Review Article

Artificial Intelligence and Machine Learning models in adsorptiveremoval of toxic heavy metals and textile dyes from wastewater

Abstract

Herein we reviewedIt also introduces Artificial intelligence (AI) and Machine learning (ML) models in the optimization and prediction of process parameters during the removal of toxic heavy metals and textile dyes. Adsorption parameters normally optimized include pH, contact time, initial concentration, adsorbent dosage, and temperature.This review focuses on common AI models such as Artificial Neural Networks (ANN), Particle Swarm Optimization, and Genetic Algorithms (GA).Furthermore, the review describes the common prediction statistical indicators such as coefficient of determination (R^2), root mean square error (RMSE), mean squared error (MSE), absolute average deviation (AAD),etc. Lastly, this review highlights the significant potential of AI and ML in revolutionizing the field of wastewater treatment and mitigating the environmental impact of industrial pollution.

Keywords:artificial intelligence, wastewater, adsorbents, toxic heavy metals, textile dyes

1. INTRODUCTION

The world's population is increasing rapidly over the last few decades, resulting in natural resource pollution. For the survival of humans, they depend on the available water sources such as the oceans, seas, rivers, lakes, and streams. Due to anthropogenic activities such as agriculture, industrialization, mining, and manufacturing a variety of pollutants have found their way into the ecosystem[1]. These pollutants are mainly due to textile dyes, toxic heavy metals, nanoplastics, fungi, pathogens, personal care products, nitrates, surfactants, insecticides, aromatic compounds, microplastics, and pharmaceuticals[2–7]. Exposure to these pollutants has a variety of side effects such as nausea, vomiting, liver damage, itching, nervous dysfunction, and hormonal imbalance[8, 9].

Several techniques have been applied to remove these pollutants from water such as reverse osmosis[10–14], membrane filtration, advanced oxidation[15–18], photolysis [19], electrochemical processes[20–22], ion exchange, chemical reduction[23, 24], biological treatment (aerobic and anaerobic) [25–27], ozonation [19], and adsorption[28–31]. Most of these have some drawbacks such as high maintenance costs, complexity in operation, and expensive. Adsorption has found wide application due to its simplicity in design, cost-effectiveness, availability, and low maintenance costs[32]. This process occurs when a substance (adsorbate) interacts on the surface of a solid (adsorbent) which occurs through chemisorption or physisorption. The common adsorbents include activated carbon[33], metal-organic frameworks (MOFs)[34, 35], graphene[36–38], carbon nanotubes[39–41], and polymers[42–45].

During analysis finding the accurate operating parameters is always a challenge during real processes particularly in the areas of science and engineering where theyare complex reactions[46]. Experimental data while highly important is alwaysenergy-intensive and time-consuming making them impractical for comprehensive analysis[47]. Due to these limitations, researchers have applied numerous traditional methods such as isotherms, thermodynamics, and kinetics, though informative have a low scope[42, 48–50]. These models operate under static conditions giving mostly information about the adsorption capacity, mechanisms, entropy changes, and Gibbs energy which all occur at fixed operating conditions[51]. Furthermore, the dependence on batch experiments that vary only one parameter at a time are costly and time-consuming therefore fail to give an insight into the interaction between the different parameters thus affecting the adsorption efficiency[52].

Mathematical modeling and optimization tools have gained large applications in the field of engineering and science. Among all the optimization tools, Response surface methodology (RSM) is the most commonly used statistical tool for process variable optimization[53]. RSM has several shortcomings when optimizing big data sets and more complex reactions thus the need for better and more sophisticated data predictive models[54, 55]. The advancement in computation power in the field of computer science has led to the emergence of Artificial Intelligence (AI) models which offer better accuracy and low run time.AI is characterized by its nonlinearity but also its ability to run complex and intricate data sets. These models are excellent at statistical modeling complex systems thus being able to give accurate insights into the

interactions between the various contributing variables and how they influence the adsorption efficiency.AI comprises of a variety models such as gradient boost decision tree (GBDT), linear regression (LG), random forest (RF), support vector regression, and artificial neural networks (ANN) which are used in adsorption studies to remove pollutants. Using various AI models provides invaluable information about the relationship between input and output parameters thus elaborating the dynamics for the reaction dynamics.

This review is aimed at giving information about the importance of artificial intelligence and machine learning models in the optimization and prediction of process parameters in the adsorptive removal of toxic heavy metals and textile dyes. It further highlights how the different AI models are applied in wastewater treatment.

2. AN OVERVIEW OF ARTIFICIAL INTELLIGENCE MODELS

AI is based on computer systems that behave like human intelligence and deal with smart systems as building blocks[56]. The objective of AI systems is to increase on functions of computers that are helpful to human beings such as perception, learning, and problem-solving[57].The optimization and prediction are based on three main categories which are deep learning, data analytics, and machine learning [56].The most commonly used AI models forwater treatment are shown in Figure 1.

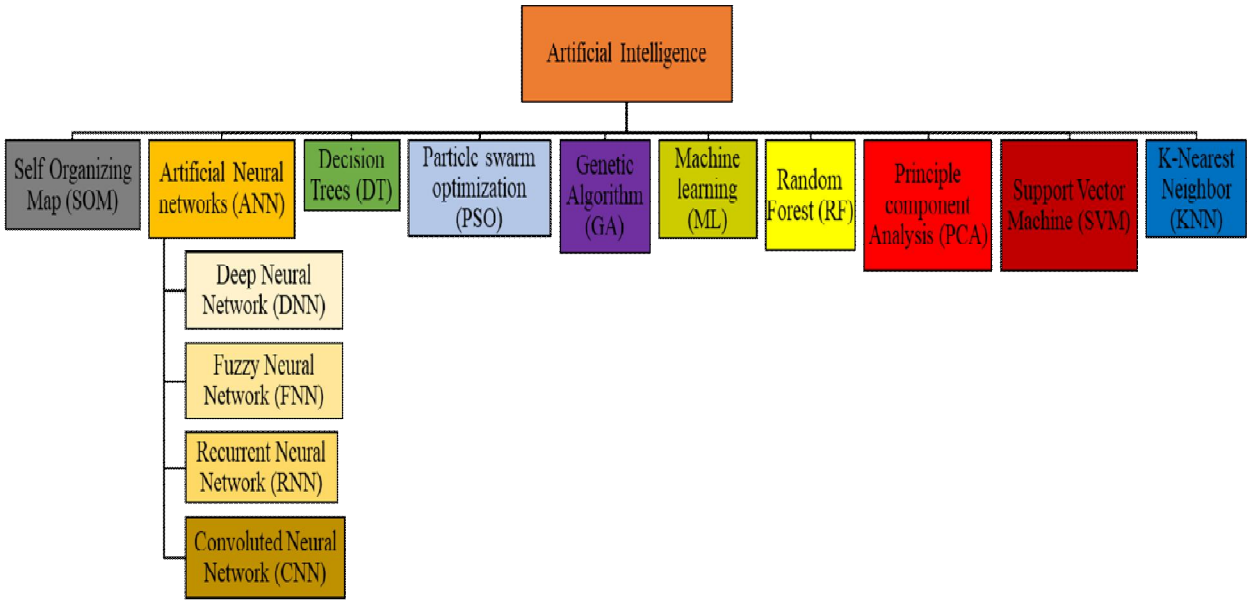

Figure 1. The most common Artificial intelligence models.

2.1 ACTIVATION FUNCTIONS

The activity of the input neurons determines the output through what is known as the activation function. It models the non-linear aspects of the world through its non-linearity. A number of expressions have been used to describe the neuron's activation function and they include step, sigmoid, tangent sigmoid, or linear function as shown in Table 1.

