

THE APPLICATION OF MACHINE LEARNING ALGORITHMS FOR PREDICTION OF PERFORMANCE ACCURACY FOR METAL(LOID) ADSORPTION IN SOIL AND UPTAKE IN WEEDS

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Abstract: The present study was attempted to predict the performance accuracy of datasets of metal(loid) contaminated and uncontaminated soil and uptake capability in weeds through machine learning (ML) classification models by using WEKA tool, version 3.8.5. Different ML algorithm models along with 4 attributes viz. Pb in soil (SPb), Cd in soil (SCd), As in soil (SAs) and effect (normal as N and abnormal as A content) as well as Pb accumulation in plant (PIPb), Cd accumulation in plant (PICd), As accumulation in plant (PIAs) and effect (N and A content) separately predicted to know overall performance accuracy as per 10-fold cross validation. In the present study, PRC values were recorded the ranged between 87% to 100% for the prediction of metal(loid) content performance accuracy in the soil while PRC values were recorded the ranged between 73% to 96% for the prediction of metal(loid) accumulation performance accuracy in the weeds. It is concluded that ML algorithms performed accurately from the dataset and obtained rich information with statistical validation. The future study in WEKA tool can easily be analysed with more dataset to predict classifier accuracy related to metal(loid) phytoremediation efficiency through weeds.

Keywords: Machine learning algorithm, Model classifier accuracy, WEKA tool, Predictive soil adsorption, Predictive plant accumulation, Metals and metalloids

1. INTRODUCTION

The municipal solid wastes (MSW) comprise different wastes viz. raw vegetable and cooked food wastes, garden wastes, papers, woods, plastics, construction and demolition wastes, glass, ceramics, electrical and electronic wastes, etc. [1] in which few are biodegradables, but majority wastes are non-biodegradable. In the municipality area, the specified barren land is used to dump MSW, which could produce environmental pollution [2,3]. The leachate runoff from open dumping sites showed dominant source of metal(loids) in the surface water and underground water, soil, and finally uptake by plants [4-14].

Several investigations have been carried out especially in and near the solid wastes dumping sites in India and abroad [15-19]. On the other hand, Mandal et al. [20] observed that soil is contaminated due to unsafe disposal of large quantity of arsenic contaminated sludge, which is generated from arsenic removal water treatment plant and arsenic could be adsorbed through waste candles containing arsenic.

In the technique of phytoremediation, several studies have been reported nationally and internationally that some weeds are also able to extract the heavy metals from the soil and could remediate easily from the medium both *in situ* as well as *ex situ* conditions [21-29]. Shahid et al. [30] revealed that metals or metalloids have tendency to accumulate and translocated to roots and aerial parts viz. stem, leaves, etc. of plant species. It was reported that root is the main target to accumulate but it translocated to the different parts of the shoot of plant species [31]. Biswas et al. [19] observed two weed species (*Lantana camara* and *Sida* sp.) accumulated Pb and Cd into the leaves as hyper-accumulator and could be efficiently used for phyto-remediation for these toxic elements from the soil around solid waste dumping ground of Berhampur Municipality, West Bengal, India.

Interestingly, recent research revealed that big data mining is demanding research in which the endeavour from dataset to valuable information through statistical interpretation. It can easily be accomplished through ML models or artificial intelligence (AI) algorithms, which is predicted the performance accuracy of the dataset [32,33]. On the other hand, several big data analysis on finance, agriculture, biomedical science, bio-science, etc. well established by many researchers [33-38], the data analysis by using ML models to establish limits in the classification of hyperaccumulator plants growing on different metals contaminated soils has already been achieved to know plant mineral composition [38] and recently many investigations are showing interest on the big data analysis by using ML and AI classification algorithms to obtain the accuracy in the big dataset [34-38].

The objective of the present study was to predict the performance accuracy of datasets of uncontaminated and contaminated soil and uptake potential in weeds through machine learning (ML) classification models in the WEKA (Waikato Environment for Knowledge Analysis) tool (version 3.8.5).

