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Designing Efficient and Sustainable Predictions of Water Quality Indexes at the Regional Scale Using Machine Learning Algorithms

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Abstract: Water quality and scarcity are key topics considered by the Sustainable Development Goals (SDGs), institutions, policymakers and stakeholders to guarantee human safety, but also vital to protect natural ecosystems. However, conventional approaches to deciding the suitability of water for drinking purposes are often costly because multiple characteristics are required, notably in low-income countries. As a result, building right and trustworthy models is mandatory to correctly manage available groundwater resources. In this research, we propose to check multiple classification techniques such as Decision Trees (DT), K-Nearest Neighbors (KNN), Discriminants Analysis (DA), Support Vector Machine (SVM), and Ensemble Trees (ET) to design the best strategy allowing the forecast a Water Quality Index (WQI). To achieve this goal, an extended dataset characterized by water samples collected in a total of twelve municipalities of the Wilaya of Naâma in Algeria was considered. Among them, 151 samples were examined as training samples, and 18 were used to test and confirm the prediction model. Later, data samples were classified based on the *WQI* into four states: excellent water quality, good water quality, poor water quality, and very poor or unsafe water. The main results revealed that the SVM classifier obtained the highest forecast accuracy, with 95.4% of prediction accuracy when the data are standardized and 88.9% for the accuracy of the test samples. The results confirmed that the use of machine learning models are powerful tools for forecasting drinking water as larger scales to promote the design of efficient and sustainable water quality control and support decision-plans.

Keywords: prediction model; regional management; drinking water quality; support decision-plans

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1. Introduction

High-quality water resources are vital in the supply of necessary drinking water for humans and natural ecosystems, but also to guarantee human activities and development [1,2]. Nowadays, it is well-studied that several factors interacting in complex systems among them such as population growth, intensive agriculture, urbanization, and industrial activity, increase the water need, especially facing an uncertain context of climate change [3]. According to a recent United Nations (UN) report, 1.5 million people die each year because of diseases caused by contaminated water because water contamination causes 80% of health problems in low-income countries [4]. In fact, five million fatalities and 2.5 billion illnesses were accounted for during the time of this report. Therefore, the assessment and prediction of water quality are required to set up whether water is suitable for a certain use and, if not, to find relevant remedies or precautions; however, water quality is determined by many measures that quantify dissolved substances. Due to this, assessing all interacting factors in a groundwater bodies (and/or in a water surface lagoon) is insufficient in low-income countries because the process is expensive and exhausting [5]. As a result, minimizing the subjectivity and the cost-effectiveness of water quality assessment is a major challenge and several tools are being developed to determine its cleanliness and purity [6,7].

The design of an accurate and adapted Water Quality Index (WQI) is a well-accepted indicator used by several international and national organizations to classify water quality at a certain location and time. Some researchers proposed modifications when calculating this indicator (WQI), for instance, Uddin, Nash [8] presented twenty-one *WQI* models for assessing drinking water quality, such as the Horton index, the National Sanitation Foundation (NSF-WQI), and the Bascaron index (BWQI), among others. In order to calculate it, physicochemical parameters must be gathered. As a result, an indicator is achieved that allows the general public to know the water quality in aquifers [9]. It can also evaluate water characteristics about human health and natural quality effects [10] or even to decipher its impact on water poverty risk [11].

Indicators such as the *WQI* often are calculated in a complex and time-consuming process. So, many methodologies are proposed to easily and accurately predict these indicators considering its application for larger scales instead of a specific municipality or small catchment. These models make it possible to expect compliance (and noncompliance) with quality requirements in the short and long terms [12]. Water quality monitoring and forecasting are carried out using a variety of methods such as computational intelligence techniques (such as genetic algorithms, artificial neural networks, and others), which have received increasing attention in environmental time-series prediction research, as they allow for modeling nonlinear systems and are robust to noise data, leading to more right results [13–15]. Thus, the machine learning helps to reduce the consumption time to compute the *WQI* for each sample. However, using equations to determine the *WQI* for 100 samples will consume more time, while using the machine learning (classification learner) will significantly save the consumed time [12–15].

Recently, traditional Machine Learning models such as the Decision Tree, which has been frequently used in many fields and applications [16,17] has been applied for water quality assessments. The Ensemble Trees (ET), which is considered a more accurate predictor than any of the individual learning algorithms has been tested [18,19]. Discriminant analysis (DA) was also utilized in several kinds of research around the world to predict water quality by generating discriminant functions (DFs) for grouping nonoverlapping data based on scores on one or more quantitative predictor variables [20,21]. Other researchers even used K-nearest neighbors (KNNs) to classify and predict the water quality [22,23].

Likewise, several new studies have been published assessing the behavior of the *WQI* by using machine learning algorithms in many regions over the world [24,25]. For instance, Support Vector Machines (SVM) can be offered as a robust technique for water quality prediction in a free-form wetland environment because of many variables influencing water quality [26]. Some approaches adopted SVM to predict sediment load concentration in an arid watershed as in India Samantaray, Sahoo [27], or to predict the boundaries of water quality limits, for example, in the Kelantan River in Indonesia by Kurniawan, Hayder [28]. Koranga, Pant [29] proposed a machine learning model to predict the water quality of Nainital Lake in India. Tan, Yan [30] used a square support vector machine to predict water quality time series data from China. Mohammadpour, Shaharuddin [13] forecasted the *WQI* in freely constructed wetlands using a support vector machine in Malaysia. Other studies have also been undertaken in Algeria to test the effectiveness of SVM [31–34] and confirmed that SVM provides accurate results in less time-consuming and can run with fewer data than other algorithms. However, there is a lack of studies that offer decision-makers effective tools for predicting water quality index to improve water resource planning and to be used at larger scales in arid areas.