Table 1. The common activation functions used in artificial intelligence

Activation	**Expression**	**Range**	**Reference**
Sigmoid	$f(x) = \frac{1}{1 + e^{-x}}$	(0,1)	[58]
Tanh	$f(x) = \tanh(x)$	(-1,1)	[59]
Linear	$f(x) = x$	(-∞,+∞)	[60]
ReLU	$f(x) = max(0,1)$	(0, +∞)	[61]
ELU	$f(x) = \begin{cases} a(e^x - 1), & x < 0 \\ x, & x \geq 0 \end{cases}$	(-a,+∞)	[62]
Heaviside	$f(x) = \begin{cases} 0, x < T_1 \\ 1, x \geq T \end{cases}$	(0,1)	[63, 64]
Leaky ReLU	$f(x) = \max(x, x)$	(-∞,+∞)	[65]
Ramp	$f(x) = \begin{cases} 0, x < T_1 \\ \frac{x - T_1}{T_2 - T_1}, T_1 \leq x \leq T_2 \\ 1, x \geq T_2 \end{cases}$	(0,1)	[66]

2.2 ARTIFICIAL NEURAL NETWORKS

A mathematical tool developed from the working neural architecture of the human brain is the Artificial neural network (ANN)[67]. This network is made of three layers: the input, hidden and outputlayers which are all interconnected by many nodes which coordinate to perform particular tasks[68]. Just like real neurons, artificial inputs are taken in and then analyzed through clever non-linear activation functions, then used to predict output according to the experimental data[69]. These neural networks can be used to predict the sorption mechanisms of pollutants in aqueous phase. For the ANN to operate, experimental data must be available to generate training, validation and test sets[70]. The neural network's effectiveness and functionality are based on

the influence of the activation function, data set, input and output normalization and its structure[71]. The working principle of the ANN is based on a number of factors such as the nodes which are normally called neurons that process the information through the use of a unitary computational processor with a transfer function and a summation function[72]. Figure 1 shows the structure of the nodes, weights, and biases which connect the neurons, input and output parameters.

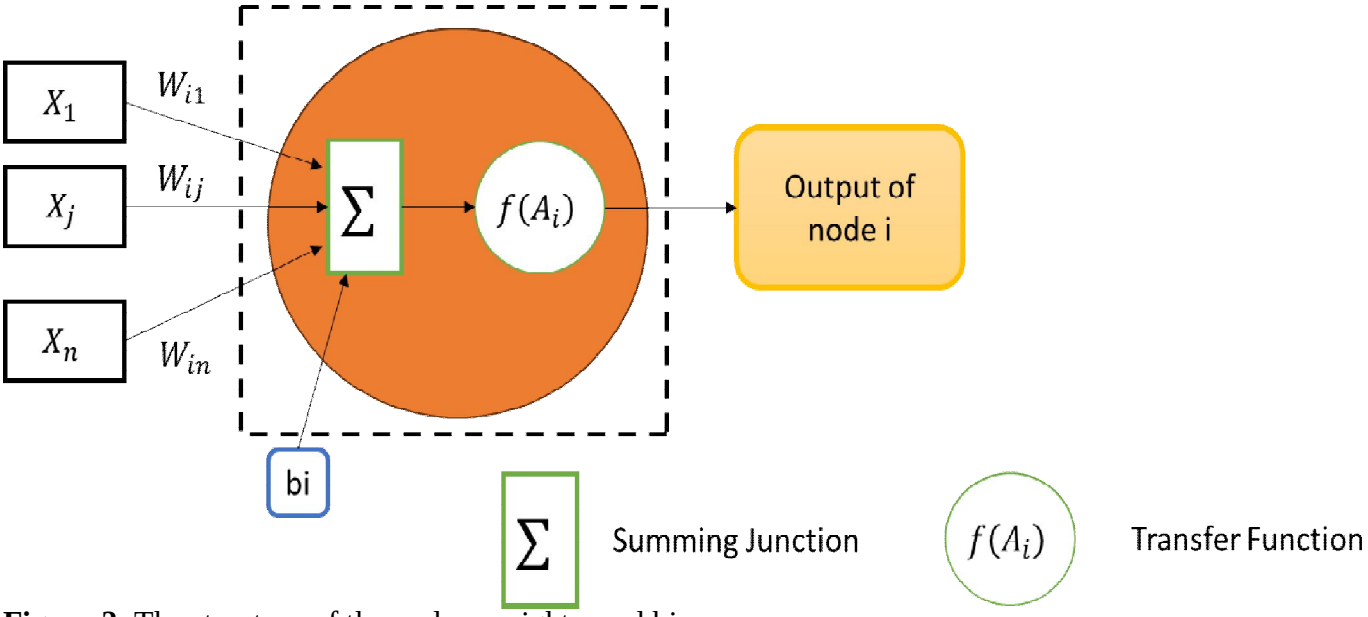

Figure 2. The structure of the nodes, weights, and biases

The neural network is described by the activation function, connecting weights, structural properties, and nodes which show the neural network [73]. The input and output layers determine the orientation of the flow of data in the neural network[74]. The three most commonly used transfer functions are the hyperbolic tangent sigmoid transfer function (tansig), linear transfer function (purelin), and the log-sigmoid transfer function (logsig), and [75, 76]. Figure 3 shows the three common transfer functions.

