS suggestions and compare together, ii) Create ML models by using algorithms such as ANN, RF, and GBM for comparing scenarios and find the best TN forecasting model, and iii) Evaluate the potential of using a state-of-the-art GBM algorithm as a new ML model for TN prediction and compared with the conventional methods (RF and ANN).

2 Methodology

2.1 Case study of WWTP and data description

In this research, a data set from North Torbat WWTP for nutrients removal which is located in the north of Iran was investigated. This WWTP is designed for a population of 350,000 PE with a mean-daily influent flow of 71,500 m^3/d. The WWTP consists of a primary sedimentation tank, anaerobic/aerobic reactors, and a clarifier. The pH and DO are monitored using online sensors, and the rest of the influent characteristics are recorded using sampling and analysis based on the standard for wastewater analysis method [27].

A data set consisting of 800 records (almost 2.5 years between 2015-2017) daily recording of total nitrogen (TN), Ammonia nitrogen (NH_4-N), biological oxygen demand (BOD), chemical oxygen demand (COD), mixed liquor suspended solids (MLSS), Mixed liquor volatile suspended solid (MLVSS), pH, dissolved oxygen (DO) for the training of models. Also, 30 days from the last data set was selected for the test of models (unseen data).

Furthermore, for obtaining an accurate model, the data set should be normalized, and unnecessary (redundant) features should be eliminated (feature selection) to avoid overfitting issues [28, 29]. One of the main points of this study is to compare different applicable feature selection methods and their effects on model precision. TN was selected as a target of prediction in this study due to the level of importance in the WWTPs as a critical influent quality index and the rest of parameters were selected as input data based on feature selection ranking.

2.2 Feature selection (FS)

The main goal of feature selection (FS) is to obtain the most relevant input data from a dataset. Considering a dataset with M features, then 2^M subsets of features are available, and the FS methods are responsible for introducing the best subset. In each method, related to the criterion and application of the model several functions are responsible to optimize and evaluate the subset. The FS methods are divided into three major categories: filters, wrappers, and embedded methods [30- 32].

Filter methods emphasize on characteristics of each feature and they evaluate the features based on the properties without employing any clustering algorithm to guide the search [30]. Wrapper methods use clustering algorithms. If the introduced subset increased the accuracy of the clustering algorithms, then the subset earns a higher score [30]. Embedded techniques combine all the advantages of wrappers and filters. They construct an ML algorithm, and it performs feature selection while training the model [33].

In this study, variance threshold [34], analysis of variance (ANOVA) [35], mutual information (MI) [36,37], Pearson correlation (PC) [38], backward elimination (BE) [39], random forest (RF) [40], and Least Absolute Shrinkage and Selection Operator (LASSO) were used [41,42]. The details of each method can be found in supplementary information.

2.3 Modeling approaches

2.3.1 Artificial neural networks (ANNs)

An artificial neural network (ANN) is a fully connected multilayer perceptron (MLP) with three layers: input, hidden, and output (Fig. 1). The network may have several hidden layers concerning the level of complexity of the data set [43, 44].

In this study, the number of input neurons of the model is equal to the number of input features which depends on the scenario (considered subset). Also, two hidden layers with 15 and 10 neurons are designed to capture the complexity of the model. For having a smooth and accurate connection between layers, we used the ReLU activation function for the hidden layers. Finally, there is a single neuron in the output layer to predict the target variable (TN). The optimization process was performed by Adam's algorithm concerning the mean squared error (MSE) as a loss function with 100 epochs.

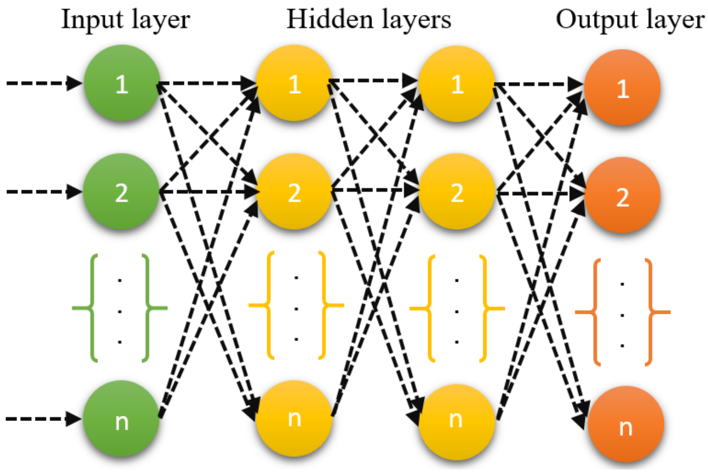


Fig. 1. Fully connected artificial neural network (ANN)

