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Predictive Performances of Machine Learning– and Deep Learning–Based Univariate and Multivariate Reservoir Inflow Predictions in the Chao Phraya River Basin

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Abstract

This study demonstrated the predictability of Machine Learning (ML)– and Deep Learning (DL)–based univariate and multivariate predictions of reservoir inflows of Bhumibol (BB) and Sirikit (SK), two major dams in the Chao Phraya River Basin. XGBoost, tree–based ensemble–, and LSTM, deep neural network–based algorithms were selected for development of daily and monthly prediction models. For univariate prediction, the inflows of the BB and SK dams were predicted separately using two individual models. In contrast, for multivariate prediction, a single model was developed to simultaneously predict the inflows of both the BB and SK dams facilitating the integrated decision–making processes. Across all prediction scenarios, ML– and DL–based models demonstrated superior performances in predicting daily reservoir inflows for BB and SK dams compared to monthly predictions, achieving NSE values of 0.86 and 0.77, respectively. Since modeling with LSTM algorithm can effectively handle larger datasets, this enables single multivariate prediction model to predict closer results to those individual univariate models performed by XGBoost and LSTM for BB and SK prediction. XGBoost models mostly outperformed LSTM when tested on the datasets for both daily and monthly univariate predictions. Among all prediction scenarios, underprediction of low reservoir inflows and overprediction of high reservoir inflows by both univariate and multivariate models were consistently existed. Therefore, extracting specific and informative insights from the results of each model type, forecasting horizon, and algorithms used can significantly enhance decision–making support for both real–time reservoir operation and long–term reservoir management planning.

Keywords: Machine Learning (ML), Deep Learning (DL), Artificial Intelligence (AI), Reservoir Inflow Prediction, Chao Phraya River Basin

1. Introduction

The increased climate variability has intensified the water–related challenges globally making the water resources management more complicated under the changing circumstances (Ngamsanroaj and Tamee, 2019). Consequently, risks of water stress and scarcity exacerbated by reservoir operation and management have substantially increased. A key factor contributing to this is uncertain water supply in the reservoir system. Reservoir inflow is commonly considered as the principal source of water supply in reservoirs. It is significantly influenced by the climate variability and hydrologic phenomena. Accurate and precise reservoir inflow prediction plays a crucial role for effective reservoir planning and management (Suprayogi et al., 2020). During critical climate events, future reservoir inflow forecast informs decision making for instant operational responses to natural disasters like floods and drought. During normal climate conditions, predictive reservoir data is used for establishment of guideline trajectory for proper reservoir operation. Predicting the precise reservoir inflow is inherently stochastic due to uncertainty of hydrological inputs and strong non–linearity of the system (Soncin et al., 2024). For decades, numerous research studies have been dedicated to reservoir inflow predictions to achieve the desired purposes for both reservoir management planning and real–time operation.

A wide range of prediction techniques including physically process–based–, conventional stochastic–based– and modern data–driven approaches like Machine Learning (ML) and hybrid models have been widely employed to enhance the model predictability. It is revealed that the process–based hydrological models usually rely on a various number of assumptions and require many physical parameters to resemble the hydrological nature of environment (Firat and Güngör, 2008; Luo et al., 2020). In addition, the conventional stochastic–based techniques such as ARMA, ARIMA for time series prediction provided good results for only linear data. However, it is not appropriate for non–

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linearity phenomenon influenced by climate, natural geography, and human activities (Valipour et al., 2013). Prediction time horizon selected has been generally ranged from short–term (hourly, daily, weekly) to long–term predictions (monthly, seasonal, yearly). Univariate prediction model is generally used to predict future values of single variable using the historical data. While, multivariate prediction model involves predicting the future values of multiple interrelated variables. However, short–term univariate prediction predicting future values of single reservoir inflow has broadly been found particularly for real–time operation and short–term planning. Predicting multiple reservoir inflows using multivariate prediction model by taking the interdependencies of influencing factors of multiple reservoirs has rarely studied and limited.

The advancement of Artificial Intelligence (AI) and Machine Learning (ML) approach has revolutionized transformative impacts across the traditional prediction methods and their disciplines. A great deal of data–driven ML approach has enhanced the predictability for hydrological prediction (Zhang et al., 2018) such as rainfall (Chen et al., 2017; Ridwan et al., 2021), streamflow (Latif et al., 2023; Kisi et al., 2024), reservoir inflow (Zhang et al., 2021; Hameed et al., 2022; Latif et al., 2024), reservoir water level (Sapitang et al., 2020; Aquil and Ishak, 2023), river water level (Ahmed et al., 2023; Zakaria et al., 2023), groundwater level (Osman et al., 2020), sediment transport (Almubaidin et al., 2023), water quality prediction (Haghiabi et al., 2018; Shams et al., 2024) and snow water equivalent (Khosravi et al., 2023).

Since 1990s, a well–known Artificial Neural Networks (ANNs) inspired by human brain structure and its function has intensively been used for hydrological prediction. It was commonly applied for both univariate and multivariate predictions. For example, univariate time series prediction of reservoir inflow was developed using ANNs to map the non–linear relationships between input and output variables (Kawade et al., 2019). Many studies also revealed that ANNs significantly outperformed than the statistically–stochastic–based prediction models like AR, MA, and ARIMA for the reservoir inflow prediction (Pradeepakumari and Srinivasu, 2019). Additionally, ANNs can be applicable for both parametric and non–parameter data (Pini et al., 2020).