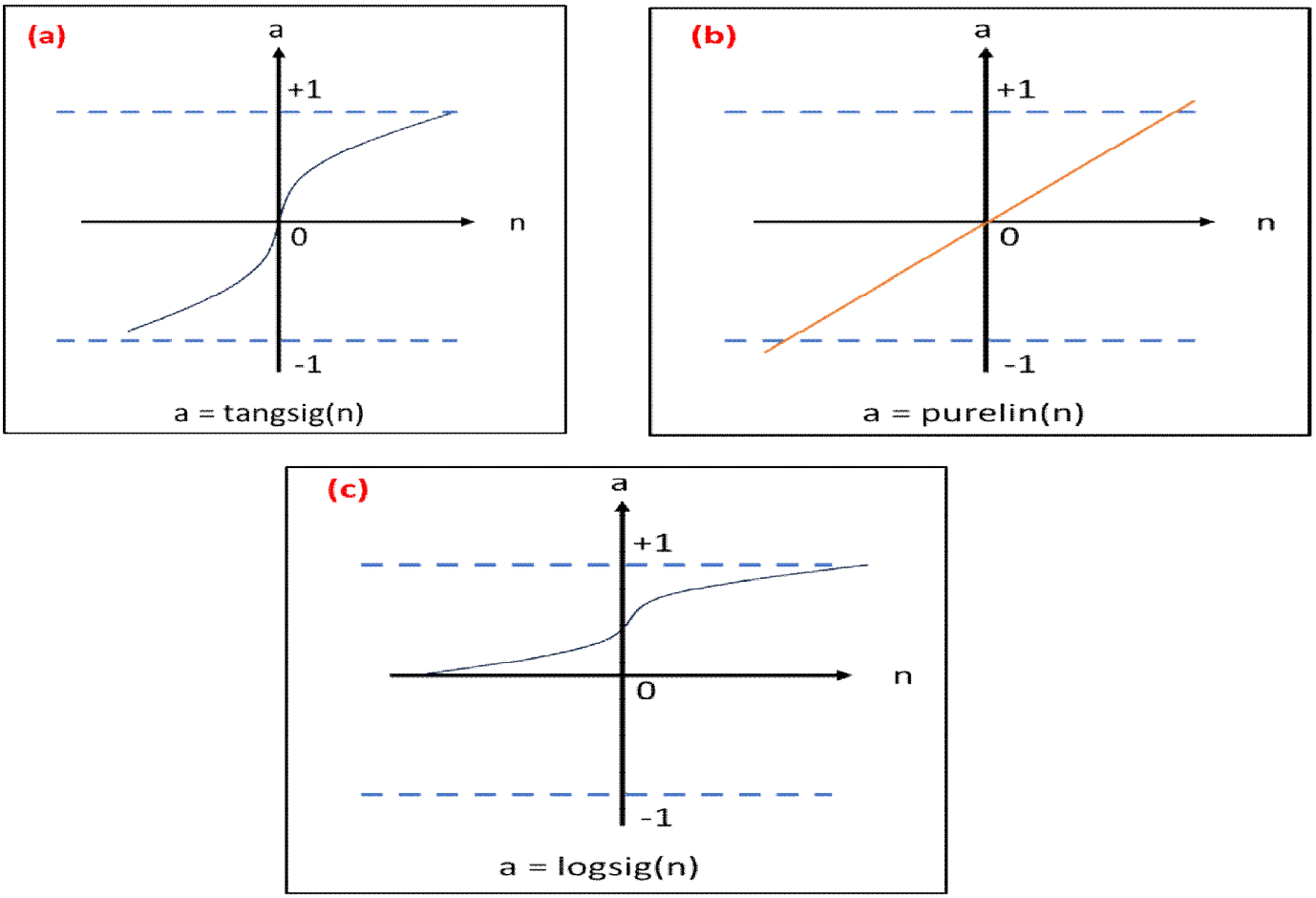

Figure 3. The three most common transfer functions

The classification of the ANN structure is based on two network architectures that is the radial basis function and back propagation network (BPN)[77]. The latter is commonly used since it is based on a reverse error spread but also its multilayer feed-forward mechanism which is known in 80 % of the neural networks [77]. A sigmoid layer, biases, and output layer are used as an approximation to the finite number of discontinuities [78]. Figure 4shows a diagrammatic representation of afeed-forward BPN.

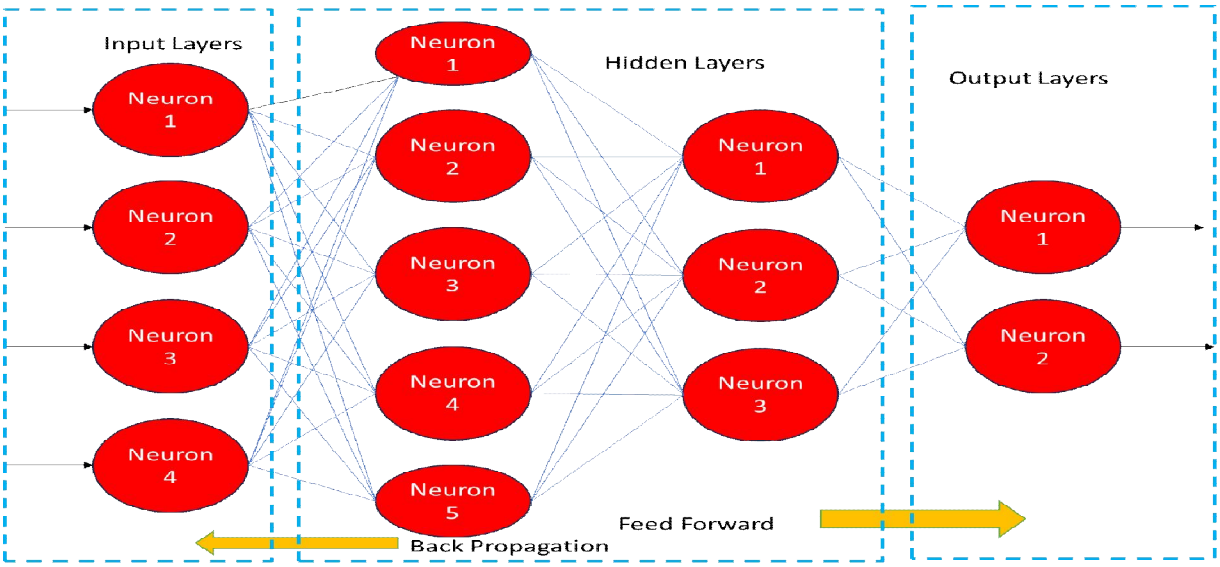

Figure 4.A diagrammatic representation of afeed-forward BPN

ANN models that have found wide application include Recurrent Neural Networks (RNNs), Fuzzy Neural Networks (FNNs), Deep Neural Networks (DNNs) and Convolutional Neural Networks (CNNs)[79–83].

2.2.1 Convolutional Neural Network (CNN)

This network is defined by a deep structure and convolutional computation and is based on a feedforward neural network. It is part of deep learning with the ability to process data in language processing and computer vision. The inputs are processed through the convolutional layers which then move to the pooling that reduces the dimensions and then regression occurs at the connected layers [84]. Figure 5 shows the basic structure of aCNN architecture.

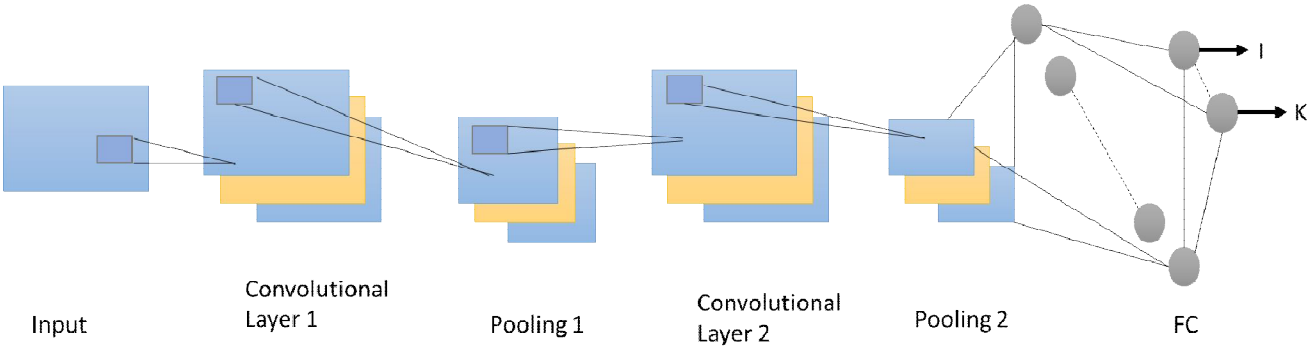

Figure 5. The basic structure of a CNN architecture

2.2.2 Deep Neural Network (DNN)

This is classified with multiple hidden layers but the output and input layers enable it to learn deep and complex data sets where high-level learning occurs through the use of successive low-level layers. It is mainly applied in mapping nonlinear data sets for the input and output layer but also in understanding the complexity of data. Figure 6shows the basic structure of a DNN.

