4. DEEP LEARNING FOR WQI PREDICTION MODELS WITH PHYSIOCHEMICAL PARAMETERS

Water quality is a significant environmental issue, and its monitoring and management are crucial for the safety and sustainability of ecosystems and human health. Accurate and timely water quality index (WQI) prediction helps to identify potential hazards and implement preventive measures. Traditional water quality monitoring methods require collecting samples and laboratory analysis, which is expensive and time-consuming. WQI prediction models are currently being developed using traditional machine learning approaches and deep learning algorithms. The capabilities of deep learning in building WQI prediction models employ sophisticated algorithms to process extensive data and generate precise WQI prediction models. This chapter elucidates the construction of WQI prediction models by training the physicochemical parameters with various deep learning architectures for regression.

WQI PREDICTION MODELS USING PHYSIO-CHEMICAL PARAMETERS AND RNN VARIANTS

The objective of this study is to construct a WQI prediction models by learning the trends in time series data containing physiochemical parameters using deep-learning architecture RNN and its variants. The water quality index prediction problem is treated as a regression task, and the regression models are developed by leveraging the knowledge obtained from the training data using RNN and its variants LSTM, and GRU. The efficacy of the WQI prediction models is evaluated through a range of performance metrics, including Mean Absolute Error, Mean Squared Error, Root Mean Squared Error, and the R2 Score value.

Methodology

Deep neural networks use the data inputs, weights and bias to accurately describe, classify and characterise the data. Deep neural networks have numerous layers of interconnected nodes, with two layers that are visible serving as the input and output layers to enhance prediction. The deep learning model consumes the pre-processed data at the input layer, and at the output layer, the final prediction is made. The structure of the proposed WQI prediction model consists of important building blocks which includes 1. data collection 2. exploratory data analysis and data pre-processing 3. construction the WQI prediction models 4. model evaluation. Fig.4.1 depicts the framework of the proposed RNN variants-based WQI prediction models.