The rapid evolution of ML algorithms has driven by the advancement and succession of computer science and technologies to increase the computational capability and handle large dataset. Consequently, the improved ML algorithms have been progressively developed incorporating supervised learning, unsupervised learning, and reinforcement learning for various tasks. Several conventional ML algorithms have commonly been employed for reservoir inflow prediction such as Support Vector Machines (SVM), K–Nearest Neighbors (KNN), Random Forest (RF), Multi–layer Perceptron (MLP), Gradient Boosting (GB), Extreme Gradient Boosting (XGBoost), and Radial Bias Function (RBF). A comparative study for daily reservoir inflow prediction was conducted using four different approaches; (1) Multiple Linear Regression (MLR), (2) Random Forest (RF), (3) Extreme Learning Machine (ELM), and (4) Regularized Extreme Learning Machine (RELM). The results showed the superiority of RELM approach that yielded higher prediction accuracy with R = 0.955 (Hameed et al., 2022). XGBoost, a relatively recent algorithm, has proven its effectiveness in reservoir inflow prediction. To forecast multi–step ahead daily and monthly reservoir inflows, XGBoost was ranked as the best prediction model compared to MLP, Support Vector Regression (SVR), Adaptive Neuro–Fuzzy Inference System (ANFIS) (Ibrahim et al., 2023). Similarly, XGBoost outperformed RF and an ensemble model combining XGBoost–RF algorithms for daily reservoir inflow prediction (Jan et al., 2024)

Recently, achievement of Deep Learning (DL) which is a subset of ML, has renowned incorporating multiple layers artificial neural networks or Deep Neural Networks (DNNs) with automatic feature learning. It is indicated that DL is powerful in extracting complex features hidden in vast amount of hydrological dataset (Huang et al., 2022). Some of the most widely used DL algorithms for time series prediction are Convolutional Neural Networks (CNNs), Recurrent Neural Networks (RNNs), Long–Short Term Memory (LSTM), and Gated Recurrent Unit (GRU). GRU is the simplified form of LSTM well–suited for faster training for time series prediction. While, LSTM is a specific type of RNNs designed to learn the long–term temporal dependency and seasonality of time series data and overcome the vanishing and exploding gradient problems of RNNs (Dtissibe et al., 2024). It is found that RNNs with input delayed time gave better predictive performances for multivariate reservoir inflow prediction than Input Delayed Neural Network (IDNN) (Coulibaly et al., 2001). Real–time reservoir inflow prediction in the case of different climate scenarios and lead time conditions (+1–Hr, +4–Hr, and +6–Hr) with three conventional ML algorithms; (1) SVM, (2) RF, (3) MLP and four DL algorithms; (1) DNNs, (2) RNNs, (3) LSTM, (4) GRU were investigated. In comparation, the results distinctly showed that DNNs outperformed than the conventional ANNs in most scenarios. However, under the extended periods of lead time prediction, underestimation of reservoir inflow by DDNs is more serious compared to ANNs (Huang et al., 2022). Encoder–Decoder LSTM (ED–LSTM) was employed for sub–seasonal reservoir inflow with multiple lead time (+1–D to +30–D) for 30 reservoirs, at 1–D ahead prediction, ED–LSTM could produce good predictive performance of NSE exceeding 0.75 for 29 reservoirs. At 30–D ahead prediction, ED–LSTM achieved NSE of more than 0.5 for most reservoirs (Fan et al., 2023). Furthermore, LSTM exhibited superior performances in

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predicting medium to long–term data compared to the conventional ML algorithms as well as RNNs (Khorram and Jehbez, 2023; Rajesh et al., 2023) and CNNs architectures (Herbert et al., 2021).

However, the biased performance of overfitting, information saturation, and under–fitting issues of ML–based prediction models has become the challenging issues. It is reviewed that ML models cannot improve the prediction accuracy without including preprocessing techniques for feature engineering (Apaydin and Sibtain, 2021). Data preprocessing is conducted at the first step of ML modeling to ensure the data quality for model training. Data cleaning, transformation, and decomposition are adopted for prediction improvement. In addition, selecting suitable ML algorithms for specific purpose of hydrological prediction is a challenging task.

This study employed two powerful ML algorithms; XGBoost and LSTM for univariate and multivariate reservoir inflow prediction of two large storage dams in the Chao Phraya River Basin (CPYRB); (1) Bhumibol (BB) and Sirikit (SK) dams as shown in Fig. 1. Predicting precise and accurate reservoir inflow for these two reservoirs is important to ensure reliable water supply sources and establish proper water allocation plan for the downstream water use in the central region. Furthermore, during the storm seasons from May. to Dec. when the flood risks are likely elevated, future inflow data is informative for the Office of National Water Resources (ONWR), key decision maker to implement effective flood mitigation strategies. Input features selection and configuration design of two different types of daily and monthly reservoir inflow prediction models; (1) univariate prediction with XGBoost and LSTM algorithms and (2) multivariate prediction with LSTM algorithm, were definitely highlighted. In the last step, predictability of predicting low and high reservoir inflow values of these models were accordingly explored to assess their statistical performances.