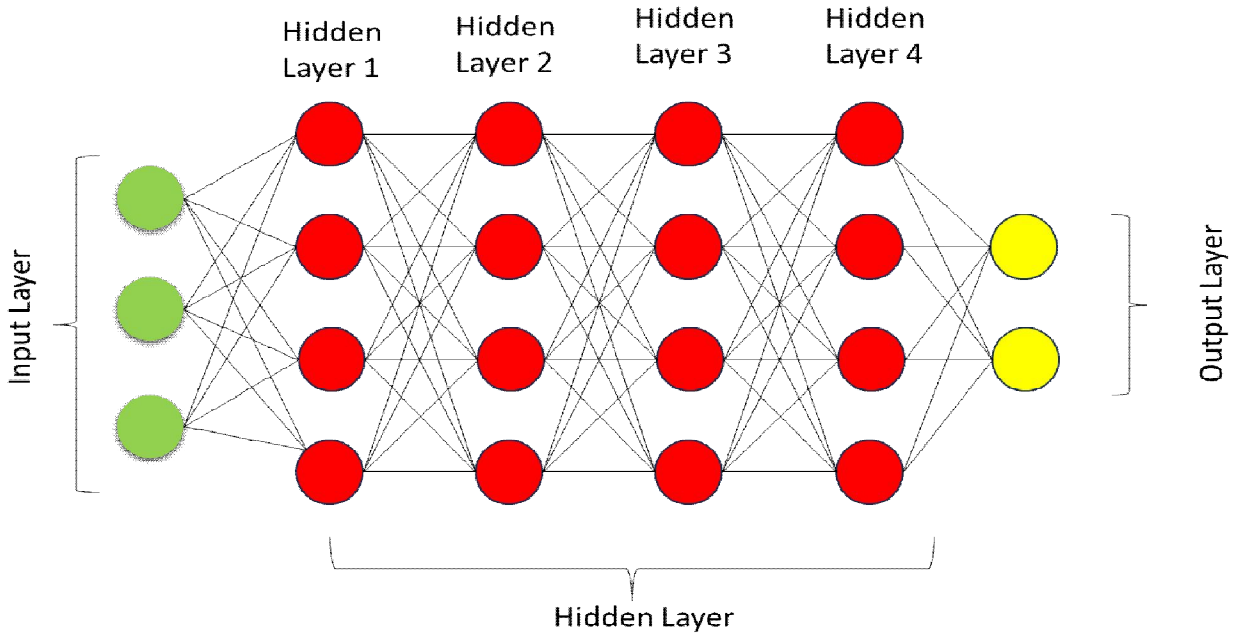

Figure 6. The basic structure of a DNN

2.2.3 Recurrent Neural Network (RNN)

RNN is based on connections of feedback which takes the input data in the form of a sequence and makes recursions to the sequence through the evolution direction. It can determine the nonlinear characteristics of the time series problems through its abilities of parameter sharing, memory, and turing completeness. Long short-term memory (LSTM), is the commonly used RNN through its capacity to have gated units which help to solve the gradient disappearance problem. The basic RNN architecture is shown in Figure 7.

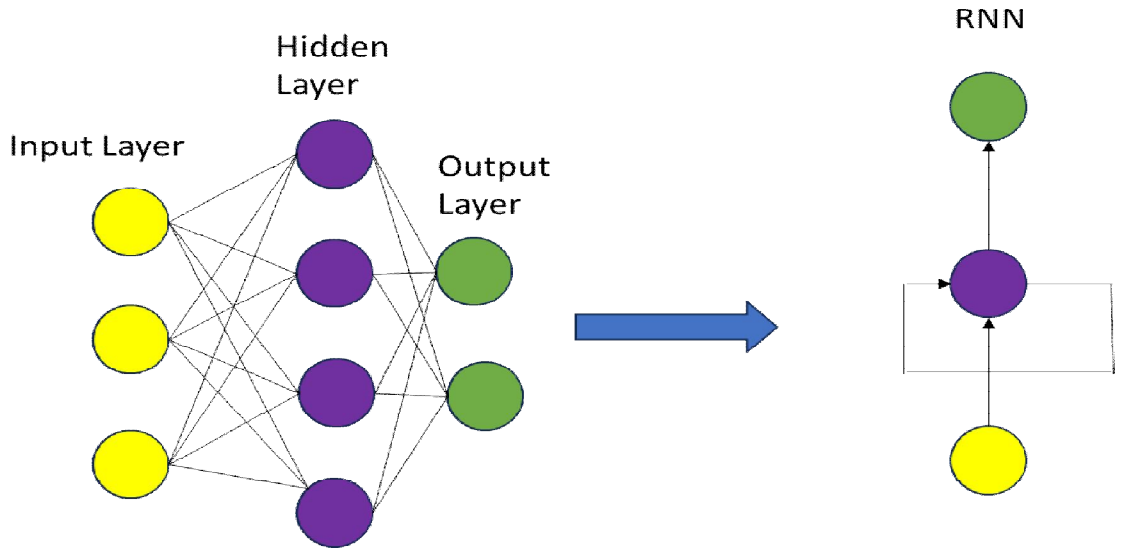

Figure 7.The basic RNN architecture

2.2.4 Fuzzy Neural Network (FNN)

FNN uses both the ANN and fuzzy logic to simulate and predict data sets with uncertainty. Fuzzy logic is applied in the processing of the input data while ANN trains and outputs the data. It uses the membership function, normalization, and inference to describe the relationship between input and output data while describing the neuron connections by the weights.The basic FNN architecture is shown in Figure 8.

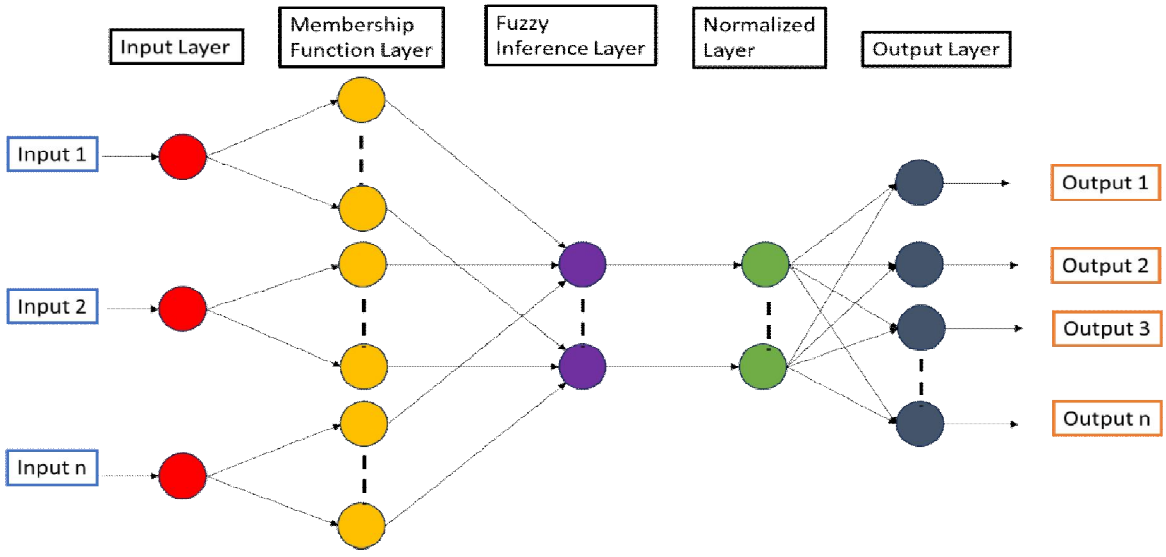

Figure 8. The basic FNN architecture

2.3 MACHINE LEARNING (ML)

This is a sub-category of AI aimed at developing statistical models and algorithms that enable systems to learn from data without having prior knowledge of the data sets[85]. Its objective is to make accurate decisions and predictions based on predictive models and what it has learned from the raw data [86]. Figure 9 shows the common machine learning models.