2.3.2 *Random forest (RF)*

Ensemble learning is a technique that combines the prediction results of multiple algorithms to obtain a better final result. Random forest (RF) is an ensemble method that uses bootstrap aggregation to generate decision trees. The final output of the model is an aggregation of the prediction based on the decision trees (Fig. 2). This method helps to consider all potential features fairly and prevents trees to become highly correlated [45]. In this study, after many trials and errors, a random forest tree was developed considering, 400 trees in the forest, a maximum depth of 70 for each tree, minimum of 4 samples at a leaf, and a minimum number of 10 samples required to split.

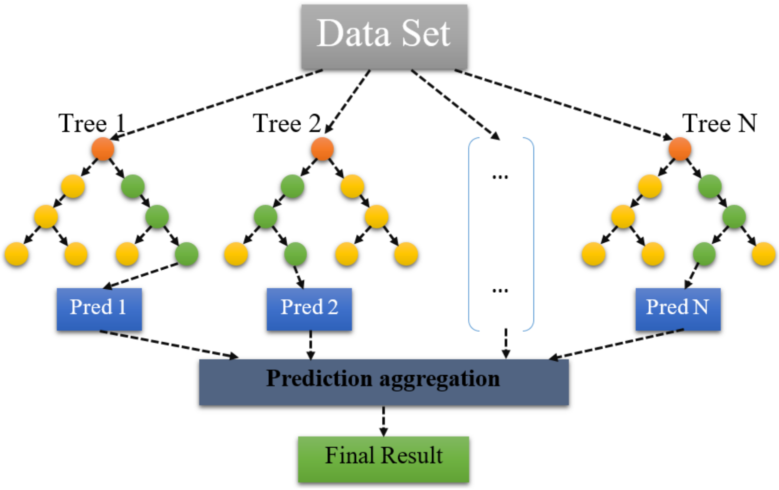


Fig. 2. Random forest architecture

2.3.3 *Gradient boosting machine (GBM)*

Gradient boosting machine is a decision tree based ML algorithm similar to RF, but it has a different constructive strategy of the ensemble formation. In a boosting approach, we add new trees to the ensemble sequentially according to the error of the whole ensemble prediction. As we add new trees with a constant learning rate, the estimation error regarding the dependent variable shrinks continuously until reaching the maximum possible precision. Due to the nature of GBM, hyper-parameters justification is extremely important [46]. In the current research, after many trials, we used a gradient boosting machine with considering the learning rate of 0.05 for training, 2000 trees in the forest, subsampling of a total of 0.8, a min sample leaf of 50, a tree depth of 6, and 600 as minimum split samples.

2.4 Model construction

The total data set was divided into two groups: train data (almost 90% of total data-set) and test data (10% of the total data set) as unseen data, followed by applying to preprocess, and feature selection methods. Furthermore, four scenarios were defined to compare the feature selection methods. Also, for the prediction of the target (TN), three prediction models containing fully connected artificial neural network (ANN), random forest (RF), and state-of-the-art gradient boosting machine (GBM) were selected and applied for all sub-data-sets. The normalized data were used as input data for training and testing all models. After defining different scenarios and model structures, the TN concentration was forecasted by noted models, then the predicted values were compared to the real data to evaluate the model accuracy (Fig. 3~~5~~).