Therefore, in this research, classification techniques were used to predict the *WQI* for several water samples collected from an arid area, in particular, the Naama province in Algeria which depicts clear signals of water pollution and scarcity. To accomplish this objective, the MATLAB tool was considered because it contains a set of classification learner methods, such as the SVM among others [35]. The main goals of this study can be summarized as follows: (i) assess the physicochemical properties of different water points (samples) on a large scale (12 municipalities); (ii) determine the water quality of the study area, depending on the *WQI*; (iii) apply the learner technique to develop a classification model for dry areas estimating the model's accuracy about *WQI* values. These data were divided into classes such as excellent, good, poor, and very poor or unsafe water in order to facilitate its consideration; (iv) predict the *WQI* by using the best classifier, which develops the based prediction accuracy, and (v) offer decision-makers with effective tools for predicting water quality index to improve water resource planning and management in arid areas. We hypothesize that the proposed prediction model will reduce the time to determine the water quality state based on conventional equations.

2. Materials and Methods

2.1. Description of the Study Area and Data Collection

This research was carried out in the region of Naâma (Figure 1), which is located in the southwestern part of Algeria (from 32°9.284′ N to 34°19.492′ N; and from 1°39.568′ W to 0°1.781′ E). It is part of the high plains of southern Oran, a region affected by desertification processes [36], and specifically, the case study area is situated between the Tell Atlas and the Saharan Atlas in the western part of Algeria.

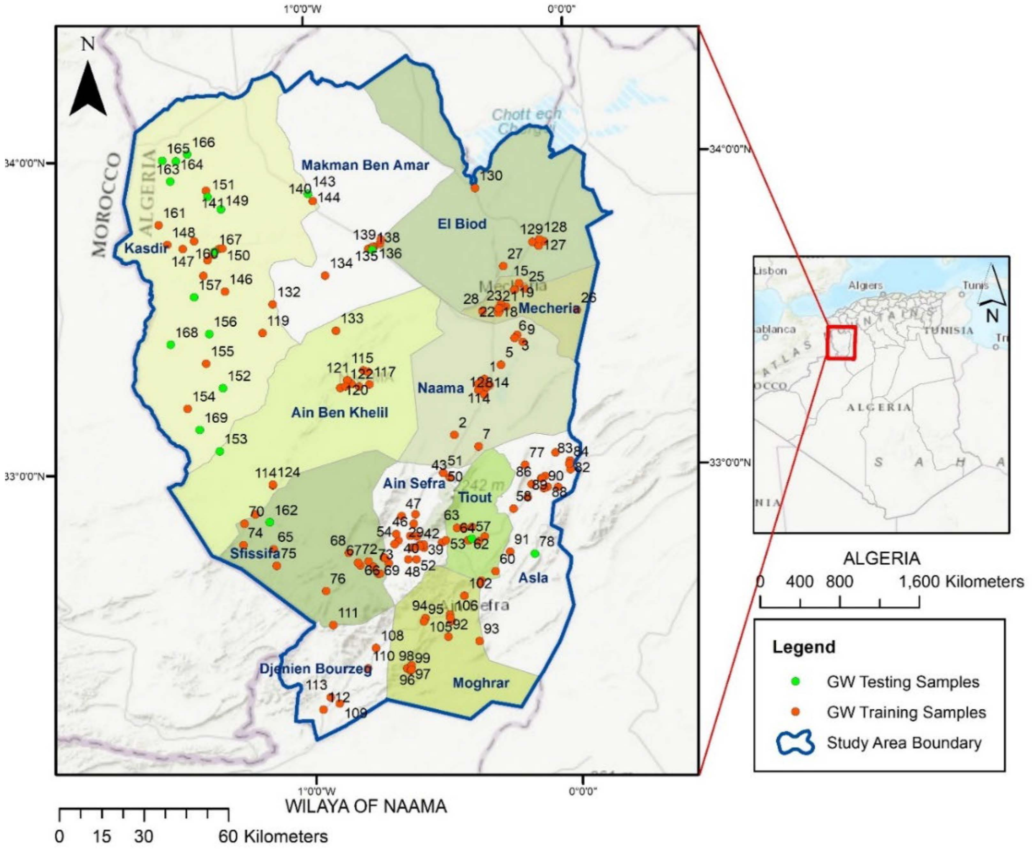


Figure 1. Localization of the study area and sampling points.

The north region of the Naâma is characterized by pastoral activities, particularly in hilly areas. In contrast, in the south region, agricultural fields with olive orchards, cereals, vegetables, and livestock can be found [37]. Naâma receives most of its rainfall from the north direction, with an estimated average of 287 mm [38]. The evaporation can reach 2000 mm, which affects the groundwater quality. The average temperatures range from 7.22 to 30.03 degrees Celsius. Summer temperatures can reach 48 °C, while in winter, they can drop below 0 °C [39].

The case study area depicts about 29,825 Km^2 (i.e., three times the area of Lebanon). Rangelands occupy about 74% of the total area (22,070.50 Km^2) and the southern pre-Saharan zone extends over the remaining 14% (4175.50 Km^2) [40]. Elevation ranges from 768 to 2239 m.a.s.l. Geologically, Naâma is composed from the Triassic to the Quaternary formations [41]. The vegetation is characterized by a steppe except in the mountains, where remains of Aleppo pine forests (*Pinus halepensis* Mill.) are identified [42].