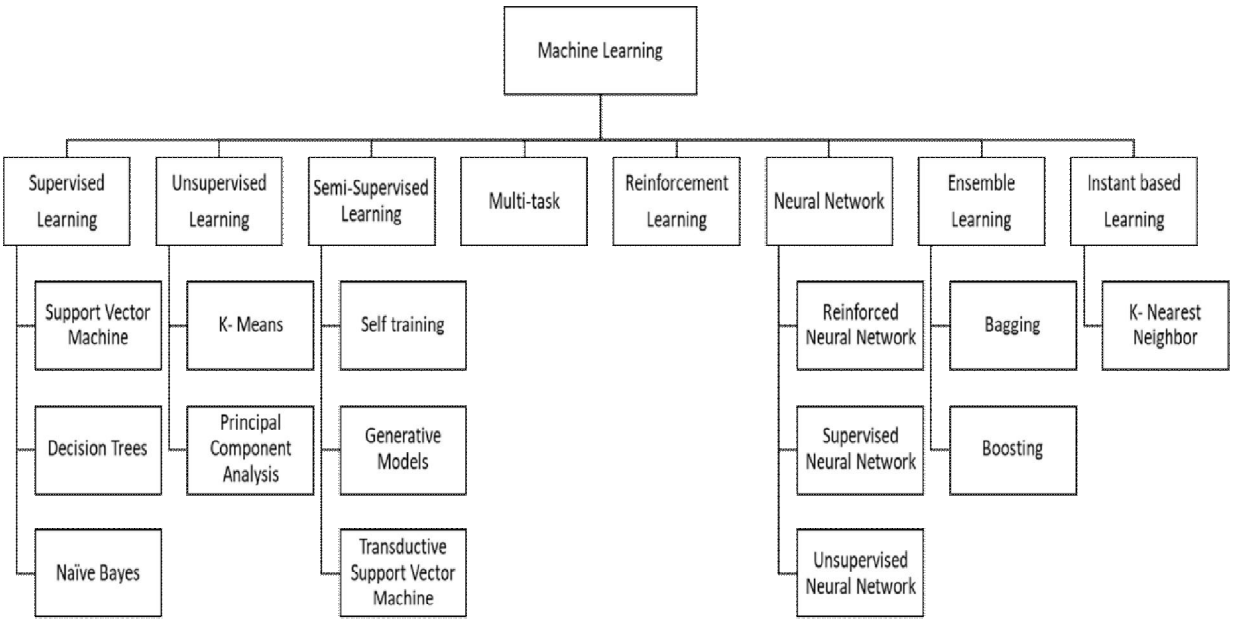

Figure 9. Thecommon machine learning models

2.4 ADAPTIVE-NETWORK-BASED FUZZY INFERENCE SYSTEM (ANFIS)

This is an intelligent modeldesigned using neural networks and fuzzy logic for prediction, regression, and classification. It is modeled using the neural network's learning capacity plus the fuzzy inference ability of the fuzzy logic to increase the learning of the inference systems [87]. It is used in the modeling of multivariable and nonlinear systems which help in its application in areas such as classification and prediction. Figure 10 shows the basic structure of ANFIS.

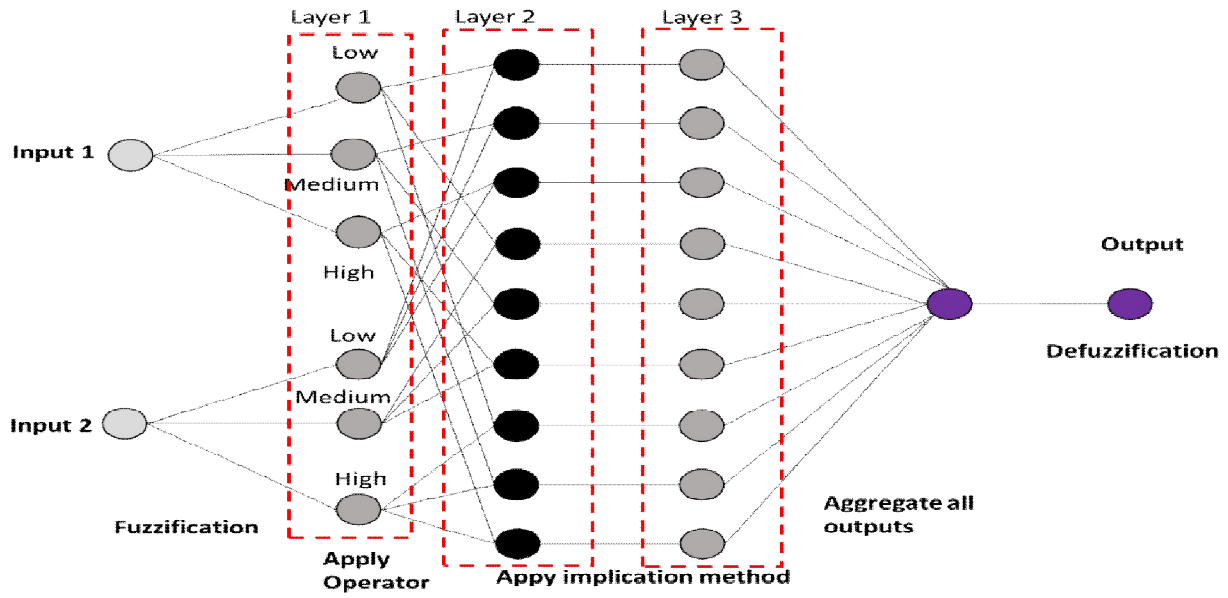

Figure 10. The basic structure of ANFIS

2.5 RANDOM FOREST (RF)

It is normally used to increase the stability and accuracy of the model through the application of multiple decision trees. Through the decision tree training on different random data sets, the accuracy of the model can be improved. Averaging multiple decisions helps in optimization and classification [88]. Figure 11shows the basic structure of RF.

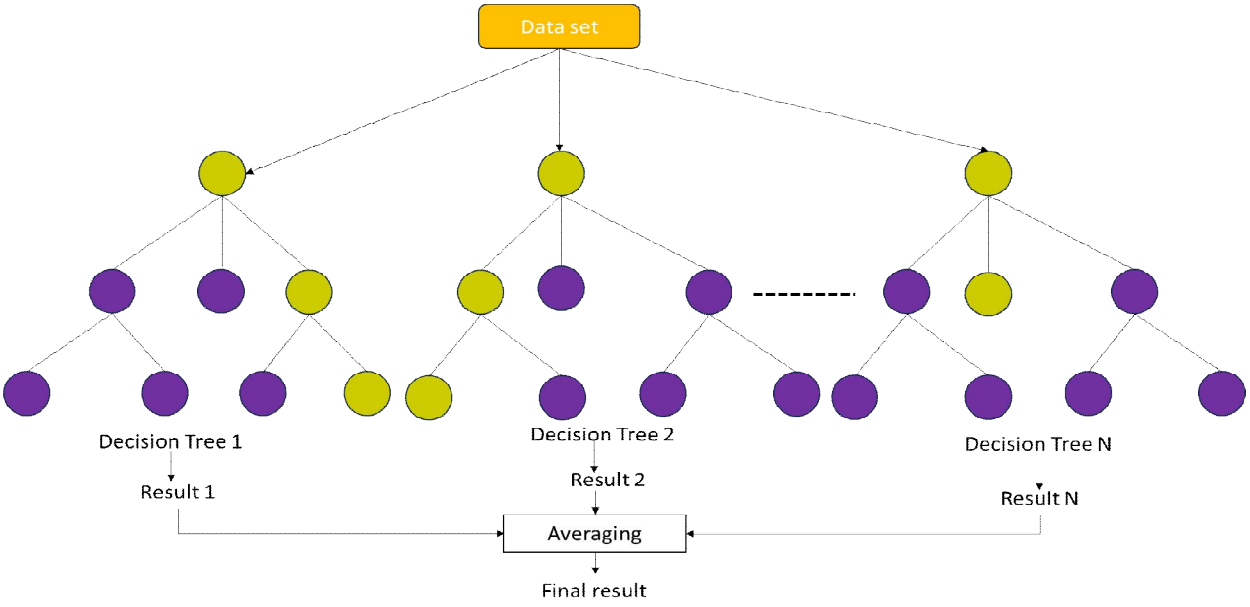

Figure 11. The basic structure of RF

2.6 K-NEAREST NEIGHBORS (k-NN)

This is another algorithm that is simple and commonly used in the regression and classification of data sets. It simulates the category of a new data point based on K neighbors closest to this point through the use of the training sets. Using different data point distance measurements, it can easily modify complex models and deal with nonlinear relationships between the output and input data.

Figure 12shows a schematic representation of a KNN model.