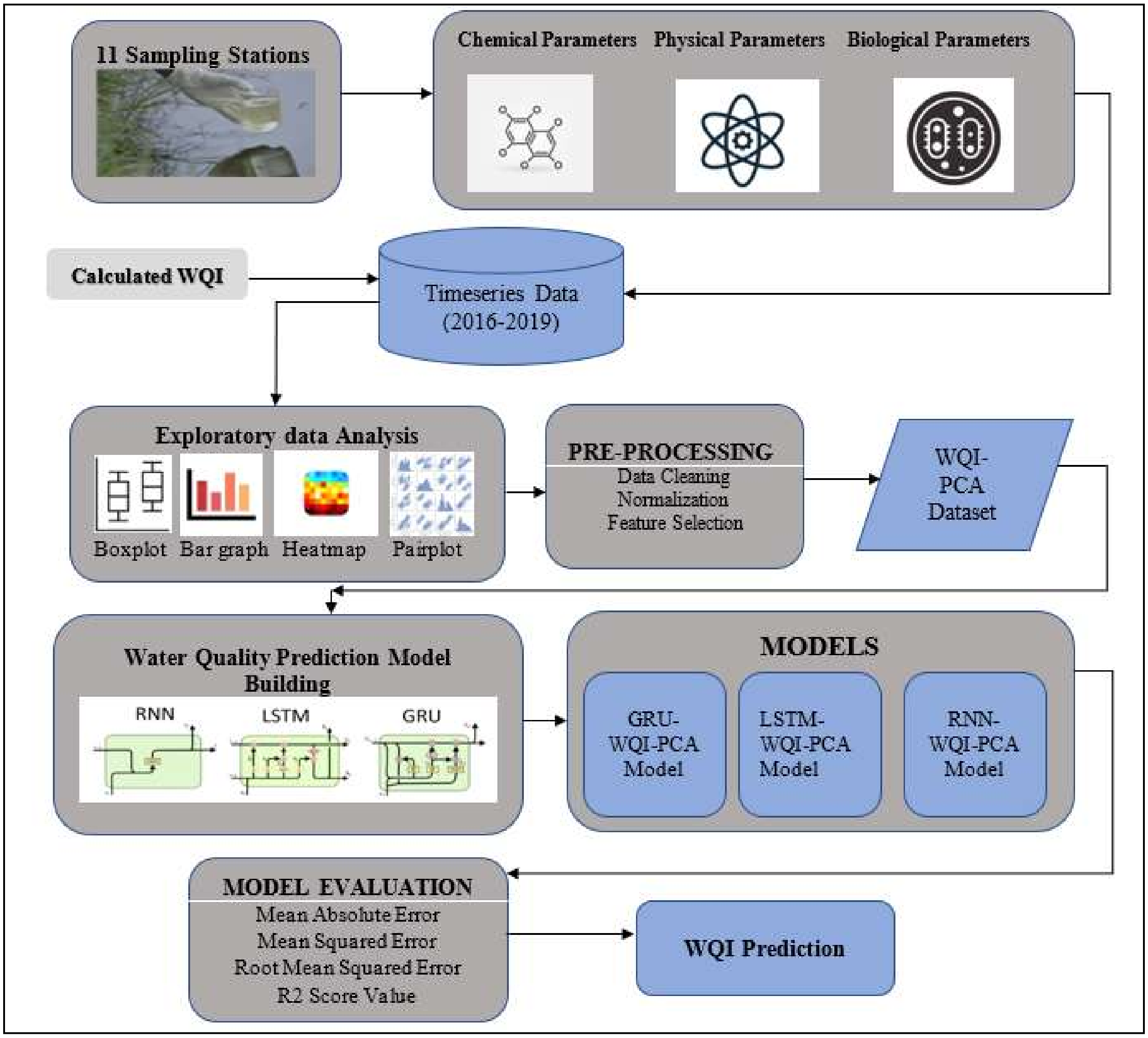

Fig.4.1 Framework of the WQI Prediction Model using RNN and Variants

Data Collection and Dataset Preparation

Around 10560 instances are collected from the 11 monitoring stations situated across the Bhavani River for the period from January 1st, 2016 to December 31st, 2020. The observations for 26 physicochemical parameters such as pH, conductivity, turbidity, phenolpth alkalinity, total alkalinity, chloride, chemical oxygen demand, total Kjeldahl nitrogen, ammonia, hardness, Ca.hardness, Mg. hardness, sulphate, sodium, total suspended solids, total dissolved solids, fixed dissolved solids, phosphate, boron, potassium, biological oxygen demand, fluoride, nitrate, dissolved oxygen, total coliform and faecal coliform, and the spatial parameters such as longitude, latitude, station ID, and temporal parameter date, have been derived for the water samples. The water quality index value for each sample is calculated using the Indian Standards for Drinking Water Specification and assigned to the corresponding sample as the target variable. A time series data with 31 attributes and 10560 tagged instances has been prepared.

The EDA is applied to this time series data to understand the characteristics of the data and to analyse the importance of each parameter in determining the water quality index. The detailed report on EDA is presented in Chapter 3. The results of EDA suggested few preprocessing requirements, which have been carried out. The Select k best feature selection method is used and more relevant features are considered. Finally, the dataset with 10560 instances and 28 attributes along with calculated WQI has been developed and is called as WQI-PCA dataset for reference as mentioned in Table XII of Chapter 3.

Model Building

The WQI prediction models are built using deep learning architectures such as RNN, LSTM and GRU. Recurrent Neural Networks are a class of neural networks designed for sequential data processing, capable of retaining information from past inputs through recurrent connections. Long Short-Term Memory is a specialized type of RNN that overcomes the vanishing gradient problem by incorporating gated cells, enabling it to learn and retain information for longer periods. Gated Recurrent Unit is another variant of the traditional RNN, similar to LSTM but with fewer gates, resulting in a simpler architecture. Although the Gated Recurrent Unit may not possess the same level of sophisticated control over information flow as the Long Short-Term Memory model, it still maintains computational efficiency and has demonstrated competitive performance across a range of sequential data tasks.

The model training involves selecting the optimal hyperparameters to improve the efficiency of the model in mapping the input features as independent variables to the target variable as the dependent variable. The hyperparameters used in deep learning architectures are hidden layers, dense layers, optimizer, epoch, momentum, batch size, activation function and dropout. The layers that exist between the input and output layers are known as hidden layers. A dense layer is a layer in which each layer receives input from all layers in the previous and thus, it is densely connected. Dense layers improve overall accuracy and the range is set to 5 to 10 units. Optimizers are techniques used to modify the neural network's properties, such as its weights and learning rate, in order to minimize losses and address optimization issues. The epoch size determines how many complete iterations of the dataset must be run. Momentum is a special hyperparameter that allows the search direction to be determined by the accumulation of gradients from prior steps rather than just the gradient from the current step. Activation functions are used to introduce nonlinearity into the model. This allows deep learning models to learn nonlinear prediction bounds. The activation function can split them into different layers and get a reduced output of the density layer. The dropout layer improves in avoiding overfitting in training by bypassing randomly selected layers, limiting sensitivity to particular layer weights. The learning rate determines the speed at which a deep model replaces an already learned concept with a new one.