The main water resources refer to groundwater used for irrigation and drinking in the region. From a hydrogeological perspective, the Wilaya of Naâma has four main groundwater aquifer systems: the Jurassic sandstone aquifer, the lower cretaceous sandstones aquifer, the tertiary limestones aquifer, and the quaternary alluvial aquifer [43]. Those aquifers offer water supplies to 208,136 people living and there are supplies to 1,792,076 animals grazing in this area. These resources irrigate 43,688 ha of agricultural area. Because of the population growth and several activities developed throughout the study area, it is necessary to assess the water demand and the supply of resources. The dataset in this research was gathered from twelve different communes in the Naâma Province.

2.2. Data Collection, Analysis, Sampling, Preprocessing and Water Quality Index Calculation

A total number of 169 samples were collected to analyze eleven elements. Electric Conductivity (EC), Mineralization, and Hydrogen Power (pH) were measured in situ using a portable HANNA type multiparameter (HI98194) during the sampling procedure in the laboratory at the University Center of Naâma. Then, in the Algerian Water Unit of Naâma (ADE) laboratory, a flame photometer was used to measure Sodium (Na) and Potassium (K). The UV-Vis spectrophotometer recognized Sulphate (SO_4) and Nitrate (NO_3), and the complex metric titration method was used to identify Calcium (Ca), Magnesium (Mg), Chloride (Cl), Bicarbonate (HCO_3). These values were then used to rank the water samples according to many terms that affect water quality [44,45].

This study considers the collected dataset to test the proposed model, and eleven significant water quality parameters are included. *WQI* has been calculated using the following Formula (1):

$$WQI = \frac{\sum_{i=1}^{N} q_i \, w_i}{\sum_{i}^{N} w_i} \tag{1}$$

where WQI, is the water quality index; N represents the total number of parameters used to calculate the *WQI*. q_i means the rating scale of each parameter, which is determined using Equation (2), where S_i denotes the drinking water standards, and C_i denotes the concentration of each chemical parameter (Table 1). Detail information of these equations can be found in [8,9].

$$q_i = (C_i / S_i) \times 100 \tag{2}$$

Table 1 depicts the relative weight of each physicochemical parameter. In particular, weights were attributed to each of the study's 11 physicochemical parameters, according to their relative significance on the total quality of drinking water. Thus, nitrates received a maximum weight of 5, due to their high impact on groundwater quality, while magnesium was assigned the minimum value of 1, due to its low influence on the water quality of drinking. Weights between 2 and 4 were attributed to other physicochemical parameters.

The values of *WQI* were classified into four classes as below [46]: Class I: excellent water class and $WQI < 50$; Class II: good water class and $50 < WQI < 100$; Class III: poor water class and $100 < WQI < 200$; and, Class IV: very poor water class and $WQI > 200$.

Table 1. The weighting of each physicochemical parameter.

PC-Parameters	Units	Permissible Limits	Weight (Wi)	Relative Weight (Wi)
pH		8.5	4	0.118
Electrical Conductivity	μδ/cm	2800	4	0.118
Mineralization	mg/L	2000	4	0.118
Magnesium	mg/L	50	1	0.029
Calcium	mg/L	200	2	0.059
Potassium	mg/L	12	2	0.059
Sodium	mg/L	200	2	0.059
Chlorides	mg/L	500	3	0.088
Sulphates	mg/L	400	4	0.118
Nitrates	mg/L	50	5	0.147
Bicarbonates	mg/L	120	3	0.088
			34	1

2.3. Data Classification

The results obtained from the data samples were divided into training and testing ones (151 and 18 samples, respectively). The limitation of the samples number imposed on us to reduce the number of test samples. A total number of 151 samples were used for training to be efficient and to get a robust classifier model. Although the number of test data is small, it contains all classes. On the other hand, the accuracy of the model will be calculated based on the correct number of predicted samples to the total number of test samples. Thus, the number of samples for each class of the sample data is selected to be sufficient for determining the prediction accuracy. The number of test samples for each *WQI* class is shown in Table 2.

Table 2. Distribution of the training and testing samples according to the *WQI* class.

Samples	Excellent (1)	Good (2)	Poor (3)	Very Poor or Unsafe (4)	Total
Training	20	101	24	6	151
Testing	5	5	5	3	18
Total	25	106	29	9	169

2.4. Data Standardization

In this study, the original classifiers were applied to the raw data without normalization, and the forecast model was built up. The data standardization was accomplished to study the transformation process of the data on the prediction accuracy of the classification process. It is not easy to compare data from different sources, such as analyses and tests. Therefore, data standardization is an important task to analyze, process, and compare more accurately and efficiently. Each variable value as X is subtracted from the sample's mean (μ) and divided by the standard deviation (σ). The mean and standard deviation of each data sample of each variable will be zero and 1, respectively. The new standard magnitude of each variable in each sample can be determined as in Equation (3):

$$X_n = \frac{X_c - \mu}{\sigma} \tag{3}$$

where μ and σ are the mean and standard deviation of each variable for all samples in the training process, respectively.

2.5. Classification Techniques

2.5.1. Decision Tree

The decision tree (DT) is a prediction tool or a classification tool, which uses machine learning [33,45]. The decision tree is a binary tree that means for every parent, there are at most two offspring. Each node in the tree refers to a variable and also a separation point for that variable. Each leaf of the tree represents the result (output) that was used to predict. To build the prediction DT model, the following procedures must be followed: (i) the variables from the data that will build the model should be selected, (ii) choose the values by which separate each variable based on the rules that have been built; and, (iii) tree construction ends upon arrival with a certain stop condition (for example, the lowest number of instances of tree leaves were identified).