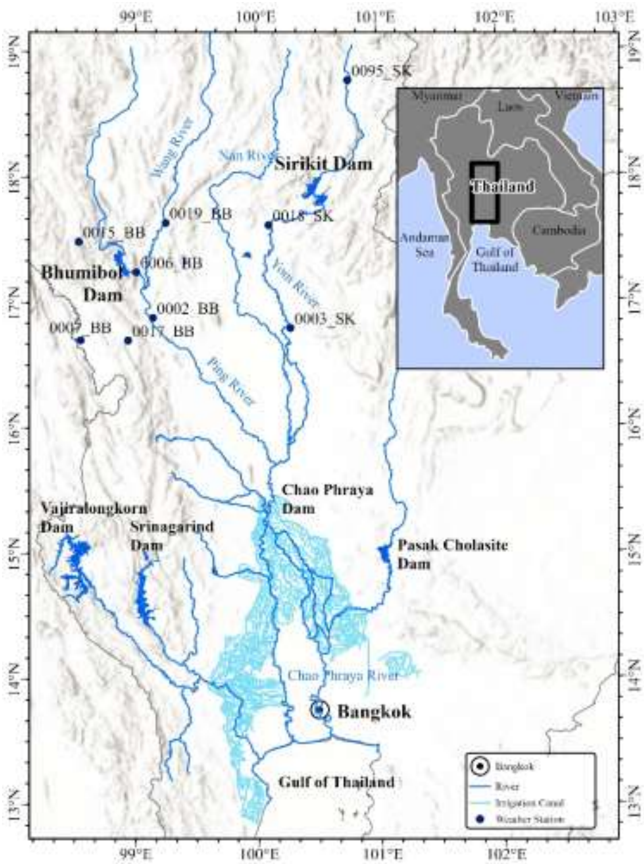

Fig. 1 Study area in the Chao Phraya River Basin and weather stations

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2. Material and methods

2.1. Input features for reservoir inflow prediction models

The development of ML prediction models relied on the historical observation data from 2000 to 2020 including reservoir inflows of BB and SK reservoirs, and climate data gathered from the nearest weather stations as summarized in Table 1. As input feature selection is definitely critical to the success of ML– and DL–based prediction models, consequently, the statistical correlation analysis was performed to assess the strength and direction of relationships between climate data from adjacent weather stations and reservoir inflow. By doing this, the daily observed climate data (air humidity, air pressure, temperature, and rainfall) was collected from six Thai Meteorological Department (TMD) stations (0002, 0006, 0007, 0015, 0017, and 0019) located in Tak, Sukhothai, and Lampang provinces near BB dam. Additionally, climate data from the Climate Data Services (CDS) publicly provided by NASA was gathered for locations with geographic coordinates matching those of the TMD stations. Likewise, the daily observed climate data near SK dam was collected from three TMD and NASA stations (0003, 0018, and 0095) located in Phitsanulok, Uttaradit, and Nan provinces, respectively.

For the univariate prediction, single reservoir inflows of BB and SK dams were aimed to individually predict for both daily and monthly models. A number of daily and monthly prediction scenarios with different model configuration using XGBoost and LSTM algorithms were accordingly developed. For the multivariate prediction, reservoir inflows of two main reservoirs, BB–SK dams were expected to achieve simultaneously from single prediction model for both daily and monthly prediction. Consequently, LSTM was selected for multiple output prediction as it can learn and capture the complicated relationship of relevant multiple input variables.

Table 1 Data used for reservoir inflow prediction modelling

Data	Description	Data Type	Unit	Data Length
Reservoir Inflow_BB	Reservoir Inflow of BB Dam	Daily, Monthly	MCM	1/1/2000–31/12/2020
Reservoir Inflow_SK	Reservoir Inflow of PS Dam	Daily, Monthly	MCM	1/1/2000–31/12/2020
Weather	Avg. Humidity at 9 Stations	Daily, Monthly	%	1/1/2000–31/12/2020
	Avg. Air Pressure at 9 Stations	Daily, Monthly	hPa	1/1/2000–31/12/2020
	Avg. Temperature at 9 Stations	Daily, Monthly	°C	1/1/2000–31/12/2020
	Rainfall at 9 Stations at 9 Stations	Daily, Monthly	mm	1/1/2000–31/12/2020
	Station ID	Station Name	Location: Lat.–Long.	
	0002_BB	Tak	N 16°52’48” – E 99°08’24”	
	0006_BB	Bhumibol Dam	N 17°14’37” – E 99°00’08”	
	0007_BB	Mae Sot	N 16°41’60” – E 98°32’31”	
	0015_BB	Si Samrong	N 17°29’11” – E 99°31’36”	
	0017_BB	Doi Muser	N 16°41’60” – E 98°56’07”	
	0019_BB	Tone	N 17°38’12” – E 99°14’44”	
	0003_SK	Phitsanulok	N 16°47’47” – E 100°16’33”	
	0018_SK	Uttaradit	N 17°37’00” – E 100°05’60”	
	0095_SK	Nan	N 18°46’01” – E 100°45’47”	

Note: meter above mean sea level– m. msl.|Million Cubic Meter–MCM|Cubic Meter per Second–CMS

Selecting input features for each univariate and multivariate prediction model was based on the physical river–reservoir system and statistical cross correlation between past reservoir inflow and relevant climate data as summarized in Table 2. This ensured that the prediction model can effectively capture the strong relationship between the inputs and predicted outputs.