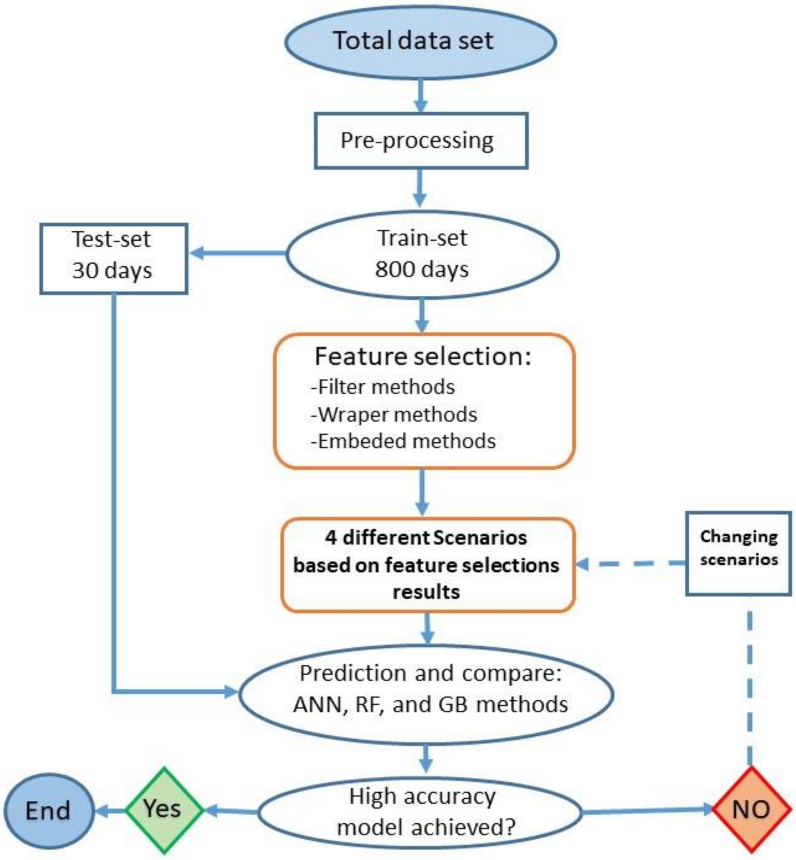


Fig. 3. Modeling and prediction structure

2.5 Model evaluation

To measure the quality and performance of a model, several model metrics can be employed depending on the model task, data types, and scenarios. In this article, models are scored based on the coefficient of determination (R^2) (Eq.1), root mean square error (RMSE) (Eq.2), and mean absolute error (MAE) (Eq.3) [47].

$$R^2 = 1 - \frac{\sum(a_i - p_i)^2}{(a_i - \mu_a)^2} \quad (1)$$

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(a_i - p_i)^2} \quad (2)$$

$$MAE = \frac{1}{n}\sum_{i=1}^{n}|a_i - p_i| \quad (3)$$

Where $i = 1,2,..n$ is the number of observations, and n is the total number of records. Considering a_i for output, p_i as real values, and μ_a as mean value.

3 Results and discussion

3.1 Data statistical information

A brief demonstration of primary statistical properties (Min, Mean, Max, and standard deviation) is represented in Table 1.

Table 1

Data set statistical properties

Parameters	**Units**	**Min**	**Mean**	**Max**	**SD**
pH	-	6.94	7.26	7.90	2.14
DO	mg/L	1.22	1.34	1.80	2.18
NH_4-N	mg/L	26.11	68.78	93.94	3.14
BOD	mg/L	205.40	505.83	858	4.21
COD	mg/L	367.36	1063.85	1881.6	4.87
MLSS	mg/L	148.80	554.17	1041.5	3.64
MLVSS	mg/L	99.7	366.39	697.87	3.51
TN	mg/L	35.81	91.60	125.73	3.16

3.2 *Summary of selected feature procedure*

Each FS method has a particular subset suggestion as described in Table 2. The variance threshold revealed the redundant features. Filter methods (ANOVA and MI) suggesting very similar subsets, and PC is indicating NH_4-N with the highest correlation to the target variable.

TN as the target of the prediction displayed a strong correlation with NH_4-N, COD, and BOD respectively, and a weak correlation with pH and DO as can be seen in the Pearson correlation result (supplementary file, Fig.S6). The highest correlation (~1.0) among input parameters belonged to MLSS and MLVSS, and the lowest value was related to BOD and pH.