2. MATERIALS AND METHODS

In the present study, we used data mining tool namely WEKA (Waikato Environment for Knowledge Analysis) tool (version, 3.8.5) developed by Frank et al. [39] in which performance accuracy could be achieved through ML modelling algorithms. The WEKA explorer was developed with data pre-processing, classification, regression, and association rules [40]. In pre-processing, all the data were made through unsupervised instance and 10-fold cross validation data was used.

The predictive accuracy of dataset on normal and abnormal metal(loid) content in soil and maximum accumulation in the weeds of MSW dumping ground through ML modelling algorithms especially different classifiers viz. BayesNet (BN), NaiveBayes (NB), logistic regression (LR), Lazy.KStar (K*), decision tree (DT) J48, Random forest (RF), Random tree (RT) and Class implementing minimal cost-complexity pruning (CART) along with 4 attributes viz. Pb in soil (SPb), Cd in soil (SCd), As in soil (SAs) and effect (normal as N and abnormal as A content) as well as Pb accumulation in plant (PIPb), Cd accumulation in plant (PICd), As accumulation in plant (PIAs) and effect (N and A content) separately studied from dataset to predict the overall performance accuracy from the dataset of our earlier study of Biswas et al. [19].

The performance accuracy of above-mentioned ML model classifications related to correctly and incorrectly classified instances, Kappa statistics (KS), mean absolute error (MAE) and root mean squared error (RMSE) were studied for 10-fold cross validation test as per earlier study by Talapatra et al. [37] and Bhattacharya et al. [41]. As per Bouckaert et al. [42], the results for each algorithm model summary were retrieved from WEKA tool. The prediction accuracy of studied ML models as per 10-fold cross validation test was retrieved from summary results and the statistical parameters such as true positive (TP), false positive (FP), Matthew's correlation coefficient (MCC), receiver operating characteristic (ROC) and Precision-recall curve (PRC), respectively were recorded.

3. RESULTS AND DISCUSSION

In the pre-processing step, graphical representation of statistical data of different attributes (SPb, SCd, SAs and effect (N and A) (Fig 1) as well as (PIPb, PICd, PIAs and effect (N and A) (Fig 2) were obtained. It is not always possible to identify that which part of plants accumulate metal(loids) and these problems can easily be explained by resorting to big data mining, which is the abstraction of implicit, previously unknown, and potentially useful information in data [40]. Generally, ML is used to extract information from raw data of metal(loids) adsorbed soil and accumulated plants [38]. The process is based on abstraction in which data were collected, with all their defects, and the underlying structure is represented [40].

In Fig 1, visual qualitative and quantitative understanding of the distribution class (class effect N as blue coloured and A as red coloured under nominal) in which SPb attribute was obtained ranged between 3.79-26.05 for N category and 26.05-48.32 for A category (11 nos. in each), SCd attribute was obtained ranged between 1.59-3.40 (18 nos.), 3.40-5.22 (2 nos.) and 5.22-7.03 (2 nos.), SAs was found ranged between 2.39-4.54 (5 nos.), 4.54-6.68 (9 nos.) and 6.68-8.83 (8 nos.) and effect attribute viz. N and A category were obtained 11 nos. in each case.

In Fig 2, visual qualitative and quantitative understanding of the distribution class (class effect N as blue coloured and A as red coloured under nominal) in which PIPb attribute was obtained ranged between 0.19-9.68 (12 nos.), 9.68-19.18 (6 nos.) and 19.18-28.67(4 nos.), PICd attribute was obtained ranged between 0.38-1.01 (16 nos.), 1.01-1.64 (3 nos.) and 1.64-2.27 (3 nos.), SAs was found ranged between 0.35-1.38 (9 nos.), 1.38-2.40 (6 nos.) and 2.40-3.43 (7 nos.) and effect attribute viz. N and A category were obtained 11 nos. in each case.