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Table 2 Correlation coefficient between climate data and reservoir inflows of the Bhumibol and Sirikit dams

Weather Station	Climate Data	TMD Data Source	NASA Data Source	Weather Station	Climate Data	TMD Data Source	NASA Data Source
0002_BB	Avg. humidity (%)	**0.402**	**0.521**	0019_BB	Avg. humidity (%)	**0.460**	**0.505**
	Avg. air pressure (hPa)	–0.117	–0.148		Avg. air pressure (hPa)	–0.090	–0.146
	Avg. temperature (°C)	–0.115	–0.190		Avg. temperature (°C)	–0.091	–0.133
	Rainfall (mm/day)	**0.284**	**0.365**		Rainfall (mm/day)	**0.191**	**0.355**
0006_BB	Avg. humidity (%)	**0.402**	**0.518**	0003_SK	Avg. humidity (%)	**0.428**	**0.536**
	Avg. air pressure (hPa)	–0.007	–0.146		Avg. air pressure (hPa)	–0.328	–0.322
	Avg. temperature (°C)	–0.103	–0.173		Avg. temperature (°C)	–0.020	–0.144
	Rainfall (mm/day)	**0.289**	**0.369**		Rainfall (mm/day)	**0.038**	**0.376**
0007_BB	Avg. humidity (%)	**0.401**	**0.491**	0018_SK	Avg. humidity (%)	**0.499**	**0.503**
	Avg. air pressure (hPa)	–0.164	–0.179		Avg. air pressure (hPa)	–0.023	–0.339
	Avg. temperature (°C)	–0.096	–0.076		Avg. temperature (°C)	–0.019	–0.017
	Rainfall (mm/day)	**0.197**	**0.360**		Rainfall (mm/day)	**0.167**	**0.406**
0015_BB	Avg. humidity (%)	**0.319**	**0.521**	0095_SK	Avg. humidity (%)	**0.535**	**0.469**
	Avg. air pressure (hPa)	–0.021	–0.139		Avg. air pressure (hPa)	–0.379	–0.358
	Avg. temperature (°C)	–0.027	–0.178		Avg. temperature (°C)	0.092	0.101
	Rainfall (mm/day)	**0.162**	**0.363**		Rainfall (mm/day)	**0.002**	**0.392**
0017_BB	Avg. humidity (%)	**0.212**	**0.491**				
	Avg. air pressure (hPa)	0.003	–0.479				
	Avg. temperature (°C)	0.006	–0.076				
	Rainfall (mm/day)	**0.034**	**0.360**				

Note: Thai Meteorological Department–TMD|
National Aeronautics and Space Administration–NASA

The correlation analysis revealed strong correlations between observed reservoir inflows and both humidity and rainfall at both BB and SK dams. The correlation coefficient between reservoir inflow of BB dam and humidity data at Station 0006 reaches up to 0.402 and 0.518 for TMD and NASA data sources, respectively. Rainfall data from Station 0006 also exhibited a strong correlation with reservoir inflow of BB dam, with correlation coefficients of 0.2886 and 0.3693 for TMD and NASA data sources, respectively. The substantial correlation between reservoir inflow of SK dam and climate data from Station 0018 particularly from NASA data source, was apparently found with the correlation coefficient of 0.503 and 0.406 for humidity data and precipitation data, respectively. Based on these analysis, humidity and rainfall data were accordingly selected to specify input structures of ML– and DL–based prediction models. Autocorrelation of past reservoir inflow was also analyzed to identify optimal lag times and number of moving average parameters for input feature selection. This analysis revealed the importance of closer lag time (t to t–7) which exhibited high correlation coefficients exceeding 0.67 with the recent reservoir inflow data for both BB and SK dams. Accordingly, information of past reservoir inflows with closer lag time t to t–7 was incorporated into the structure of the prediction models to predict reservoir inflow at lead time t+1.

Following this analysis, four daily and monthly univariate prediction scenarios with various model configurations varying input features using XGBoost and LSTM algorithms for each of BB and SK dams; S1–S4, were designed. For the multivariate prediction model, two daily and monthly prediction scenarios; S5–S6, using LSTM algorithm were established. Major inputs of these prediction models are past reservoir inflow at time t, moving average of past reservoir inflow at time t–3 and t–7, rainfall at time t, and humidity at time t as summarized in Table 3. It is illustrated that univariate models structured the specific individual inputs for single reservoir inflow prediction at lead time t+1. For example, the input features of daily reservoir inflow prediction for BB dam are BB past inflow at time t, moving average of BB past inflow at time t–3 and t–7, rainfall and humidity at time t collected from the nearest weather stations to BB dam. In contrast, the multivariate prediction models incorporate inputs of both BB and SK dams to predict two reservoir inflows at lead time t+1.