2.5.2. Ensemble Tree

A combination of several DTs to get the highest predictive performance than only one DT is referred to ensemble method. It is based on combining the weak learners to compose a strong learner. There are two techniques used in ensemble decision trees, the first one is bagging and the other is boosting [47,48]. The bagging (Bootstrap Assembly) is used when it is necessary to reduce the variance in the DT. The bagging technique basis consists on create several datasets from the randomly selected and replaced training sample. Then, each subset of data is used to train the decision trees. The mean of all predictions is used for various trees and is stronger than a single decision tree. The other ensemble technique is boosting used to create an aggregation of predictors. The learners act consecutively: the first learners adapt simple models to the data, and then the errors are analyzed. It means that consecutive trees (random samples) were adjusted to resolve the net error of the previous tree.

2.5.3. K Nearest Neighbors (KNN)

It is a supervised machine learning classification algorithm and the simplest and most frequently used classifier. In KNN, a new data point is categorized based on similarity in a particular group of neighboring data points. For a given data point in the set, the KNN identifies the distances between this point and all other K points in the dataset close to the initial point and then, votes for the class which is the most common. Usually, the Euclidian distance is taken as a distance measurement. Thus, the resulting final model is just the labeled data placed into space. KNN is used in different applications such as genetics, forecasting, etc. [49].

2.5.4. Discrimination Analysis (DA) Classifier

Discrimination analysis (DA) proposes that various classes produce data based on various Gaussian distributions. For training a DA classifier, the fitting function assesses the parameters of a Gaussian distribution for each class. For predicting the classes of new data, the trained classifier finds the class with the lowest cost of misclassification [50].

2.5.5. Support Vector Machine (SVM)

The SVM classification technique gave the highest classification and prediction accuracy of the *WQI* in the current study. It is a machine learning tool that separates the data into two-class data via a hyperplane [51]. This hyperplane must achieve the greatest distance between the points of each class; then, accurate classifying can occur. If any point lies outside the hyperplane margin, it belongs to a different class. Greater features lead it more difficult to separate among different classes. Figure 2 illustrates the margin condition of SVM. A good classification can occur when a large margin exists [52,53].

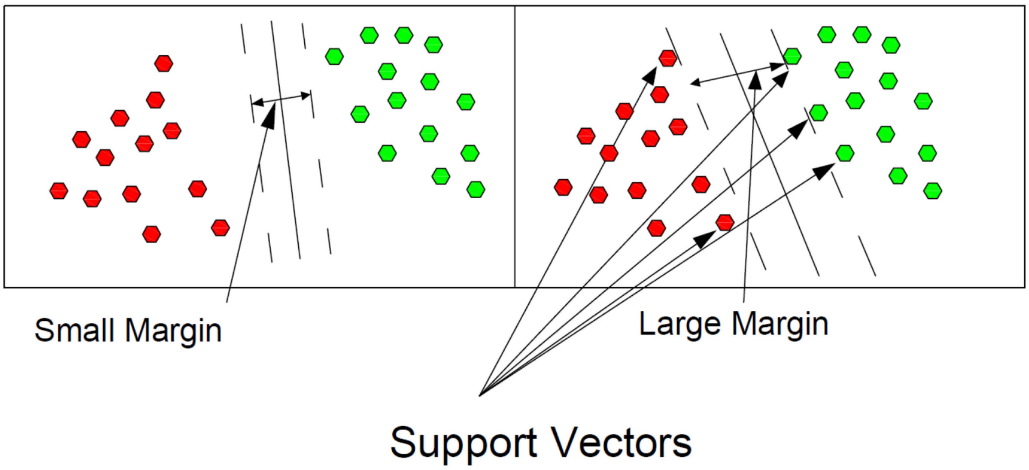


Figure 2. SVM algorithm indicates the margin separating two classes.

Hyperplanes can separate all samples in each *WQI* class in SVM in multidimensional space. The hyperplanes distinguish between every two *WQI* classes (Y_i and Y_j) of *WQI* of two different input vectors (X_i and X_j) [54]. The hyperplane with the greatest margin must be found among these hyperplanes. An orthogonal vector ω to the hyperplane can be defined as in Equation (4):

$$\omega = [\omega_1, \omega_2, \ldots, \omega_k] \tag{4}$$

The hyperplane function, h, can be identified as mentioned in Equation (5) [54]:

$$h(X_i) = w^T.\, X_i + \omega_0 = \omega_0 + \sum_{i=1}^{k} \omega_i.x_i \tag{5}$$

where ω_0 is the bias term to determine the separating hyperplane position (i.e., h (X) = 0). One by one learning strategy is chosen, where X_i is the class 1 when h (X_i) ≥ 0 and is -1 elsewhere. If X_i and X_j are the two closest points on each side of the hyperplane (i.e., different classes), the hyperplanes h (X_i) and h (X_j) are:

$$h(X_i) = w^T \cdot X_i + \omega_0 = 1 \tag{6}$$

$$h\left(X_j\right) = w^T \cdot X_j + \omega_0 = -1 \tag{7}$$

Differencing these equations and dividing both sides by the magnitude of the ω, we obtain:

$$\mathrm{X}_i - \mathrm{X}_j = \frac{2}{||\omega||} \tag{8}$$

where $X_i - X_j$ is the distance between the two hyperplanes.