By properly configuring the deep neural algorithms RNN, LSTM, and GRU with hyperparameters setting and training the instances of the WQI-PCA dataset, the WQI prediction models have been built. These models are referred to as RNN-WQI-PCA, LSTM-WQI-PCA, GRU-WQI-PCA and the performance of these models is evaluated using the metrics such as MAE, MSE, RMSE, and R2 score.

Experiment and Results

The experiments have been carried out by implementing deep learning algorithms such as RNN, LSTM, and GRU, using WQI-PCA dataset and implemented using Python libraries Tensor Flow, Keras and Scikit learn. The training dataset contains 8124 tagged instances of the WQI-PCA dataset. The evaluation of the prediction models is carried out using the metrics such as MAE, MSE, RMSE and R2 score values with the test data set containing 2009 tagged instances of the WQI-PCA dataset.

The prediction models such as RNN-WQI-PCA, LSTM-WQI-PCA, and GRU-WQI-PCA are defined with various hyperparameters as tabulated in Table XIII, such as dense layer values from 5 to 10 units, optimizer as Adam optimizer. The epoch size is given as 20, 50,100,150, 200 and 500 epoch size. The momentum is set from 0.5 to 0.9, the activation functions are defined with both on and off. The batch size is fixed as either 32 or 64, the dropout unit is 0.3 and the learning rate is 0.1. The experimental results with respect to the deviation between the predicted values and actual values shown by RNN, LSTM and GRU WQI prediction models are illustrated in Fig. 4.2 and 4.3. From the figures, it is found that the deviation between the actual values and the predicted values in the case of the GRU prediction model is less than the threshold value when compared with LSTM and RNN.

Table XIII. Hyperparameters Setting for Training Deep Neural Networks

Hyperparameter	Values	Hyperparameter	Values
Optimizer	Adam	Dropout	0.2, 0.3
Dense Layer	5 to 10	Momentum	0.5 or 0.9
Epoch	20, 50, 100, 150, 200	Learning rate	0.1
Batch size	32/64	Activation function	Relu