Table 3 Input features for univariate and multivariate reservoir inflow prediction models

Prediction Model	Reservoir Inflow ID	Prediction Scenario	Model Type and Prediction Lead Time	Model No.	Input Features					
					Past Inflow_BB	Past Inflow_SK	Avg. Past Inflow	Avg. Past Inflow	Rainfall	Humidity
–	–	–	t+1		t	t	t–3	t–7	t	t
Univariate Prediction	BB	S1: XGBoost	Daily	dBB–01, dBB–02, dBB–03	✓	–	✓	✓	✓	✓
		S2: LSTM	Daily	dBB–01, dBB–02, dBB–03, dBB–04, dBB–05, dBB–06	✓	–	✓	✓	✓	–
	SK	S1: XGBoost	Daily	dSK–01, dSK–02, dSK–03	–	✓	✓	✓	✓	✓

Prediction Model	Reservoir Inflow ID	Prediction Scenario	Model Type and Prediction Lead Time	Model No.	Input Features					
					Past Inflow_BB	Past Inflow_SK	Avg. Past Inflow	Avg. Past Inflow	Rainfall	Humidity
–	–	–	t+1		t	t	t–3	t–7	t	t
		S2: LSTM	Daily	dSK–01, dSK–02, dSK–03, dSK–04, dSK–05, dSK–06	–	✓	✓	✓	✓	–
	BB	S3: XGBoost	Monthly	mBB–01, mBB–02, mBB–03	✓	–	✓	✓	✓	✓
		S4: LSTM	Monthly	dBB–01, dBB–02, dBB–03, dBB–04, dBB–05, dBB–06	✓	–	✓	✓	✓	–
	SK	S3: XGBoost	Monthly	mSK–01, mSK–02, mSK–03	–	✓	✓	✓	✓	✓
		S4: LSTM	Monthly	mSK–01, mSK–02, mSK–03, mSK–04, mSK–05, mSK–06	–	✓	✓	✓	✓	–
Multivariate Prediction	BB&SK	S5: LSTM	Daily	dBBSK–01	✓	✓	✓	–	✓	✓
	BB&SK	S6: LSTM	Monthly	mBBSK–01	✓	✓	✓	–	✓	✓

Note: Acronyms–Bhumibol dam–BB|Sirikit dam–SK|Daily Univariate prediction model of BB dam–dBB|Daily univariate prediction model of SK Dam–dSK|Daily multivariate prediction model of BB&SK dams–dBBSK|Monthly multivariate prediction model of BB&SK dams–mBBSK

2.2. Prediction algorithms selected

2.2.1. Extreme gradient boosting (XGBoost)

Extreme Gradient Boosting (XGBoost), a powerful machine learning algorithm initiated by Tianqi Chen in 2014 (Chen and Guestrin, 2016), was used to develop the daily and monthly univariate prediction models for reservoir inflow in CPYRB. XGBoost is a decision–tree–based ensemble machine learning as illustrated its structure in Fig. 2. Its efficiency, scalability, and flexibility have been widely demonstrated and proven in hydrological prediction applications (Rajesh et al., 2022). In general, the supervised XGBoost learning primarily involves minimizing objective function which consists of two main components; (1) loss function and (2) regularization term as expressed in Eq. (1). This loss function measures the discrepancy between the predicted and observed values in the model training process as given mean squared error in Eq. (2). The regularization term in Eq. (3) is crucial in preventing model overfitting and complexity for improved prediction performance.

$$Obj(\theta) = L(\theta) + \Omega(\theta) \tag{1}$$

$$L(\theta) = \frac{1}{2}\sum_{i=1}^{n}(y_i - p_i)^2 \tag{2}$$

$$\Omega(\theta) = \gamma T + \frac{1}{2}\lambda\sum_{i=1}^{T}O_{value}^2 \tag{3}$$

where, $L(\theta)$ is the training loss function term. For robust regression tasks, the common loss functions are Mean Squared Error (MSE), Mean Absolute Error (MAE), and Huber loss which is the combination of MSE and MAE. $\Omega(\theta)$ is regularization term. θ denotes the optimal parameter values that best fits the training inflow data (y_i) to the predicted inflow output (p_i). γ is a hyperparameter controlling the strength of the regularization term which influences the decision to make a further partition on a leaf node of a tree–based model. T is a number of leaf nodes in the tree and λ is a hyperparameter used to scale the regularization term. A larger number of leaf nodes signifies the model complexity potentially leading to overfitting. A larger λ indicates the increased penalty to model encouraging the reduction of model complexity. O_{value} is a measure of the impurity or heterogeneity of the data points within the leaf node. For tree building process, a prediction for one given data is made by traversing the tree from the root node to a leaf node. The tree is built from a root node and recursively split into left and right child nodes. This process continues until a specific stopping criterion is met as graphically shown in Fig.2. Similarity score (*Sim*) is used to assess the homogeneity of data within a node to guide for leaf node splitting. The larger value of similarity score signifies the similar data within a leaf node that further splitting might not be necessary. Similarity score is computed to indicate a score of each node by using Eq. (4).