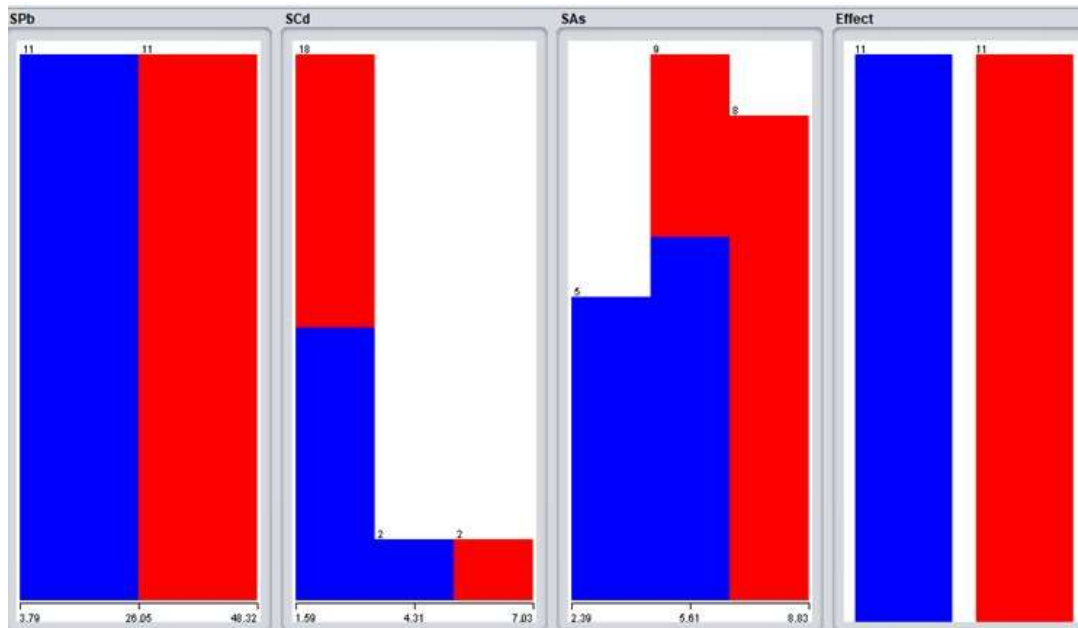


Figure 1: Representation of different attributes of soil after pre-processing in WEKA tool

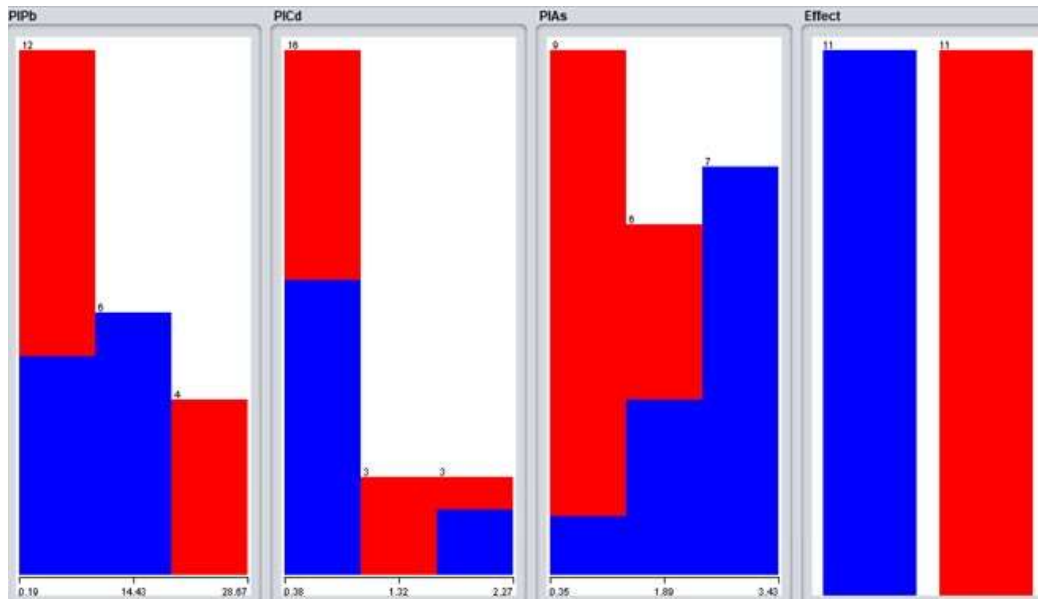


Figure 2: Representation of different attributes of weeds after pre-processing in WEKA tool