The maximization of the margin of Equation (8) implies the minimization of the weight vector ω defining the hyperplane. In addition, a soft-margin SVM is utilized for nonlinear classes to allow the model to misclassify some data points by minimizing the number of such samples [55].

3. Results

3.1. Description of the Physicochemical Analysis of the Sampling Points

The results of eleven (11) physicochemical parameters obtained from 169 samples of groundwater in the Wilaya of Naâma are shown in Table 3.

Table 3. Descriptive statistics of groundwater parameters of the Wilaya of Naâma.

	Min Value	Max Value	Mean Value	Standard Values [56]	Standard Deviation	Coefficient of Variation (%)
Ca^{++}	12.00	832.00	137.69	75–200	122.50	88.97
Mg^{++}	3.00	560.00	76.03	50	68.85	90.56
Na^{+}	5.00	2967.00	186.40	200	315.33	169.17
K^{+}	1.00	59.00	8.97	12	8.47	94.38
Cl^{-}	10.00	443.00	118.95	250	62.90	52.88
SO_4^{2-}	38.00	2370.00	376.78	250	437.83	116.20
HCO_3^{-}	20.00	529.00	237.85	120	63.92	26.87
NO_3^{-}	1.00	390.00	26.82	50	36.85	137.40
Cond.	290.00	8660.00	1556.82	1500	1306.60	83.93
Miner.	186.00	5493.00	1076.67	-	877.30	81.48
pH	6.58	10.60	7.71	6.5–8.5	0.51	6.64

3.2. *Water Quality Index Assessment*

The results obtained to evaluate the groundwater quality through the Wilaya of Naâma using the *WQI* method are presented in Table 4, and in Figure 3.

Table 4. Summary of *WQI* evaluation in the Wilaya of Naâma.

Classes	Type	Number of Samples	%
I	Excellent	25	14.8
II	Good	106	62.7
III	Poor	29	17.2
IV	Unsafe	9	5.3

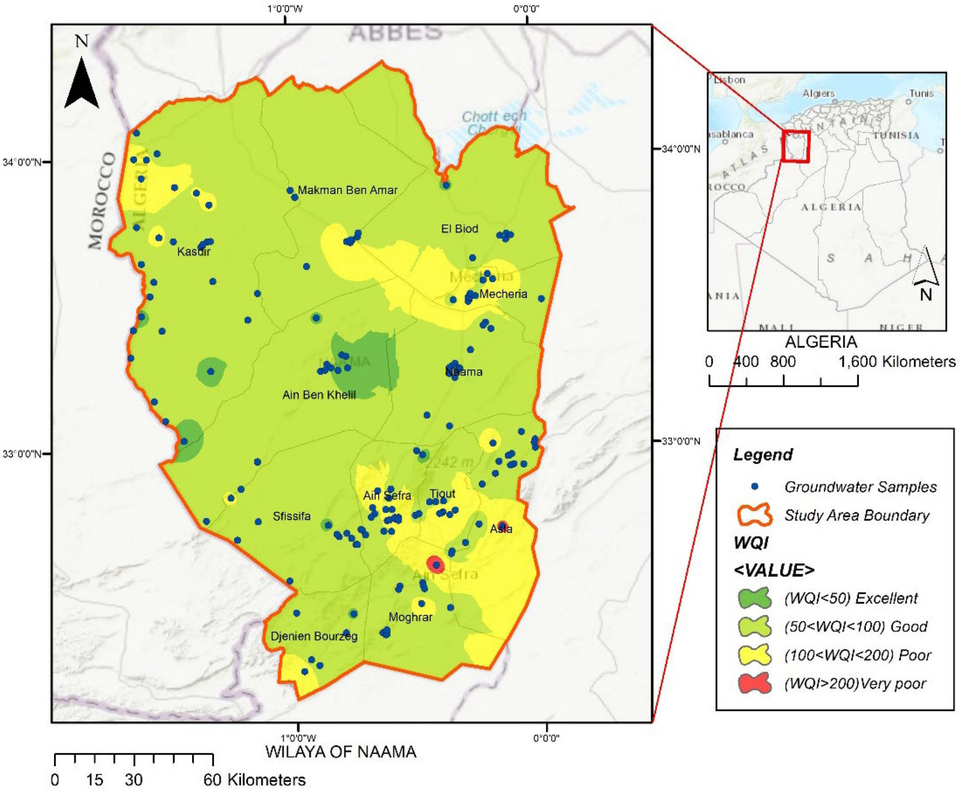


Figure 3. Spatial distribution of *WQI* in the study area.

3.3. Results with Raw Data

The procedures to predict the *WQI* via the classifiers will be illustrated. The data (169 samples) is classified based on the *WQI* in Excellent, good, poor, and very poor classes (Table 2). A total number of 151 samples were used for training and the remain (18 samples) were used for testing the model. The training and testing samples were selected to include all classes. The 151 samples were trained with all classifiers to investigate which one is the best (achieves high prediction accuracy). This process was accomplished by feeding the classification learner tool in MATLAB with the input data of each sample and its output (WQI). So, the classifiers learn the relation between the inputs and outputs (extraction the features). Each class will contain the samples that have similar features. After learning the classifier, the constructed weighted matrix (identifying the features of each class) was exported to the worksheet in MATLAB and then the test data were applied without its output and then the prediction results will be developed based on the feature in weighted matrix for each class. Then the accuracy of the constructed classifier will be computed dividing the number of the correct prediction to the total number of test data (18 Samples).