Generally, FS algorithms are pointing at (NH_4-N, COD, and BOD) as the best possible subset, while LASSO is showing a different result. Besides, four scenarios as shown in Table 3 were grouped based on FS suggestions and they were compared with ANN, RF, and GBM techniques to introduce the best scenario. Details for the result of each FS process can be found in the supplementary information file.

Table 2

Summary of feature selection application on the data set

Method	**Subset**	**Description**
Variance	COD, MLSS, MLVSS, BOD, NH_4-N	Dropping redundant features
ANOVA	NH_4-N, COD, BOD, MLSS	Ranking based on the importance level
Mutual Information	NH_4-N, COD, BOD, DO	Ranking based on the importance level
Pairwise correlation	NH_4-N	Choosing highly correlated features (> 0.8) with target
Backward	NH_4-N, COD, BOD	Choosing features that increase the regression model performance reasonably
Random Forest	NH_4-N, COD, BOD, MLSS	Ranking based on Gini importance level
LASSO	NH_4-N, MLSS, MLVSS	Ranking based on the importance level

Table 3

Different scenarios defined in this study based on different feature selection methods

Scenario	Number of features	Suggested by	Name of features
I	1	Pairwise correlation	NH_4-N
II	3	LASSO	NH_4-N, MLSS, MLVSS
III	4	ANOVA, Random Forest, Backward Elimination	NH_4-N, COD, BOD, MLSS
IV	4	Mutual Information	NH_4-N, COD, BOD, DO

3.3 Prediction results

After training the models in various scenarios, the whole dataset was predicted by models (Fig. 4), then model metrics were calculated (R^2, RMSE, and MAE) for both training and test dataset. The model metrics of each scenario are described in both data sets (Table 4).

According to scenario I, with only one feature (NH_4-N), RF has the best performance on the training set, but its performance dropped significantly on the test data set which shows serious overfitting issues. Similarly, ANN and GBM lost their precision, but with a lower difference. These two models with R^2=0.52 had a better outcome for this scenario on the test data-set.

In scenario-II, although more features were introduced to the models and accuracy on the training set was increased, the performance on the test data-set was decreased. This result is indicating the introduced subset is not adding precision to the models, but it is causing overfitting issues. For these features, GBM has the best result on the test dataset with R^2=0.52.

In scenario-III, the RF has the highest accuracy on the training dataset and the lowest performance on the test dataset. In this scenario, ANN performance was increased slightly, so it is showing that this subset has a better outcome than the subset in scenario-II for neural network algorithms, while it is causing overfitting issues for decision tree algorithms (GBM and RF).

The last scenario (IV) showed better results compared to previous scenarios. As indicated in Table 4, the RMSE of test data of this scenario is 0.092, 0.095, and 0.095 for GBM, RF, and ANN respectively. In this scenario, RF had less overfitting, ANN performance was increased, and GBM had the best performance both on training set R^2=0.88 and test data-set R^2=0.58.

GBM has the highest precision followed by RF and ANN in scenario-IV. Also, among FS methods, Mutual Information has better performance, because it was the only technique that considered DO as effective variable.

The results revealed that how sensitive is ANN to selecting the wrong features. In scenario-II and scenario-III, with adding more features to the subset, the ANN metrics decreased on the test dataset. Similarly, RF with very high performance on the training dataset suffered from more overfitting issues due to introducing inefficient subsets in scenario-II and scenario-III. In contrast, GBM showed a more robust model. Introducing wrong features to GBM didn’t change the model performance considerably, and more or less it kept the performance level similar to previous subsets, but with introducing the best subset (scenario-IV), GBM showed an exceptional improvement in model evaluation. So, generally, it can be said that decision tree algorithms (RF and GBM) showed better performance than the neural network model (ANN).