Table 1 describes the summary results of studied ML algorithm models such as BayesNet (BN), NaiveBayes (NB), logistic regression (LR), Lazy.KStar (K*), decision tree (DT) J48, Random forest (RF), Random tree (RT) and Class implementing minimal cost-complexity pruning (CART) related to 4 attributes of soil. The performance of model accuracy of above-mentioned ML algorithm classifications as per correctly and incorrectly classified instances, Kappa (K) statistics, mean absolute error (MAE) and root mean squared error (RMSE) were studied as per 10-fold cross validation test. In the case of algorithm model classification, the higher values were observed in BN, NB, LgR, RF and CART (100.00%) followed by J48 (95.45%), and lower value in RT (90.91%) as per 10-fold cross validation test.

Table 1: Results on different classified instances and statistical values for different algorithm models for soil

Classifier model	Correctly classified instances	Incorrectly classified instances	KS	MAE	RMSE
BN	100.0	0.0	1	0.03	0.07
NB	100.0	0.0	1	0.00	0.00
LgR	100.0	0.0	1	0.00	0.00
K*	100.0	0.0	1	0.0005	0.002
J48	95.45	4.54	0.91	0.04	0.21
RF	100.0	0.0	1	0.03	0.06
RT	90.91	9.09	0.82	0.09	0.30
CART	100.0	0.0	1	0.03	0.06

BN = Bayes Network; NB = NaiveBayes; LgR = Logistic Regression; K* = Lazy.KStar; J48 = Pruned and unpruned decision tree C4; RF = Random Forest; RT = Random tree; CART = Class implementing minimal cost-complexity pruning; KS = Kappa Statistics; MAE = Mean Absolute Error; RMSE = Root Mean Squared Error

Table 2 describes the summary results of studied ML algorithm models such as BayesNet (BN), NaiveBayes (NB), logistic regression (LR), Lazy.KStar (K*), decision tree (DT) J48, Random forest (RF), Random tree (RT) and Class implementing minimal cost-complexity pruning (CART) related to 4 attributes of weeds. The performance of model accuracy of above-mentioned ML algorithm

classifications as per correctly and incorrectly classified instances, Kappa (K) statistics, mean absolute error (MAE) and root mean squared error (RMSE) were studied as per 10-fold cross validation test. In the case of algorithm model classification, the higher values were observed in K* (95.45%) followed by LogR (86.37%), RF (86.36%), NB and RT (81.82%), J48 and CART (72.72%) and lower value in BN (68.18%) as per 10-fold cross validation test.

Table 2: Results on different classified instances and statistical values for different algorithm models for weeds

Classifier model	Correctly classified instances	Incorrectly classified instances	KS	MAE	RMSE
BN	68.18	31.82	0.36	0.38	0.48
NB	81.82	18.18	0.63	0.17	0.36
LgR	86.37	13.64	0.73	0.17	0.34
K*	95.45	4.54	0.91	0.07	0.22
J48	72.72	27.27	0.45	0.32	0.48
RF	86.36	16.64	0.73	0.24	0.24
RT	81.82	18.18	0.64	0.18	0.43
CART	72.72	27.27	0.45	0.32	0.47

BN = Bayes Network; NB = NaiveBayes; LgR = Logistic Regression; K* = Lazy.KStar; J48 = Pruned and unpruned decision tree C4; LMT = Logistic Model Tree; RF = Random Forest; RT = Random tree; CART = Class implementing minimal cost-complexity pruning; KS = Kappa Statistics; MAE = Mean Absolute Error; RMSE = Root Mean Squared Error

Table 3 describes the representation of the detailed accuracy of studied models for the studied dataset. In case of the accuracy of a class of values of TP, FP, precision, MCC, ROC and PRC, the better performances were observed in BN, NB, LgR, RF and CART followed by J48 and RT for soil. In the present study, PRC values were recorded the ranged between 87% to 100% for the prediction of metal(loid) content performance accuracy in the soil. The ROC curve is depicted (Figs 3, 4 and 5).