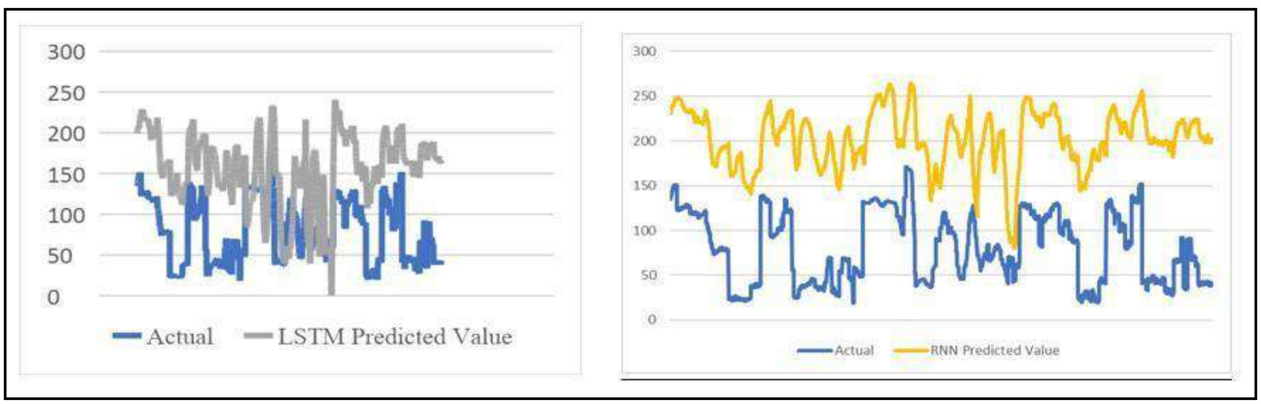

Fig. 4.2. Actual vs Predicted Values of LSTM and RNN Based WQI Models

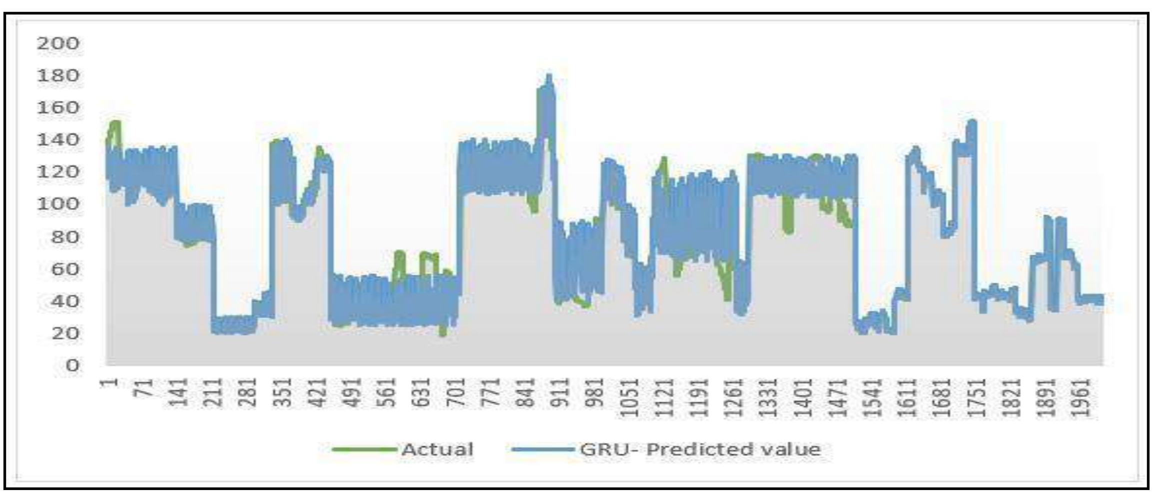

Fig. 4.3. Actual vs Predicted Value of GRU Based WQI Models

The results of the RNN-based WQI prediction model (RNN-WQI-PCA model) have experimented with various epochs such as from 20 to 500 where various metrics are measured at different epochs. The metrics used for evaluation are MAE, MSE, RMSE, and R2 Score. At epoch 500, the MAE value is 0.512, indicating the average absolute difference between the predicted and actual values. The MSE is 0.408, representing the average of squared differences, and the RMSE is 0.6387, which is the square root of the MSE. The R2 score, measuring the goodness of fit, is 0.8, indicating a high level of prediction accuracy.

Similarly, at epoch 200, the MAE increases slightly to 0.523, while the MSE becomes 0.416. The RMSE also increases to 0.6450. However, the R2 score remains at 0.79. As the number of epochs decreases, the MAE and MSE values continue to increase gradually, indicating a larger difference between the predicted and actual values. At epoch 150, the MAE is 0.536, and the MSE is 0.432, resulting in an RMSE of 0.6573 and an R2 score of 0.783. At epoch 100, the MAE increases further to 0.548, and the MSE becomes 0.467. The RMSE is 0.6834, and the R2 score drops slightly to 0.775. With only 50 epochs, the MAE reaches 0.569, and the MSE increases to 0.471. The RMSE becomes 0.6863, while the R2 score remains at 0.761. Finally, at epoch 20, the MAE is 0.573, the MSE is 0.484, and the RMSE is 0.6957. The R2 score drops to 0.742. These values reflect the performance of the model on the WQI-PCA dataset at different epochs, providing insight into the prediction results which are tabulated in Table XIV.

Table XIV Prediction Results of the RNN-WQI-PCA Model for Various Epochs

Dataset	Epochs	MAE	MSE	RMSE	R2 Score
WQI-PCA	500	0.512	0.408	0.6387	0.8
	200	0.523	0.416	0.6450	0.79
	150	0.536	0.432	0.6573	0.783
	100	0.548	0.467	0.6834	0.775
	50	0.569	0.471	0.6863	0.761
	20	0.573	0.484	0.6957	0.742

The prediction results of the LSTM-based WQI prediction model (LSTM-WQI-PCA model) observed for different epochs are tabulated in Table XV. For epoch 500, the LSTM-WQI-PCA model achieves an MAE of 0.393, indicating the average absolute difference between the predicted and actual values. The MSE is 0.2401, representing the average of squared differences, while the RMSE is 0.49, which is the square root of the MSE. The R2 score, measuring the goodness of fit, is 0.838, indicating a high level of prediction accuracy. At epoch 200, the MAE slightly increases to 0.401, and the MSE becomes 0.267. The RMSE is calculated as 0.5167, and the R2 score remains high at 0.83. As the number of epochs decreases, the MAE and MSE values continue to increase gradually, indicating a larger difference between the predicted and actual values.