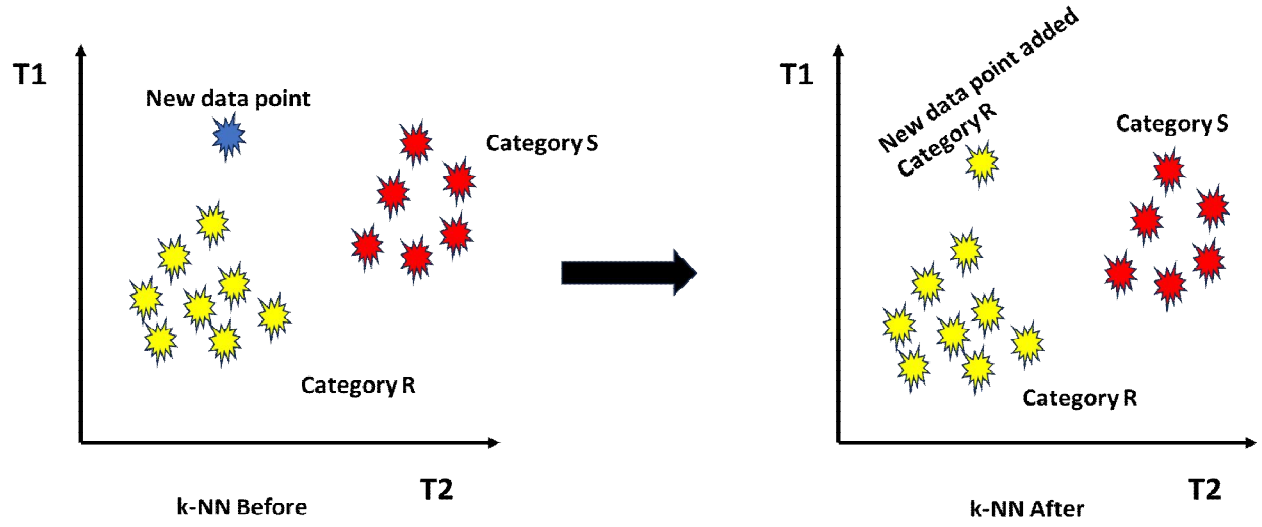

Figure 12. A schematic representation of a KNN model

2.7 DECISION TREE

This model follows a tree where the node shows the input, the edge describes the probable outputs and the leaf node denotes the real output[89]. It uses simple learning decision rules to generate training data that is used for class or data prediction. It isfavoured becauseof its ease of implementation and high accuracy. In this model all problems are looked at starting with the leaves, stem up to the roots which results in many possible solutions. Figure 13 shows the basic structure of a decision tree.

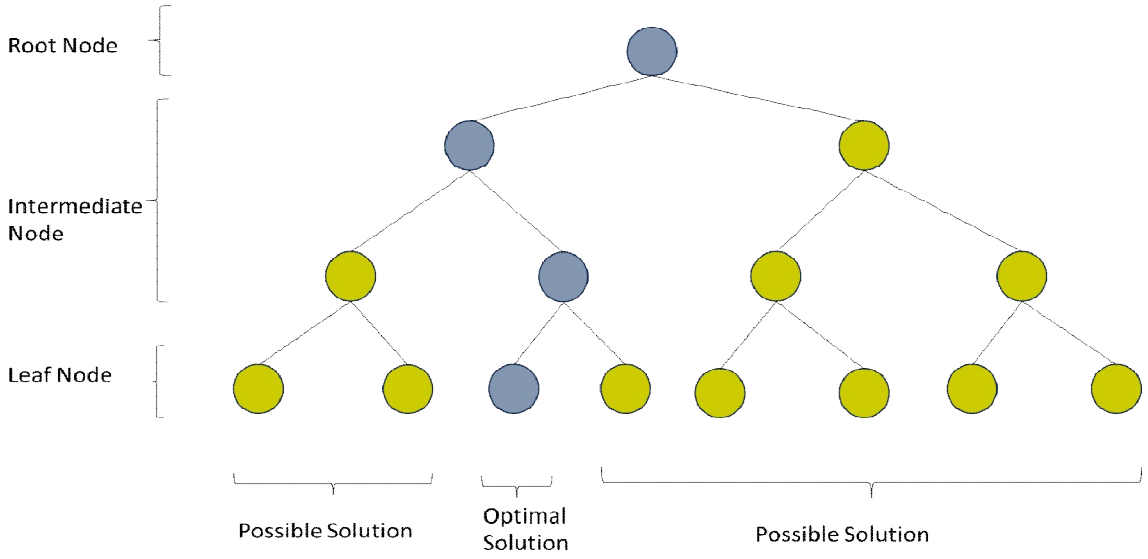

Figure 13.The basic structure of a decision tree.

2.8 PRINCIPAL COMPONENT ANALYSIS (PCA)

It is an algorithm used to train high-dimension data to low-dimension data through a reduction technique and ensure that during the orthogonal transformation, the original data is retained [90]. It is applied in noise filtering, clustering, and language processing. Figure 14 shows a diagrammatic representation of Principle Component Analysis.

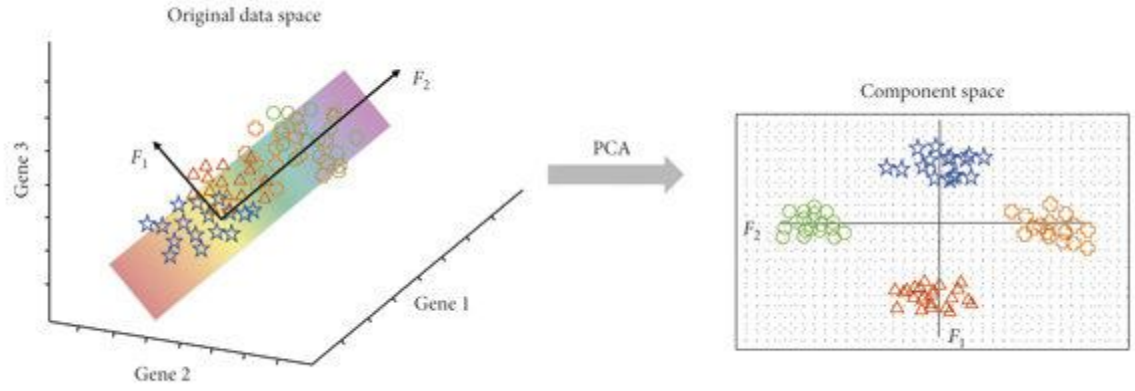

Figure 14. A diagrammatic representation of Principle Component Analysis[91].

2.9 PARTICLE SWARM OPTIMIZATION (PSO)

PSO describes the behavioral patterns of biological systems such as birds, whales, or fish through its ability to optimize the velocity and position to achieve an optimal solution.After each iteration based on the optimal position and the algorithm-defined rule, the individual particles will migrate to the best position through modification of their position and velocity [92]. The

position and velocity of the particle is shown by the blue bold lines, P_{best} describes the individual best position, and G_{best} describes the best global position in a given search space. The representation of the Particle Swarm Optimization model is shown in Figure 15.