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$$Sim = \frac{\sum_{i=1}^{n} (y_i - p_i)^2}{n + \lambda} \tag{4}$$

Gain value is termed to measure the accuracy improvement resulted from a specific splitting. It helps assess the optimality of potential splits in a tree structure as expressed in Eq. (5). A higher positive gain value indicates a better split in improving the model predictive performance. When the gain values are negative, the tree branch is removed as shown in Fig. 3.

$$Gain\ value = (Simleft + Simright) - Simroot \tag{5}$$

where, *Simleft*, *Simright*, and *Simroot* denote the similarity score of the left leaf node, right leaf node, and root node of the branch, respectively. The tree structures are iteratively built for T iterations until the desired number of models is reached. In each iteration, the output value (O_{value}) for all leaf nodes is computed using Eq. (6).

$$O_{value} = \frac{\sum_{i=1}^{n} (y_i - p_i)}{n + \lambda} \tag{6}$$

In addition, the precision and speed of convergence of the prediction model is governed by learning rate (ε). Learning rate determines level of model improvement to handle the prediction error made by previous iterations. A larger values of learning rate can accelerate the training process leading to faster convergence. However, overfitting can simply find if not properly fine–tuned. In contrast, the smaller values of learning rate can help reduce overfitting but speed of convergence is definitely lower. In the final step, XGBoost can make updated prediction (p_i^t) by combining the initial prediction (p_i^0) with the gradient of the loss function and the regularization term multiplied with learning rate as expressed in Eq. (7).

$$p_i^t = p_i^0 + \varepsilon [\, \textstyle\sum_{i=1}^{n} L\, (y_i, p_i^0 + O_{value}) + \frac{1}{2} \lambda O_{value}^2] \tag{7}$$

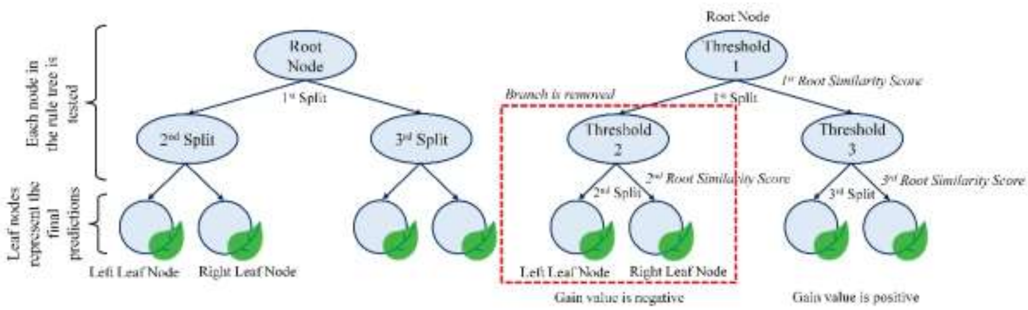

Fig. 2 XGBoost tree–based structure

2.2.2. Long Short–Term Memory (LSTM)

Long Short–Term Memory (LSTM) is a well–suited type of deep learning algorithm designed to process sequential data. It was initially introduced by Hochreiter and Schmidhuber in 1997 (Hochreiter and Schmidhuber, 1997). LSTM is an evolution of Recurrent Neural Networks (RNN) which is a type of Artificial Neural Networks (ANNs) having memory to process sequential inputs. However, the complications to learn and capture long–term dependencies due to vanishing and exploding gradient problems become the significant drawback of RNN. To overcome this, LSTM is specifically developed to learn long–term dependencies and retain previous information over extended periods. The LSTM model is commonly structured as a chain of units as illustrated in Fig. 3. Each LSTM unit is composed of a cell state and three gates namely, (1) input gate, (2) forget gate, and output gate. Cell state is functioned as core component of LSTM to store and carry information through time steps. Input gate regulates new information from current input to be stored in a cell state. Forget gate decides to discard or keep information from previous cell state. Output gate determines which part of cell state should be the current prediction output (Khorram and Jehbez, 2023; Rajesh et al., 2023).

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In the initial step, forget gate examines the current input at time t (x_t), previous hidden state (h_{t-1}) which is the output at previous time t–1, and long–term memory from previous cell state at time t–1 (C_{t-1}). It calculates a value in a range of 0 and 1 for each element in the previous cell state as expressed in Eq. (8). Subsequently, the input gate calculates two values; input gate at time t (i_t) and cell state input at time t ($\check{C}_t$) to regulate the new information into the current cell state as defined in Eq. (9) and Eq. (10). Then, the new cell state at time t (C_t) in Eq. (11) is updated by combining the new information of previous cell state at time t–1 (C_{t-1}), forget gate at time t (f_t), and input gate at time t (i_t, $\check{C}_t$). Eq. (12) is employed to compute the current prediction output at time t (o_t). The hidden state (h_t) indicating LSTM output at time t, is finally calculated by multiplying the output gate at time t (o_t) with the tanh of the new cell state at time t (C_t) as shown in Eq. (12) and Eq. (13). By doing this through iteration process, LSTM can handle the sequential data and make accurate and precise prediction.

$$f_t = \sigma(W_f * [h_{t-1}, x_t] + b_f) \tag{8}$$

$$i_t = \sigma(W_i * [h_{t-1}, x_t] + b_i) \tag{9}$$

$$\check{C}_t = tanh(W_C * [h_{t-1}, x_t] + b_C) \tag{10}$$

$$C_t = f_t * C_{t-1} + i_t * \check{C}_t \tag{11}$$

$$o_t = \sigma(W_o * [h_{t-1}, x_t] + b_f) \tag{12}$$

$$h_t = o_t * tanh(C_t) \tag{13}$$

Where $W_{f/i/C}$ is corresponding weight matrix, $b_{f/i/C}$ is corresponding bias and σ is the sigmoid activation function.