At epoch 150, the MAE is 0.417, the MSE is 0.294, resulting in an RMSE of 0.542. The R2 score decreases to 0.824, indicating a slightly lower level of prediction accuracy. At epoch 100, the MAE further increases to 0.434, and the MSE becomes 0.341. The RMSE is 0.5840, and the R2 score decreases to 0.82. With only 50 epochs, the MAE increases to 0.457, and the MSE further increases to 0.383. The RMSE becomes 0.6189, while the R2 score decreases to 0.81. Finally, at epoch 20, the MAE reaches 0.512, the MSE is 0.408, and the RMSE is 0.6387. The R2 score drops to 0.8. These values illustrate the performance of the LSTM-WQI-PCA model on the WQI-PCA dataset at different epochs, providing insights into the prediction results.

Table XV Prediction Results of the LSTM-WQI-PCA Model for Various Epochs

Dataset	**Epochs**	**MAE**	**MSE**	**RMSE**	**R2 Score**
WQI-PCA	500	0.393	0.2401	0.4900	0.838
	200	0.407	0.267	0.5167	0.83
	150	0.417	0.294	0.5422	0.824
	100	0.434	0.341	0.5840	0.82
	50	0.457	0.383	0.6189	0.81
	20	0.512	0.408	0.6387	0.8

The prediction results of the GRU-based WQI prediction model (GRU-WQI-PCA model) for different epochs are tabulated in Table XVI. At epoch 500, the GRU-WQI-PCA model achieves an MAE of 0.364, which represents the average absolute difference between the predicted and actual values. The MSE is 0.2098, indicating the average of squared differences, while the RMSE is calculated as 0.4580, which is the square root of the MSE. The R2 score, measuring the goodness of fit, is 0.845, indicating a high level of prediction accuracy. Moving to epoch 200, the MAE increases slightly to 0.375, and the MSE becomes 0.2355. The RMSE is 0.4853, while the R2 score remains high at 0.84. As the number of epochs decreases, the MAE and MSE values gradually increase, indicating a larger difference between the predicted and actual values.

At epoch 150, the MAE is 0.393, the MSE is 0.2401, resulting in an RMSE of 0.49. The R2 score decreases to 0.837, indicating a slightly lower level of prediction accuracy compared to previous epochs. At epoch 100, the MAE further increases to 0.415, and the MSE becomes 0.2645. The RMSE is 0.5143, while the R2 score slightly decreases to 0.825. With only 50 epochs, the MAE reaches 0.432, and the MSE further increases to 0.2861. The RMSE becomes 0.5349, while the R2 score decreases to 0.825. Finally, at epoch 20, the MAE is 0.46, the MSE is 0.3023, and the RMSE is 0.5498. The R2 score drops to 0.82. These values demonstrate the performance of the GRU-WQI-PCA model on the WQI-PCA dataset at different epochs, providing insights into the prediction model accuracy.

Table XVI. Prediction Results of the GRU-WQI-PCA Model for Various Epochs

Dataset	**Epochs**	**MAE**	**MSE**	**RMSE**	**R2 Score**
WQI-PCA	500	0.364	0.2098	0.4580	0.845
	200	0.375	0.2355	0.4853	0.84
	150	0.393	0.2401	0.4900	0.837
	100	0.415	0.2645	0.5143	0.83
	50	0.432	0.2861	0.5349	0.825
	20	0.46	0.3023	0.5498	0.82

Various experiments have been carried out with different dropout rates such as 0.2 and 0.3 for building WQI prediction models using the WQI-PCA dataset and the experimental results concerning the same evaluation metrics are shown in Table XVII.