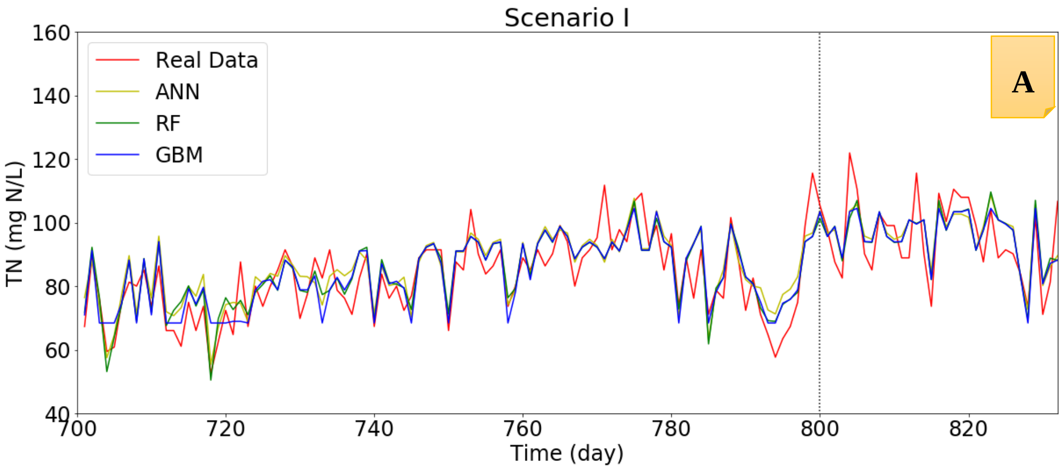
Table 4

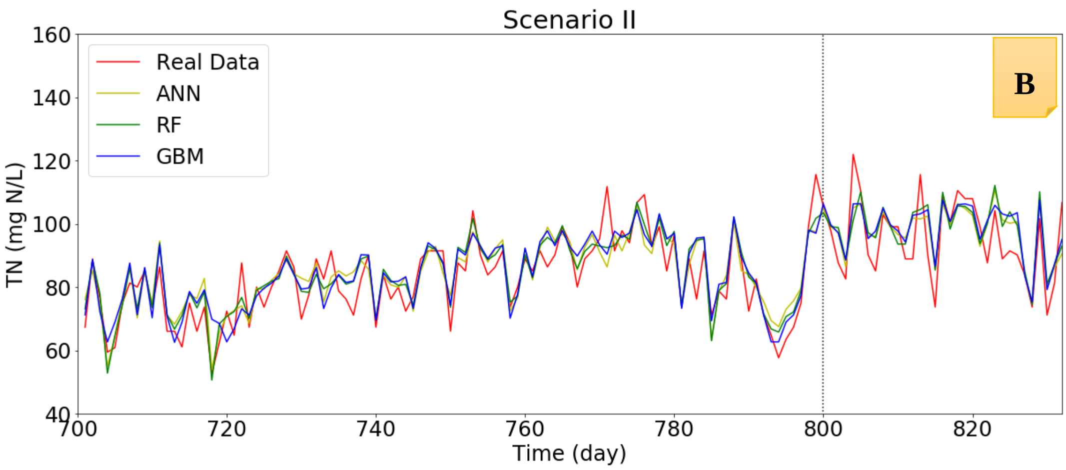
Model Metrics (accuracy and errors) of each prediction models

		Training Data			Test Data (unseen)		
	Model	R^2	RMSE	MAE	R^2	RMSE	MAE
Scenario I	ANN	0.77	77E-3	8E-5	0.52	94E-3	83E-4
	GBM	0.76	78E-3	3.5E-5	0.52	95E-3	57E-4
	RF	0.80	96E-3	5E-5	0.50	96E-3	104E-4
Scenario II	ANN	0.75	79E-3	18E-3	0.42	104E-3	51E-3
	GBM	0.81	72E-3	1E-3	0.52	95E-3	34E-3
	RF	0.88	60E-3	1.4E-3	0.46	100E-3	34E-3
Scenario III	ANN	0.79	74E-3	-5E-5	0.51	96E-3	28E-3
	GBM	0.84	68E-3	11E-4	0.51	96E-3	31E-3
	RF	0.89	55E-3	12E-4	0.48	98E-3	28E-3

Scenario IV	ANN	0.81	73E-3	56E-4	0.55	95E-3	22E-3
	GBM	**0.88**	**68E-3**	**4E-4**	**0.58**	**92E-3**	**17E-3**
	RF	0.83	55E-3	9E-4	0.55	95e-3	19E-3

According to Table 4 and Fig.4, comparing Scenario-I with scenario II and III, the accuracy of models on capturing the complexity of the training dataset was increased, while the model performance on the test dataset was not improved. This means that the model learned the training dataset very well, but not able to generalize the patterns perfectly. Among all models, RF has had the best match with real data on the training data set and faced more with overfitting issues. In Scenario-IV, GBM showed the best matching with real data, as well as, a great improvement in generalizing the patterns for the unseen dataset.