Table 3: Statistical data for prediction accuracy of studied algorithms for soil

Classifier model		TP Rate	FP Rate	Precision	Recall	F-Measure	MCC	ROC area	PRC area
BN	N	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	A	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
NB	N	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	A	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
LgR	N	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	A	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
K*	N	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	A	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
J48	N	0.91	0.0	1.0	0.91	0.95	0.91	0.95	0.95
	A	1.0	0.09	0.92	1.0	0.96	0.91	0.95	0.92
RF	N	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	A	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
RT	N	0.91	0.09	0.91	0.91	0.91	0.82	0.91	0.87
	A	0.91	0.09	0.91	0.91	0.91	0.82	0.91	0.87
CART	N	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0
	A	1.0	0.0	1.0	1.0	1.0	1.0	1.0	1.0

BN = Bayes Network; NB = NaiveBayes; LgR = Logistic Regression; K* = Lazy.KStar; J48 = Pruned and unpruned decision tree C4; LMT = Logistic Model Tree; RF = Random Forest; RT = Random tree; CART = Class implementing minimal cost-complexity pruning; TP = True positive; FP = False positive; MCC = Matthew's correlation coefficient; ROC = Receiver operating characteristic; PRC = Precision-recall curve

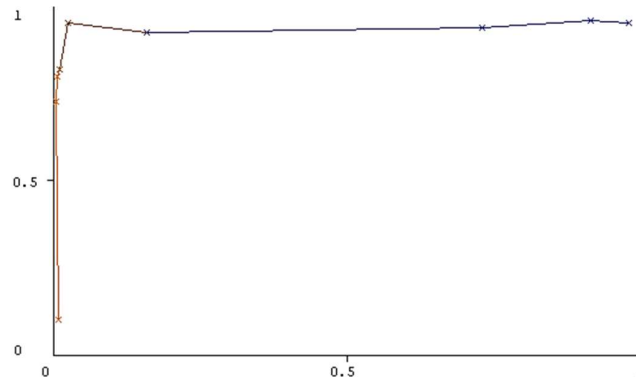


Figure 3: Area under ROC (=1) plot for BN, NB, LgR, K*, RF and CART algorithms of N and A effect for soil

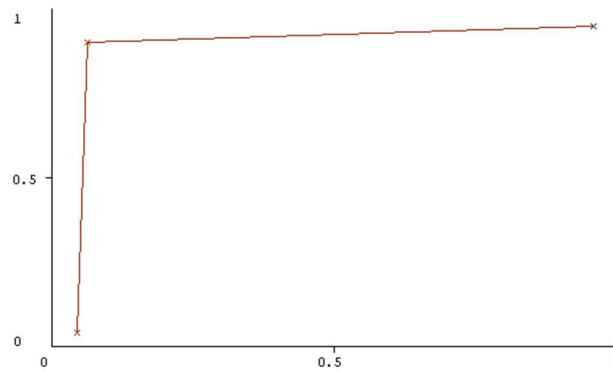


Figure 4: Area under ROC (=0.95) plot for J48 algorithm of N and A effect for soil