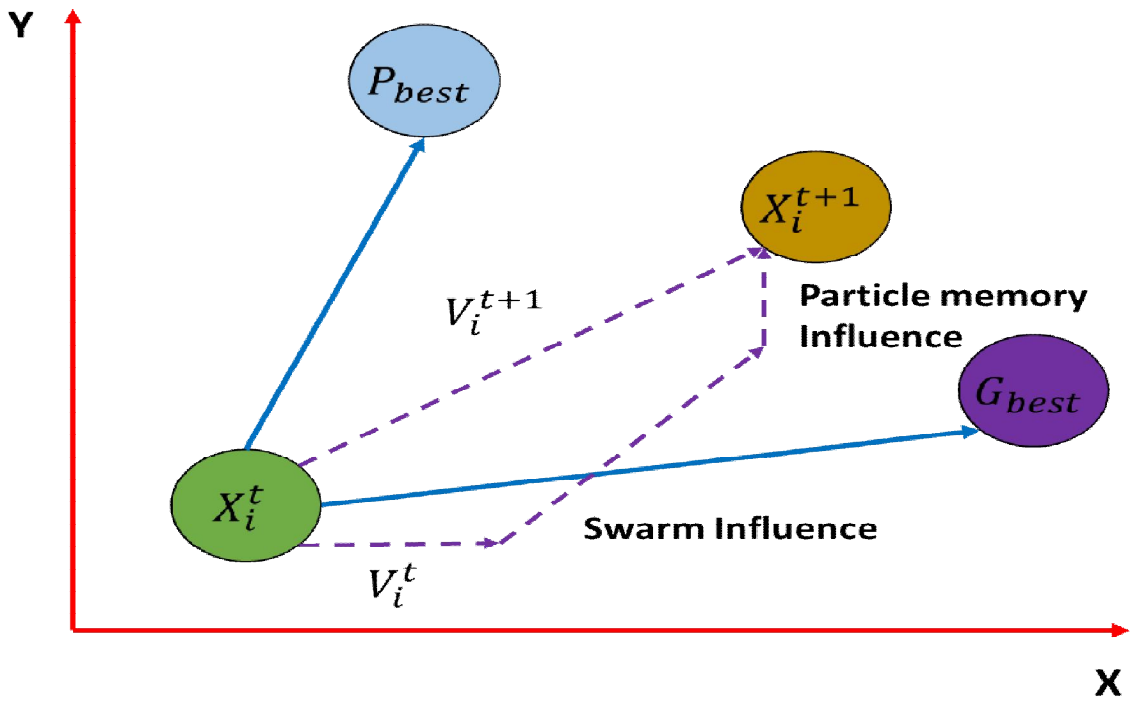

Figure 15. A representation of the Particle Swarm Optimization model

2.10 SUPPORT VECTOR MACHINE (SVM)

SVM deals with training data that is labelled to determine the next step of each category and is based on the mapping of the input vector via a high dimensional space. The basis for the mapping is obtained using a variety of kernel functions such as polynomial andradial basis whereas the datasets determine the function selection [29]. It is mainly used in pattern recognition where a hyperplane is drawn which causes the differentiation between two data sets in the space thus creating a margin for classification. Figure 16 shows a diagrammatic representation of a Support Vector Machine model.

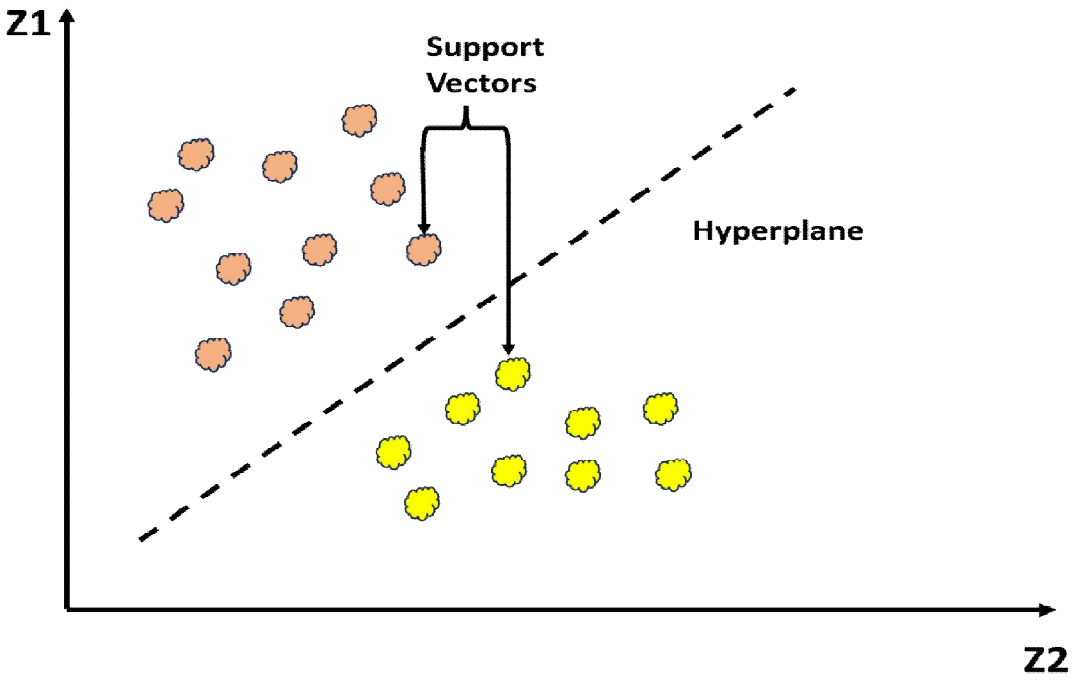

Figure 16.A diagrammatic representation of a Support Vector Machine model

2.11 SELF-ORGANIZING MAP (SOM)

It is based on the input and output layers and is commonly applied in dimensional reduction and clustering. It uses an associated competitive process for input data that projects high dimensional to low dimensional input data without affecting the topology of the data thus making it simple to classify and visualize data points [93]. Figure 17 shows a diagrammatic representation of a Self-Organizing Machine model.

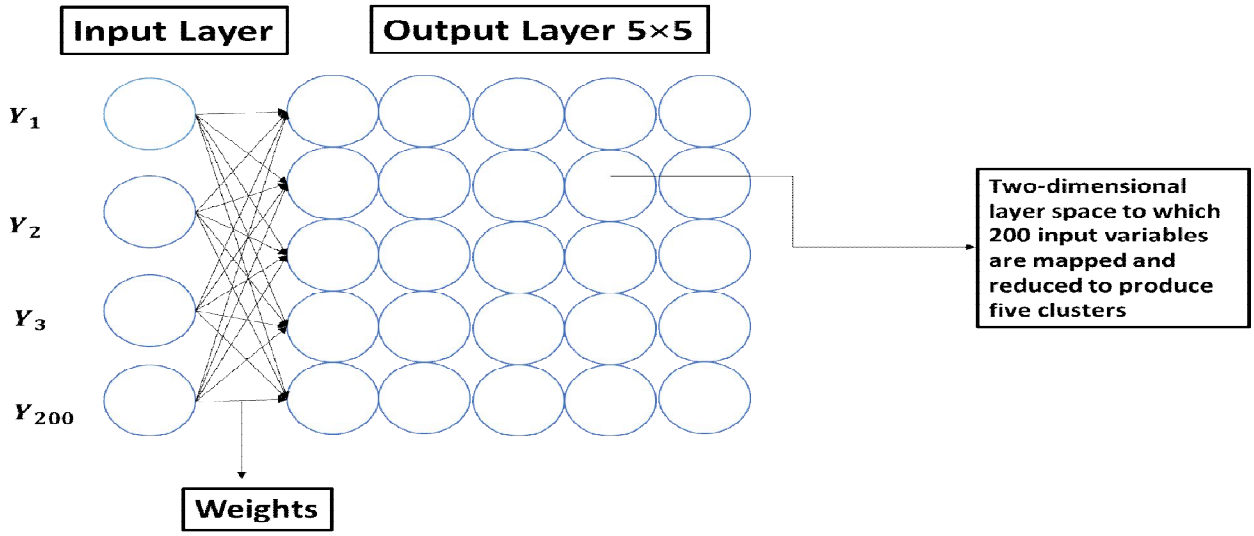

Figure 17. A diagrammatic representation of a Self-Organizing Machine model

2.12 GENETIC ALGORITHM (GA)

It is an optimization and search method based on the evolution of biological systems. Through genetic manipulation, it copies the genetic process of nature leading tooffspring that are best adapted to the environment. The local optimal solution does not limit it but rather can be able to search the multidimensional space for the optimal solution through either mutation, crossover, and selection which causes it to deal with complex nonlinear optimization challenges [94].

Figure 18shows a genetic algorithm with selection, crossover, and mutation processes.