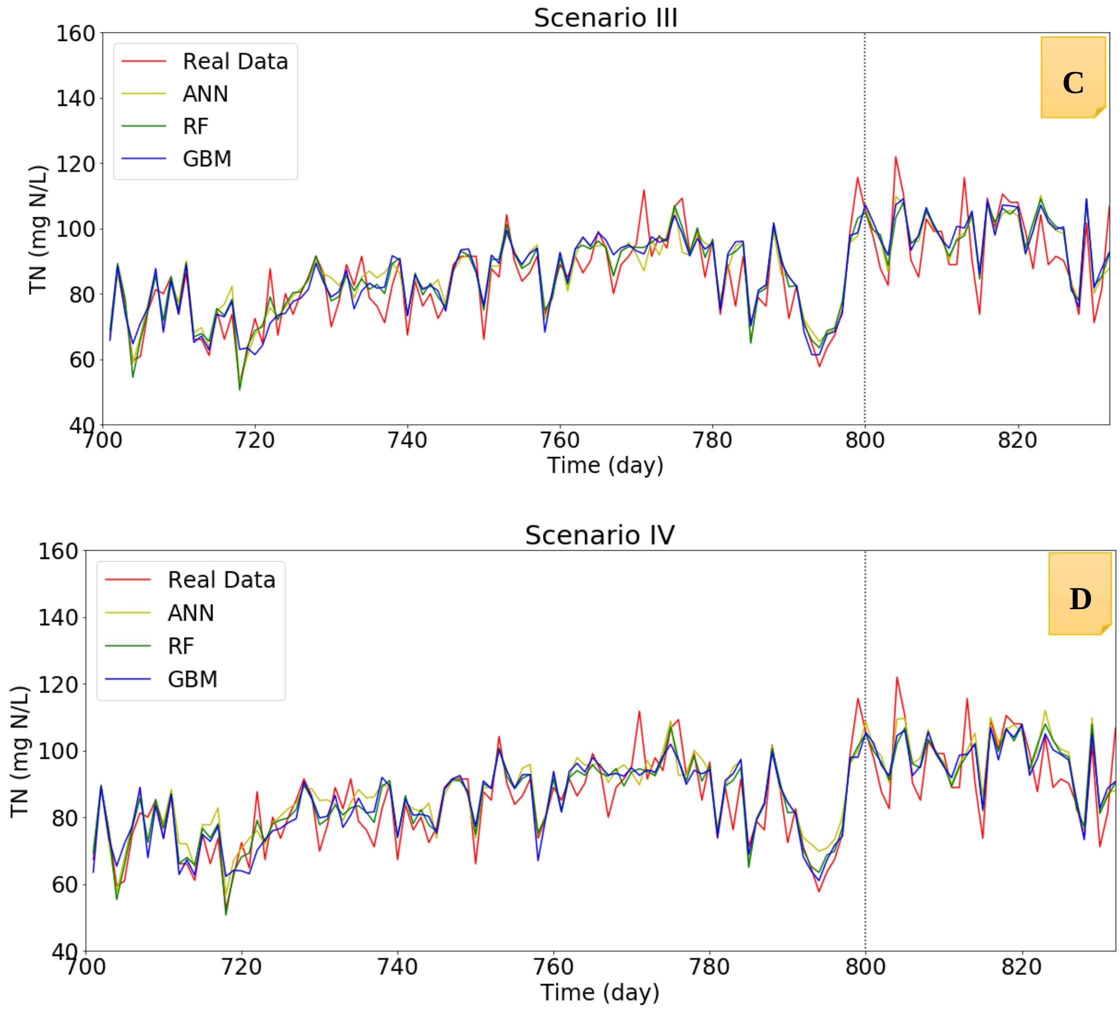


Fig. 4.- prediction of TN concentration for two sub-set of training (0-800 days) and unseen test data (800-830 days) for different scenarios, A) Scenario I, B) Scenario II, C) Scenario III, and D) Scenario IV

Prediction of critical characteristics like TN in the WWTP influent is a topic in which many researchers attempt to propose various methods to enhance precision. In recent approaches with ML methods and data-driven decision techniques, better results are demonstrated (Table 4).