Table XVII. Results of WQI Prediction Models for Different Dropout Rates

Dataset	Algorithm	Dropout	MAE	MSE	RMSE	R2 Score
WQI-PCA	RNN	0.3	0.512	0.408	0.6387	0.8
		0.2	0.536	0.432	0.6573	0.783
	LSTM	0.3	0.393	0.2401	0.49	0.838
		0.2	0.417	0.294	0.5422	0.824
	GRU	0.3	0.364	0.2098	0.458	0.845
		0.2	0.393	0.2401	0.49	0.837

The R2 score value of GRU based WQI prediction model shows 0.845 and is high when compared to other prediction models. The R2 score value of the RNN prediction model yields 0.8 and the LSTM prediction model is 0.838 with an epoch size set to 500. The WQI prediction results showed the least mean absolute error value of 0.364 for the GRU prediction model, 0.393 for the LSTM prediction model and 0.512 for the RNN prediction model, with epoch size 500. The regression model results of prediction results observed that the root mean squared error value of the GRU prediction model trained with epoch size 500 is 0.4580, the LSTM prediction model is 0.49 and the RNN prediction model is 0.6387. The comparative performance results of the deep learning model concerning the metrics mean absolute error, root mean squared error and R2 score variation. The performance results of the deep learning model concerning the metrics MAE, MSE, RMSE and R2 score values are shown in Table XVIII.

Table XVIII. Overall Performance of Deep Learning based WQI Prediction Models

Models	MAE	MSE	RMSE	R2 Score
RNN-WQI-PCA	0.512	0.408	0.6387	0.8
LSTM-WQI-PCA	0.393	0.2401	0.4900	0.838
GRU-WQI-PCA	**0.364**	**0.2098**	**0.4580**	**0.845**

Comparison of Deep Learning WQI Models with Traditional Machine Learning WQI Models

A pilot study was carried out prior to this work and traditional machine learning algorithms such as random forest, linear regression, support vector regressor, and MLP regressor have been implemented by training the WQI-PCA dataset with default parameter settings. The prediction results obtained with respect to metrics such as MAE, MSE, RMSE and R2 Score, are given in Table XIX.

Table XIX. Performance of ML Based WQI Models

Models	**MAE**	**MSE**	**RMSE**	**R2 Score**
Linear Regression	0.659	0.4872	0.698	0.6375
MLP Regressor	**0.714**	**0.5821**	**0.763**	**0.7342**
Support Vector Regressor	0.763	0.7921	0.89	0.6132
Random Forest	0.709	0.6288	0.793	0.6923

The performance of the deep learning-based WQI prediction models is compared with the prediction results of WQI models based on random forest, linear regression, support vector regressor, and MLP regressor. Regression model prediction results show that the GRU prediction model trained with the least mean absolute error value with epoch size 500 is 0.364 and for MLP regressor obtains a 0.714 error value. The WQI prediction results showed that the least root mean squared error value of 0.4580 for the GRU prediction model with epoch size 500 and the MLP regressor acquires a 0.763 error rate. The WQI prediction models are built using the Bhavani River water dataset, comparing the R2 score value of deep learning prediction models with traditional machine learning approaches. It is found that GRU based WQI prediction model shows the R2 score value as 0.845 and the MLP regressor obtains 0.7342. The results of the prediction models are evaluated using different metrics such as mean absolute error, root mean squared error, mean squared error and R2 score.

The GRU-based WQI prediction model yields less error rate as compared to all other prediction models used in predicting water quality index using the river water quality dataset. It is proven from the evaluation results that the GRU prediction model yields high accuracy and less error rate. The comparative performance results of the WQI prediction model are shown in Table XX and the comparative performance analysis is illustrated in Fig 4.4.

Table XX. Performance Comparison of DL vs MLWQI Prediction Models

Models	MAE	MSE	RMSE	R2 Score
LR-WQI-PCA	0.659	0.4872	0.698	0.6375
MLP-WQI-PCA	0.714	0.5821	0.763	0.7342
SVR-WQI-PCA	0.763	0.7921	0.89	0.6132
RF-WQI-PCA	0.709	0.6288	0.793	0.6923
RNN-WQI-PCA	0.512	0.408	0.6387	0.8
LSTM-WQI-PCA	0.393	0.2401	0.4900	0.838
GRU-WQI-PCA	**0.364**	**0.2098**	**0.4580**	**0.845**