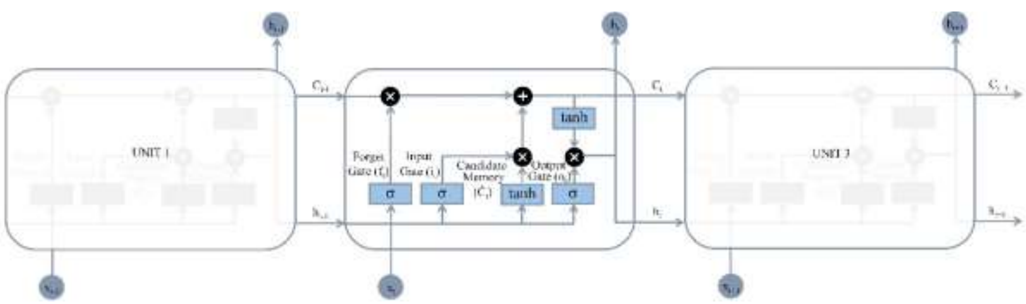

Fig. 3 LSTM chain–like structure and its unit

2.3. Model configuration design and prediction modelling

Model configuration design of daily and monthly univariate and multivariate prediction models are presented in Fig. 4 and Table 4–Table 5. The input features as aforementioned in Section 2.1., designated training–testing dataset ratios (60:40, 70:30, 80:20), delayed time of moving average inflow (t–3 and t–7), and learning rates (0.001, 0.01, 0.1) were varied to optimize the model configuration and prediction performance. Implementation of training model for daily and monthly prediction by XGBoost was controlled by the hyperparameter tunning process such as gamma, maximum depth of a tree, number of iterations (nrounds), number of threads (nthreads), learning rate, number of fold (nfolds) and early stopping rounds (early_stopping_rounds) parameters as presented in Table 4. In this study, maximum depth of a tree was set to 6 in increase deeper tree model complexity. Maximum number of iterations was specified to 10,000 for model training process. Number of threads determining for parallel computation to speed up the training process and number of folds specifying for cross–validation was 10 and 2, respectively. The early stopping rounds were generally used to stop training procedures when the loss on training dataset starts increasing. In this study, the early stopping round was set every 500 iterations if the performance on RMSE was not substantially improved.

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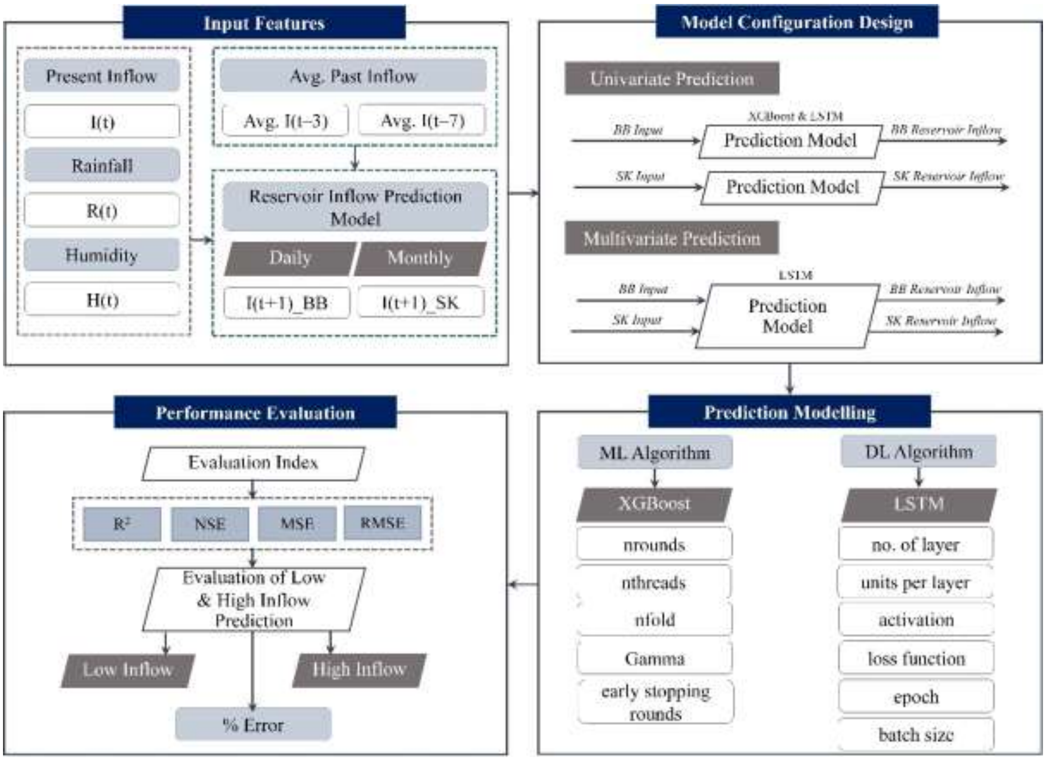

Fig. 4 Workflow diagram of this study

Table 4 Model configuration design of daily and monthly univariate prediction models using XGBoost