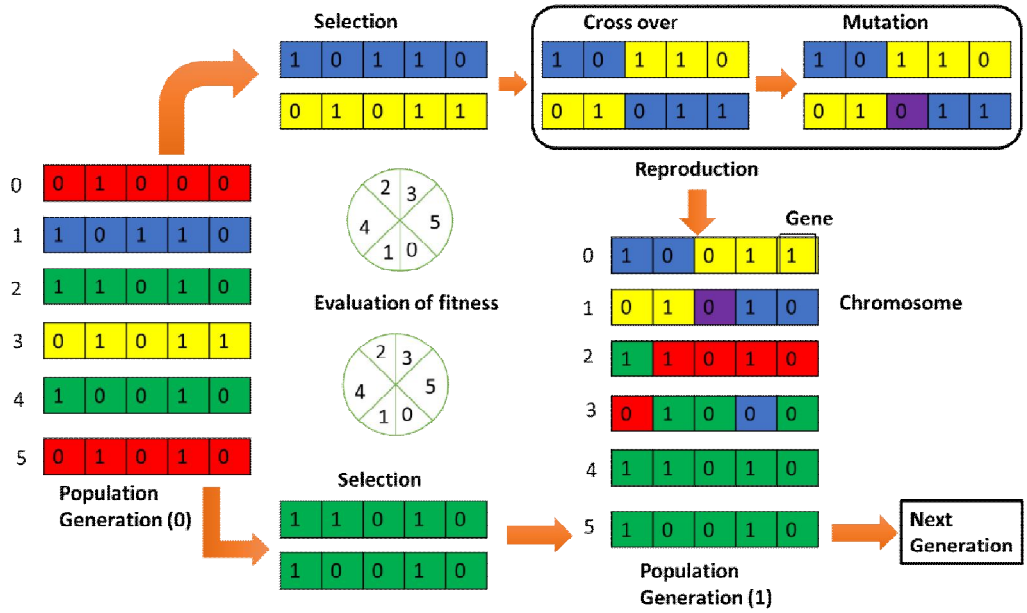

Figure 18. A diagrammatic representation of a genetic algorithm

3.0 PERFORMANCE STATISTICAL INDICATORS

AI model's performance evaluation is based on a number of statistical indicators such ascoefficient of determination (R^2), root mean squared error (RMSE), mean squared error (MSE), absolute average deviation (AAD), etc. The details of commonly used performance indicators are summarized in Table 2.

Table 2. The commonly used performance parameters

Indicator	Equation	Reference
MSE	$\frac{\sum(Z_i - Y_i)^2}{n}$	[95]

Root mean squared error (RMSE)	$\sqrt{\frac{\sum_{i=1}^{n}(Z_i - Y_i)}{n}}$	[96]
Mean absolute error (MAE)	$\frac{\sum_{i=1}^{n}(Z_i - Y_i)}{n}$	[97]
Sum of squared error (SSE)	$\sum_{i=1}^{n}(X_i - X_{mean})$	[98]
Absolute average deviation (AAD)	$\frac{\sum_{i=1}^{n}(X_i - X_{mean})}{N}$	[99]
Coefficient of determination (R^2)	$\frac{1 - \sum_{i=1}^{n}(Z_i - Y_i)}{\sum_{i=1}^{n}(Z_i - Y_{mean})}$	[100]
Adjusted R^2	$\frac{(1 - R^2)X(n-1)}{(n-k-1)}$	[101]
Normalized RMSE	$\frac{\sum_{i=1}^{n}(Z_i - Y_i)}{n}$	[102]

4.0 APPLICATION OF ARTIFICIAL INTELLIGENCE IN WASTEWATER TREATMENT

AI models have been extensively applied in wastewater treatment, particularly using the adsorption process. This study will describetwo pollutants that is textile dyes and toxic heavy metals will be discussed briefly.

Nwosu-Obieogu et al., [103] used *Luffa cylindrica* activated carbon (LAC) for the removal of chromium (VI) from wastewater. The variable parameters were contact time, pH, and adsorbent dosage using a batch experiment through ANN and ANFIS. ANN and ANFIS were determined throughR^2 and MSE. The models demonstrated significant predictive behavior with R^2 (9.9999E−1) and MSE (5.985E−14) for chromium (VI) removal.

Ahmad., [104] investigated the effect of various parameters on the removal of methyl orange dye through the use of PANI/FO nanocomposite. The ANN with a structure of 5-9-1 was used in this study it showed good predictive results. The accuracy was illustrated using R^2 square value of 0.991, RMSE value of 0.127, AAD value of 0.842 %, and MAE value of 1.418.

In this study Kumari et al., [105]applied four models that areRSM, ANN,k-NN, and ANFIS in removing crystal violet (CV) from wastewater using Sugar cane bagasse (*Saccharum officinarum*) biochar. The effect of process variables which include adsorbent dosage, pH, temperature, and initialconcentration were investigated. The ANN, RSM, k-NN, and ANFIS models obtained R^2 of 0.9685, 0.9618, 0.9421, and 0.8823, respectively. From the data obtained it was observed that ANN had the best accuracy.

The removal of Pb(II) and Cu(II) using a nanocomposite of rice straw and Fe3O4 was investigated by Khandanlou et al., [106]. Using ANN, the input parameters that is adsorbent dosage, time, and initial concentration with removal efficiency as the output variable were modeled. The model was trained using Batch Backpropagation (BBP), genetic algorithm (GA), quick propagation (QP), Levenberg-Marquardt (LM), and Incremental Back Propagation (IBP) algorithms. RMSE determined that the best training set was due to IBP and topology of 3-9-2 with a superior R^2.

Esfandyari et al., [107]studied the prediction accuracy of ANN and ANFIS in the removal of Pb (II) and Ni (II) using active sludge. The variables parameters in this study were contact time, pH, temperature, and initial concentration. A Sugeno Fuzzy for ANFIS and a multilayer perceptron for ANN were used in the modeling. The experimental and predicted data were well in agreement with correlation coefficients>98% although the ANFIS showed higher superiority compared to ANN.

Through the use of chemically modified sugarcane bagasse (SBM) bio-adsorbent Leon et al., [108]removed color from textile real water through the modeling and simulation of the data using ANN. The multilayer feed-forward neural network, with five inputs and one output, was trained with eight neurons in the hidden layer. Using this model a comparison was carried out to understand the fitness of the experimental and predicted data and an (R^2) of 0.928 and a mean square error (MSE) of 0.013 were obtained.

Khiamet al., [109]determined the effect of adsorbent dosage, pH, and contact time on the removal of methylene blue using graphene oxide/chitosan composites through the use of ANN-PSO by using experimental data obtained from RSM. ANN-PSO had a good accuracy with R^2 (=0.998) compared to RSM (R^2 = 0.981).

Lastly Rafie et al., [110]used hydrothermally synthesized $MnFe_2O_4$ and $CoFe_2O_4$ nanoparticles to remove Pb (II) and Cr (VI). The ANN-GA was used to predict the adsorption capacity at both non-equilibrium and equilibrium conditions. Using GA the training (49.5%), validation (40.5%), testing (10%), seven neurons, and input parameters that are contact time, adsorbent dosage, pH, initial concentration, and temperature. The model gave a high predictive accuracy for the modeled data with ($R^2 = 0.998$).

5.0 CONCLUSION

Artificial Intelligence (AI) and Machine Learning (ML) models arechanging the understanding of the adsorptive removal of toxic heavy metals and textile dyes from wastewater. These models exhibit exceptional predictive capabilities, accurately forecasting adsorption capacities, isotherms, kinetics, and breakthrough curves. This predictive power significantly optimizes treatment processes while minimizing the need for extensive experimental trials. Secondly, these models excel at extracting valuable insights from vast datasets. By analyzing the relationships between adsorbent properties, operating conditions, and pollutant removal efficiency, AI provides a deeper understanding of the underlying adsorption mechanisms. This enhanced understanding facilitates the development of more effective and targeted treatment strategies. Furthermore, AIalgorithms play a crucial role in optimizing various process parameters, such as adsorbent dosage, contact time, pH, and temperature. This optimization maximizes pollutant removal while minimizing operational costs and resource consumption. By continuously analyzing data streams, AI-powered systems can dynamically adjust treatment processes in response to changing conditions, ensuring efficient and continuous operation.

Author's contributions

This work was carried out in collaboration between all authors. Authors SB, MK, IK, and CTA designed the study, performed the statistical analysis, wrote the protocol, and wrote the first draft of the manuscript. AuthorsSB, MM, and P.M.B managed the analyses of the study. Authors S.K and P.M.B managed the literature searches. All authors read and approved the final manuscript."

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Ethics approval and consent to participate

Not applicable.

Consent for publication

Not applicable.

Availability of data and materials

Not applicable.

Competing interests

The authors declare no competing interests.

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