The samples' raw data was first considered by comparing its results with the standardization data. When all classification techniques are applied to the raw data, Linear SVM presents the highest accuracy of the classification process in the training stage (94.7%), as shown in Table 5. The results of training the classifiers on the raw data illustrate that the SVM classifier developed the highest accuracy rather than the other classifiers. It develops notable correctness with less computation power and is preferable in classification problems. It is also used when an understandable margin of dissociation between classes is observed. Likewise, it is suitable for high dimension spaces and considers memory systematic.

Other techniques obtained similar results, 93.4% for the quadratic SVM, and the cubic SVM and linear discrimination classifiers provide lower values, such as 90.7 and 88.7%.

The cross-validation method is used in classifier learners to investigate the constructed prediction model's robustness and to verify the model's prediction accuracy. In this method, the data samples divide into two partitions for the training and testing processes. Division of the data samples was carried out randomly into k equal size subsamples. A single subsample is kept as validation data. The remaining k-1 subsamples are used in training the model and repeated k times. The accuracy of the test data is average to develop the final model accuracy. So, all data samples are used for training and validation processes [57]. The stratified k-fold cross-validation is used in the classification learner to solve the classification problem so that the folds are selected. Each selected fold randomly includes the same features as each categorized class.

Figure 4 shows the linear SVM confusion matrix achieved with the classification technique. Figure 4a shows the corrected prediction samples for each class. The "excellent" *WQI* (class 1) was correctly classified in 17 out of 20 samples; in class 2, 99 out of 101 samples were correctly predicted. Figure 4b explained the prediction accuracy of each class, where the correct prediction of class 1 (Excellent state) was 85% (17/20), and the wrong prediction was 15% (3/20). For the very poor state, the correct and wrong predictions were 50% (3/6) and 50% (3/6), respectively.

Figure 5 shows that the predicted class 1, referring to the excellent class, appeared 19 times; 17/19 is a correct prediction class (89%), and 11% (2/19) occurred with class 2 (good state). The receiver operating characteristic (ROC) is illustrated for class 1 in Figure 6. The marker on ROC presents the current classifier performance where the false positive rate (FPR) is on the x-axis, and the true positive rate (TPR) is on the y-axis.

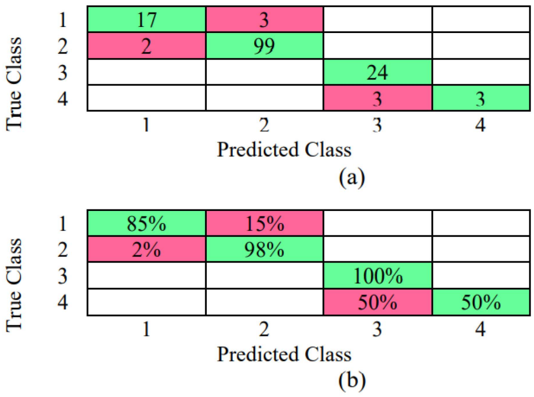
Figure 6 explained that the FPR is 0.02, i.e., 2% of the data samples were assigned incorrectly to the positive class. The TPR refers to 0.85, which explains that the classifier correctly assigns 88% of the samples to the positive class. Right angle for ROC refers to perfect classifying results. When the angle is 45°, it shows a poor classification result. The area under the curve (AUC) showed the overall accuracy of the classifier for the class.

Larger AUC values refer to better classifier performance. Figure 6 explains that the AUC is 99%, which refers to better classifying.

Table 6 shows 18 samples (randomly selected) where the chemical values gathered are shown in the left rows. The water quality index (WQI) and the quality achieved for the samples are shown in the following columns and finally, the SVM model prediction is depicted in the right column. The classification accuracy is 88.9% (16/18) due to two of the samples being wrong diagnosed (Sample 1 and sample 17).

Table 5. Comparison between different classifiers.

Classifier	Training Data	
	Raw Data	Standardization
1. Decision Tree (DT)		
Fine tree	83.4	75.5
Medium tree	83.4	75.5
Coarse tree	81.5	76.8
Linear discriminant	88.7	88.7
Quadratic discriminant	Fail	Fail
2. Support Vector Machine (SVM)		
Linear SVM	94.7	95.4
Quadratic SVM	93.4	93.4
Cubic SVM	90.7	91.4
Fine Gaussian SVM	66.9	67.5
Medium Gaussian SVM	90.1	91.1
Coarse Gaussian SVM	74.8	74.2
3. K-Nearest Neighbors (KNN)		
Fine KNN	86.1	84.1
Medium KNN	81.5	83.4
Coarse KNN	66.9	66.9
Cosine KNN	72.8	78.8
Cubic KNN	80.8	80.1
Weighted KNN	83.4	84.1
4. Ensemble Trees		
Ensemble boosted trees	66.9	66.9
Ensemble bagged trees	86.8	88.1
Ensemble subspace Discriminant	83.4	83.4
Ensemble subspace KNN	82.8	88.7
Ensemble RUSBoosted trees	75.5	78.8
5. Discrimination Analysis (DA)		
Linear Discrimination	90.7%	90.1
Quadratic Discrimination	Failed	Failed



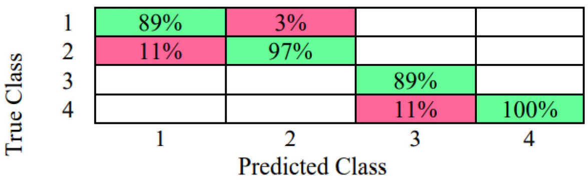
True Class \ Predicted Class	1	2	3	4
1	17	3		
2	2	99		
3			24	
4			3	3

(a)

True Class \ Predicted Class	1	2	3	4
1	85%	15%		
2	2%	98%		
3			100%	
4			50%	50%

(b)

Figure 4. Confusion matrix of linear SVM that was applied to the raw data, (Green refers to True Positive, red refers to False negative) (**a**) corrected prediction samples for each class (**b**) prediction accuracy of each class.