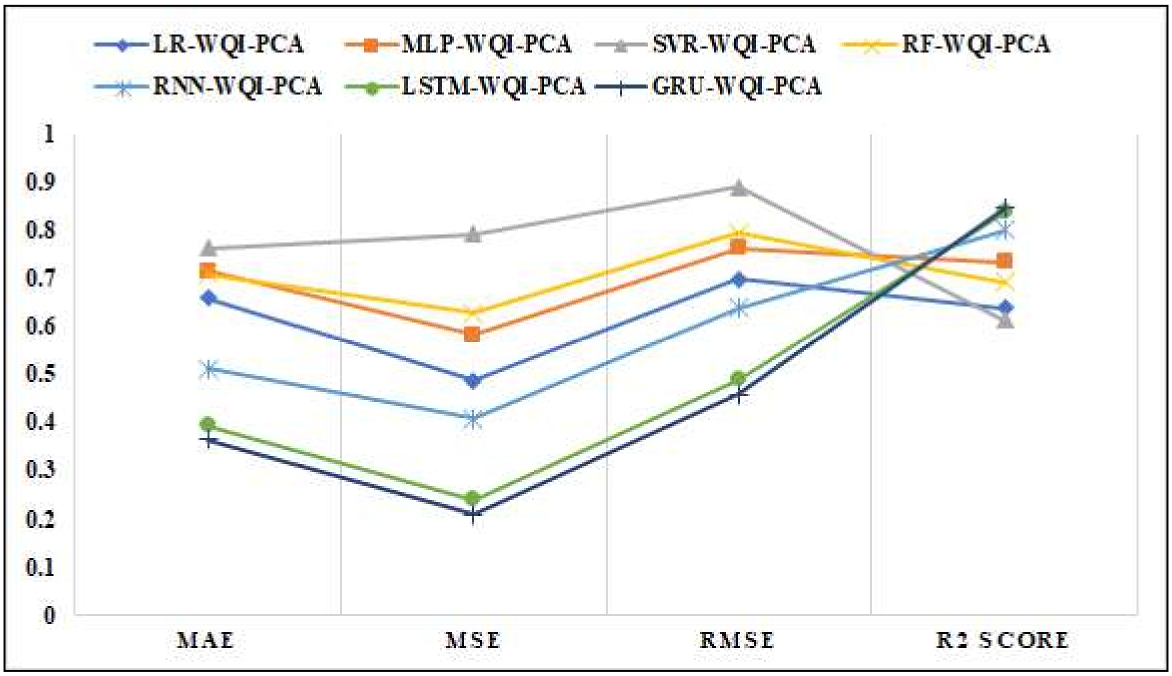

Fig. 4.4. Performance Comparison of DL vs ML WQI Regression Models

Findings

From the comparative performance analysis of various WQI predictive models, it is observed that deep learning based WQI prediction models show better performance than traditional machine learning algorithms. The machine learning approach is good for building any predictive models like water quality index prediction, but the recent deep learning approach improves the accuracy of the prediction. More powerful deep neural network architectures such as RNN, LSTM and GRU boost the recognition of the correlation between target variables and the set of predictors through representation learning. The training of self-learnt features in GRU, LSTM and RNN increases the prediction rate of models. The proper setting of hyperparameters for training the network reduces the error rate of trained models. The RNN architecture has a gradient vanishing problem in optimising the training, due to which the error rate shown by the model is higher. The GRU-based WQI prediction model performs efficiently and is more suitable for time series-based water quality datasets. The GRU prediction model yields high accuracy with less error rate as compared to other algorithms in predicting WQI.

SUMMARY

This chapter focused on the implementation of deep learning techniques for building WQI prediction models. The methodology described the formulation of the water quality index prediction problem as a regression task and the use of deep neural network architectures. The experimental results with tables and charts and the comparative analysis with traditional machine learning approaches were also presented in this chapter. In order to improve the accuracy of the WQI prediction models, the seasonal parameters which influence WQI, have been considered in the next work and the development of respective WQI predictive models will be discussed in the following chapter.

Remarks

1. *The paper titled 'Design and Development of Efficient Water Quality Prediction Models Using Variants of Recurrent Neural Networks' has been published in European Chemical Bulletin, Volume -12, Special Issue-5(Part-A) 2023.* ***(Scopus Indexed)***

2. *The paper titled "River Water Quality Prediction and index classification using Machine Learning" has been published in the Journal of Physics: Conference Series, Volume 2325, International Conference on Electronic Circuits and Signalling Technologies 2022.* ***(Scopus Indexed)***