It is noticeable that due to the sophisticated nature of different processes in WWTPs, there is no single adequate model for all types of similar issues. Consequently, this matter has required the improvement of more solid and effective models utilizing accessible information [48-52]. Table 5 shows the summarized information of recently TN prediction studies in various WWTPs

Table 5

Summary of different studies on TN prediction in the influent/effluent flow of wastewater

Feature selection methods	Prediction Algorithm	Model Accuracy (unseen data)	Remarks	References
Forward selection	parallel-serial hybrid	R^2=0.81, MSE=N/A	Combine ML models with mechanistic models (biological simulation) for increasing the model performance	Hvala et al. 2020 [50]
Latin Hypercube One factor At a Time (LH-OAT)	SVM, ANN	R^2=0.47, MSE=N/A	ANN showed better result rather than the SVM algorithm	Guo et al. 2015 [48]
Pearson Correlation	LSTM	R^2 =N/A MSE=0.015	LSTM needs lower training time and has high performance for predicting unseen dataset.	Yaqub et al. 2020 [49]
Forward Selection, Genetic algorithms, Pearson Correlation	k-fold model	N/A	five-fold cross-validation caused an increase in the accuracy of the prediction	Tomperi et al. 2017 [5]
N/A	SDAE, SVR, BNN, GBM, SAE	R^2=0.05 MSE= 1.58	Stacked denoising auto-encoders (SDAE) showed the best performance for predicting TN	Shi and Xu 2018 [53]
Analysis of variance, Mutual Information, Backward Elimination, Pearson Correlation, LASSO	ANN, RF, and GBM	R^2=0.58, MSE=0.0084	GBM model showed the best performance on training and test data-set and less vulnerable to add or remove extra features. Also, the Mutual Information feature selection method suggested the best features.	This study

Based on table 5, Guo et al. [48] utilized SVM (support vector machine) and ANN to predict TN concentration in a WWTP. The models have trained 200 records and tested during the 90 days. The model performance indicated the coefficient of determination 0.46 and 0.47 for SVM and ANN respectively. In a different approach, Tomperi [5] firstly, performed extensive feature selection methods such as stepwise selection, forward selection, and genetic algorithms, then they developed a k-fold model to predict TN with R2=0.69 without testing on unseen data. Also, Yaqub et al. [49] proposed a prediction method for TN by developing a two-layered stacked long short-term memory (LSTM) network on a large data set (6000 training and 1876 testing) with a low average model error (MSE=0.015). In addition to that, hybrid simulation can be helpful for accurate prediction of TN. For example, [50] designed a parallel-serial hybrid model (machine learning and mechanistic models) on a data set (400 train and 250 test data-set) with high accuracy (R^2=0.81). Combining external biological simulation (mechanistic modeling) to ML algorithm caused high model precision. Hence, considering based on standalone ML prediction, the proposed model by this study is a high accuracy model for TN prediction among recent similar studies.

4 Conclusions

In the present study, the importance of using suitable FS as a booster of prediction was evaluated. Also, the following conclusions were derived from this study as follows:

- Selecting a suitable feature selection for obtaining the best possible input-data increases the prediction precision (up to 20%).
- Considering the outcome of recent literature for TN prediction in the influent/effluent flow of WWTP, this study demonstrated high precision prediction by Mutual Information FS model and GBM prediction algorithm.
- Scenarios III and IV declared a more reliable performance of the model predictions which means that the wrapper feature selections (ANOVA, Random Forest, Backward Elimination, and MI) can select the level of features importance better than commonly used filter methods.
- Decision tree algorithms (RF and GBM) revealed better performance results in comparison to neural network algorithm (ANN), and GBM has the highest accuracy (R^2=0.58, RMSE=0.092, and MAE=0.017 for the test dataset respectively) followed by RF and ANN in the best scenario (IV).
- GBM is less sensitive to add or remove features to the subset. In contrast, ANN accuracy drops significantly, if redundant features are added.

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