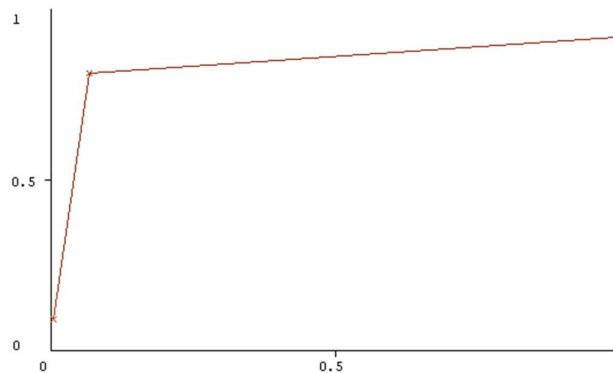


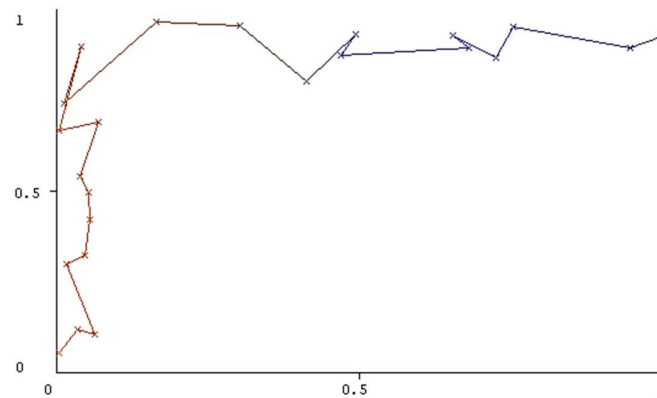
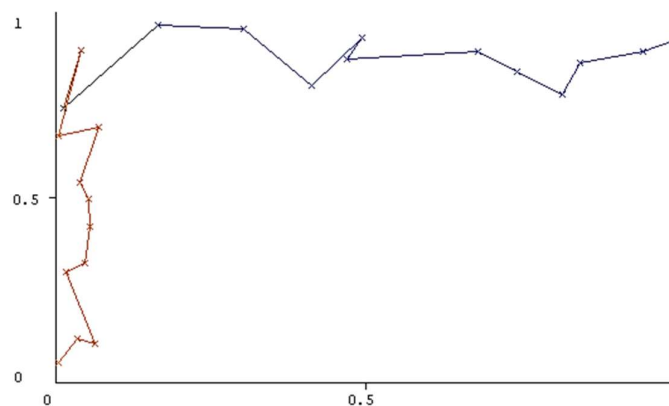
Figure 5: Area under ROC (=0.91) plot for RT algorithm of N and A effect for soil

Table 4 describes the representation of the detailed accuracy of studied models for the studied dataset. In case of the accuracy of a class of values of TP, FP, precision, MCC, ROC and PRC, the better performances were observed in BN, NB, LgR, RF and CART followed by J48 and RT for soil. In the present study, PRC values were recorded the ranged between 73% to 96% for the prediction of metal(loid) accumulation performance accuracy in the weeds. The ROC curve is depicted (Figs 6, 7, 8 and 9).

Table 4: Statistical data for prediction accuracy of studied algorithms for soil

Classifier model		TP Rate	FP Rate	Precision	Recall	F-Measure	MCC	ROC area	PRC area
BN	N	0.73	0.36	0.67	0.73	0.70	0.36	0.76	0.80
	A	0.64	0.27	0.70	0.64	0.67	0.36	0.76	0.69
NB	N	0.91	0.27	0.77	0.91	0.83	0.65	0.94	0.96
	A	0.73	0.09	0.89	0.73	0.80	0.65	0.94	0.92
LgR	N	0.82	0.09	0.90	0.82	0.86	0.73	0.89	0.94
	A	0.91	0.18	0.83	0.91	0.87	0.73	0.90	0.80
K*	N	0.91	0.00	1.00	0.91	0.95	0.91	0.92	0.96
	A	1.00	0.09	0.92	1.00	0.96	0.91	0.92	0.85
J48	N	0.64	0.18	0.78	0.64	0.70	0.46	0.72	0.68
	A	0.82	0.36	0.69	0.82	0.75	0.46	0.72	0.73
RF	N	0.91	0.18	0.83	0.91	0.87	0.73	0.89	0.93
	A	0.82	0.09	0.90	0.82	0.86	0.73	0.89	0.79
RT	N	0.91	0.27	0.77	0.91	0.83	0.65	0.82	0.74
	A	0.73	0.09	0.89	0.73	0.80	0.65	0.82	0.78
CART	N	0.64	0.18	0.78	0.64	0.70	0.46	0.76	0.74
	A	0.82	0.36	0.69	0.82	0.75	0.46	0.76	0.75