	1	2	3	4
1	89%	3%		
2	11%	97%		
3			89%	
4			11%	100%

Figure 5. Positive–negative predictive values of linear SVM confusion matrix of Raw data, (Green refers to True Positive, red refers to False negative).

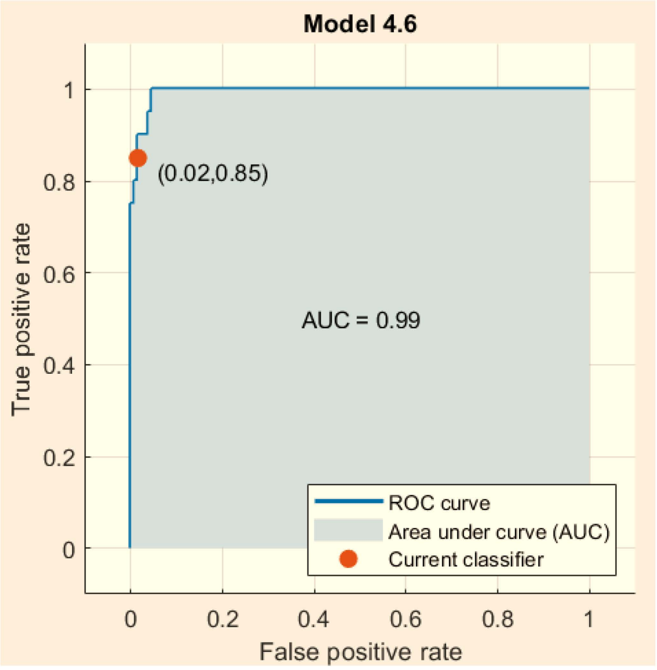


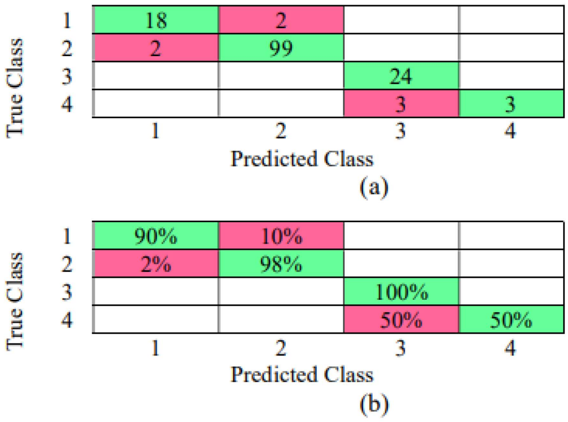
Figure 6. The ROC result of the ensemble bagged tree.

Table 6. The prediction results of the 18 testing samples with linear SVM.

Ca^{++}	Mg^{++}	Na^{+}	K^{+}	Cl^{-}	SO_4^{--}	HCO_3^{-}	NO_3^{-}	Cond.	Miner.	pH	WQI Results	Quality	Pred.
72	46	55	4	104	154	173	10	900	618	8.4	49.48	Excellent	Good
59	50	44	4	61	184	223	4	760	544	7.27	48.44	Excellent	Excellent
33	29	16	3	21	64	169	3	290	223	7.67	33.32	Excellent	Excellent
72	32	48	3	63	136	224	17	712	510	7.37	49.66	Excellent	Excellent
68	28	46	4	56	132	198	7	587	420	7.39	43.62	Excellent	Excellent
60	68	322	4	150	172	271	6	1980	1503	7.32	80.06	Good	Good
118	64	74	3	142	228	258	27	1186	900	7.53	67.70	Good	Good
73	59	41	2	78	219	217	12	867	658	7.34	52.77	Good	Good
116	48	37	2	36	363	203	8	945	717	7.22	55.10	Good	Good
91	56	35	4	99	146	284	4	890	676	6.94	54.36	Good	Good
101	99	444	17	139.6	908	106	8	2730	2073	7.34	108.02	Poor	Poor
128	124	311	12	152.5	546	201	10	2470	1875	7.5	100.95	Poor	Poor
506	290	140	19	184	2370	113	39	3520	2672	7.34	178.91	Poor	Poor
222	159	120	11	205	1020	193	25	2050	1556	7.29	107.86	Poor	Poor
303	211	85	12	116	1495	173	34	2290	1738	7.25	128.38	Poor	Poor
112.2	331	472	19	265.8	1536	182	44	4600	2852	8	241.26	Very Poor	Very Poor
451	95	1277	38	200	1320	127	1	6400	3968	8.1	220.54	Very Poor	Poor
160	452	978	26.1	172.1	1872	288	9	6200	5270	8	365.72	Very Poor	Very Poor

3.4. Results with Standardization of the Data [$(X - \mu)/\sigma$] Linear SVM

The standardization process of the data has been carried out following Equation (3). Again, linear SVM is obtained as the best classification tool, with a prediction accuracy of 95.4%. Figure 7 indicates that standardization of the raw data only enhanced the prediction accuracy of the excellent state (18/20; 90% accuracy). On the other hand, all other states are equal to those obtained with raw data. Therefore, the prediction accuracy of the test data samples was the same as that of the raw data.



True Class	1	2	3	4
1	18	2		
2	2	99		
3			24	
4			3	3

Predicted Class

(a)

True Class	1	2	3	4
1	90%	10%		
2	2%	98%		
3			100%	
4			50%	50%

Predicted Class

(b)

Figure 7. Confusion matrix of linear SVM that was applied to the standardization data (Green refers to True Positive, red refers to False negative) (**a**) corrected prediction samples for each class (**b**) prediction accuracy of each class.

The k-fold cross-validation was used to check the robustness of the constructed model for developing high accuracy classification. Tenfold cross-validation is used, which divides the data into two groups (80% of the data samples for training, and the remaining 20% is for the testing process). These processes were repeated ten times with a random collection of the samples. Then the average of the classification accuracy was determined. Standardizing the data samples slightly enhanced the training classification accuracy to 95.4% compared with 94.7% using the raw data. The testing results' classification accuracy shows that the constructed classification model is so beneficial to reduce the time needed to compute the *WQI* for each sample. The data of new samples are used as input data, and the *WQI* is directly identified.

4. Discussion

Table 3 shows that concentrations of Calcium experienced varied considerably from 12.0 to 832.0 mg/L (average value 137.69 mg/L). These values are much higher than the standards in Europe for Calcium in drinking water ranging from 75–200 mg/L [56]. Moreover, concentrations of Magnesium also varied considerably from 3.0 to 560.0 mg/L (average value of 76.03 mg/L). These values are much higher than other reference values found in literature as 78–155 mg/L (Calcium) and 28–54 mg/L (Magnesium) found in Slovakia [58] and also in Egypt, as 8–197 mg/L (Calcium) and 1.6–110 mg/L (Magnesium) [59].

Moreover, Table 3 also depicts strong variations in sodium levels of groundwater samples. The values ranged from 5.0 mg/L to 2967.0 mg/L (186.4 mg/L as average value) and an extremally variable coefficient of variation of 169.17%. Similar values (22.15–2769.5 mg/L) were found in Ghana [60] or south Africa (48–6971 mg/L) [61]. In the present study, the potassium concentration observed ranged between 1.00 to 59.0 mg/L, being these values lower than the identified in some studies carried out in Ghana (0.21–126 mg/L) [62]. The chloride concentration variation was 10–443 mg/L, while values higher to 21–110 mg/L were observed in Tunisia [63]. Sulfates concentration ranges between 38–2370 mg/L (average 376.78 mg/L) and nitrates also vary considerably from 1.0 to 390.0 mg/L (with a mean value of 26.82 mg/L) being aware that limits for drinking water are 10 mg/L in the United States and 50 mg/L according to World Health Organization [56].

The bicarbonates values in the water sampling points in our study area are between 20 and 529 mg/L, and electrical conductivity and mineralization varied considerably from 290 (μδ/cm) to 8660 (μδ/cm) and 186 mg/L to 5493 mg/L, respectively.

At different water quality levels, pH levels varied considerably from 6.58 to 10.60, spanning one order of magnitude with a mean value of 7.71 and a coefficient of variation of 6.64%. These values are not in agreement with the permissible limits (6.5–8.5 mg/L) for drinking water proposed by the World Health Organization [56].

The result shown in Table 4 revealed that 14.8% of samples fell into the excellent category (Class I; with values ranging from 33.32 to 49.48), 62.7% were classed as good (Class II; values varied from 50.9 to 99.26), 17.2% in the poor category (Class III, 100.15 to 183.82), and 5.3% are unsafe for drinking (Class IV values varied from 202.9 to 365.7). Being aware that 75% of water comes from groundwater [64] and considering the huge amount of data required to calculate *WQI*. Authors have found better values for predicting *WQI* using the SVM model than other approaches in Malaysia with the coefficient of determination (R2) equal to 0.8796 [64], or R2 = 0.9 also in Malaysia [65] using LSSVM (Least square SVM), and R2 = 0.87 in Iran [66]. However, other better results were found in Poland, where authors obtained R2 = 0.99 using neural networks [67]. Similar trustworthy results were achieved in Ethiopia, Vietnam and Brazil among others [68–71].

5. Conclusions

In order to maintain the availability of resources for drinkable water and to monitor pollution, the prediction of water quality indexes is extremely important. Thus, planning and managing water resources can greatly benefit from precise groundwater level predictions. As a result, an effort is made in this work to create a forecasting model that is effective for predicting groundwater quality by using the water quality index (WQI) in the Wilaya of Naama, placed in the southwestern region of Algeria. Based on many characteristics and indexes, conventional approaches evaluate water suitability for drinking and domestic purposes. Although these techniques are reliable tools, they can be costly and time-consuming. Therefore, this study proposes an alternative machine learning method for predicting water quality using only a few simple water quality criteria. The data used to conduct the study were collected from 169 samples of groundwater from 12 municipalities in the Wilaya of Naâma. A set of representative supervised machine learning algorithms has been used to estimate the *WQI* indicator. Based on *WQI* results, four classes were fixed: excellent, good, poor, and very poor or unsafe water. A relevant percentage (62.7%) of the considered physicochemical parameters depicted good water quality results. Related to prediction tools, main results showed that Support Vector Machine (SVM) algorithms classify groundwater quality with high accuracy (95.4%) with standardized data and lower accuracy (88.88%) for raw data. Therefore, a great correlation between observed and predicted water quality data was obtained in the present manuscript. These results offer a useful performance assessment tool for decision-makers, and further investigation can be undertaken by integrating the findings of this research on a large scale in arid areas. In conclusion, the SVM model is a simple and effective empirical model to simulate water quality, and the method presented in this work is sufficiently general to be applied to a wide range of arid areas.

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