BN = Bayes Network; NB = NaiveBayes; LgR = Logistic Regression; K* = Lazy.KStar; J48 = Pruned and unpruned decision tree C4; LMT = Logistic Model Tree; RF = Random Forest; RT = Random tree; CART = Class implementing minimal cost-complexity pruning; TP = True positive; FP = False positive; MCC = Matthew's correlation coefficient; ROC = Receiver operating characteristic; PRC = Precision-recall curve

**Figure 6: Area under ROC (=0.94) plot for NB algorithm of N and A effect for weeds****Figure 7: Area under ROC (=0.92) plot for K* algorithm of N and A effect for weeds**

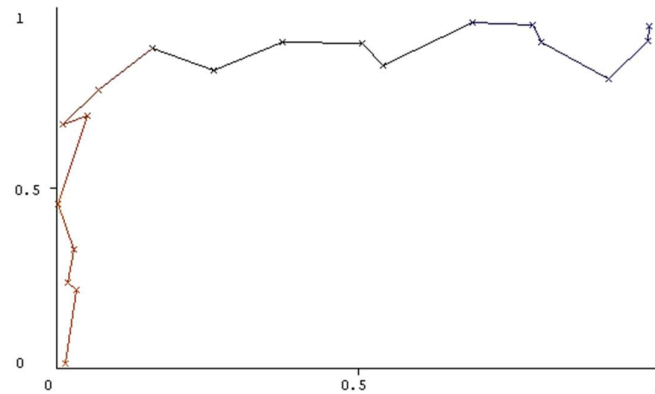


Figure 8: Area under ROC (=0.89) plot for RF algorithm of N and A effect for weeds

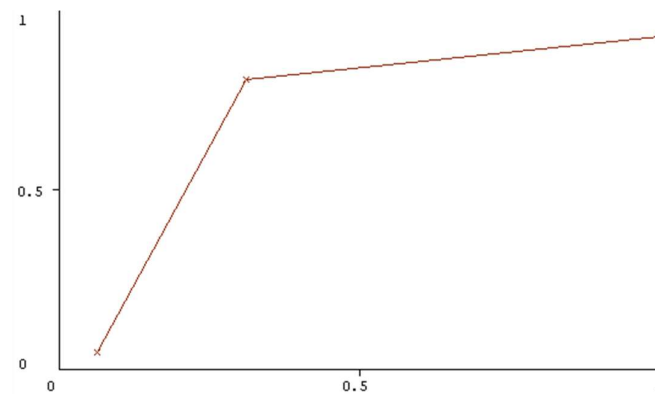


Figure 9: Area under ROC (=0.82) plot for RT algorithm of N and A effect for weeds

Several studies on ML algorithms have been carried out on biological science, [34-36,38,41] etc. but the analysis of dataset through ML modelling algorithm for soil adsorption and plant accumulation of metal(loids) to predict the classifier performance accuracy by using WEKA tool is the first-time endeavour.

4. CONCLUSION

In the present study, PRC values were recorded the ranged between 87% to 100% for the prediction of metal(loids) content performance accuracy in the soil while PRC values were recorded the ranged between 73% to 96% for the prediction of metal(loids) accumulation performance accuracy in the weeds. In conclusion, ML algorithms performed accurately from the dataset and obtained rich information with statistical validation and future study in WEKA tool can easily be analysed with more dataset to predict classifier accuracy related to metal(loid) phytoremediation through weeds.

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Conflict of interest

Authors declare no conflict of interest.

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