Model No.	Input Feature	Training:Testing Ratio	Learning Rate	XGBoost Parameter							
				Objective	Gamma	Max. Depth	Evaluation	nrounds	nthreads	nfolds	Early stopping rounds
Daily and Monthly Prediction of BB Reservoir Inflow											
dBB–01, mBB–01	Past Inflow, Avg. Past Inflow	60:40, 70:30, 80:20	0.001, 0.01, 0.1	regression: linear	0	6	RMSE	10,000	10	2	500
dBB–02, mBB–02	Past Inflow, Avg. Past Inflow, Rainfall	60:40, 70:30, 80:20	0.001, 0.01, 0.1	regression: linear	0	6	RMSE	10,000	10	2	500
dBB–03, mBB–03	Past Inflow, Avg. Past Inflow, Rainfall, Humidity	60:40, 70:30, 80:20	0.001, 0.01, 0.1	regression: linear	0	6	RMSE	10,000	10	2	500
Daily and Monthly Prediction of SK Reservoir Inflow											
dSK–01, mSK–01	Past Inflow, Avg. Past Inflow	60:40, 70:30, 80:20	0.001, 0.01, 0.1	regression: linear	0	6	RMSE	10,000	10	2	500
dSK–02, mSK–02	Past Inflow, Avg. Past Inflow, Rainfall	60:40, 70:30, 80:20	0.001, 0.01, 0.1	regression: linear	0	6	RMSE	10,000	10	2	500
dSK–03, mSK–03	Past Inflow, Avg. Past Inflow, Rainfall, Humidity	60:40, 70:30, 80:20	0.001, 0.01, 0.1	regression: linear	0	6	RMSE	10,000	10	2	500

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Similarly, model configuration using LSTM for both univariate and multivariate prediction models was designed by varying input features and tuning key hyperparameters such as number of layers, number of units per layer, activation function, optimizer, epoch, and batch size, etc. as summarized in Table 5. In this study, number of layers was set to 2 and units per layer referring number of neurons in a specific layer of LSTM network was set to 64 or 32. Rectified Linear Unit (ReLU), a famous activation function used in deep neural networks was specified in all univariate prediction experiments while Sigmoid, a traditional activation function was used for multivariate prediction. Adam optimizer which is an optimization algorithm, was employed to update weights during training process. MSE was used as loss function for both univariate and multivariate prediction models. Additionally, number of epochs involving the passing numbers through the entire training dataset was varied between 50, 100, and 500. Similarly, batch size incorporating number of samples processed before updating the model's weights was set to 16, 32, and 64.

Table 5 Model configuration design of daily and monthly univariate and multivariate prediction models using LSTM

Model No.	Input Feature	Standardization Technique	LSTM Parameter in Keras							
			Steps	Number of Layers	Units per Layer	Activation	Loss Function	Optimizer	Epoch	Batch Size
Daily Univariate Prediction Models of BB Dam										
dBB–01	Past Inflow, Avg. Past Inflow	Standard	3	2	64/32	ReLU	MSE	Adam	50	16
dBB–02	Past Inflow, Avg. Past Inflow	Standard	7	2	64/32	ReLU	MSE	Adam	50	16
dBB–03	Past Inflow, Avg. Past Inflow	Standard	14	2	64/32	ReLU	MSE	Adam	50	16
dBB–04	Past Inflow, Avg. Past Inflow, Rainfall	Standard	3	2	64/32	ReLU	MSE	Adam	50	16
dBB–05	Past Inflow, Avg. Past Inflow, Rainfall	Standard	7	2	64/32	ReLU	MSE	Adam	50	16
dBB–06	Past Inflow, Avg. Past Inflow, Rainfall	Standard	14	2	64/32	ReLU	MSE	Adam	50	16
Daily Univariate Prediction Models of SK Dam										
dSK–01	Past Inflow, Avg. Past Inflow	Standard	3	2	64/32	ReLU	MSE	Adam	50	16
dSK–02	Past Inflow, Avg. Past Inflow	Standard	7	2	64/32	ReLU	MSE	Adam	50	16
dSK–03	Past Inflow, Avg. Past Inflow	Standard	14	2	64/32	ReLU	MSE	Adam	50	16
dSK–04	Past Inflow, Avg. Past Inflow, Rainfall	Standard	3	2	64/32	ReLU	MSE	Adam	50	16
dSK–05	Past Inflow, Avg. Past Inflow, Rainfall	Standard	7	2	64/32	ReLU	MSE	Adam	50	16
dSK–06	Past Inflow, Avg. Past Inflow, Rainfall	Standard	14	2	64/32	ReLU	MSE	Adam	50	16
Monthly Univariate Prediction Models of BB Dam										
mBB–01	Past Inflow, Avg. Past Inflow	MinMax	3	2	64/32	ReLU	MSE	Adam	100	16
mBB–02	Past Inflow, Avg. Past Inflow	MinMax	3	2	64/32	ReLU	MSE	Adam	100	32
mBB–03	Past Inflow, Avg. Past Inflow	MinMax	3	2	64/32	ReLU	MSE	Adam	100	64
mBB–04	Past Inflow, Avg. Past Inflow, Rainfall	MinMax	3	2	64/32	ReLU	MSE	Adam	100	16
mBB–05	Past Inflow, Avg. Past Inflow, Rainfall	MinMax	3	2	64/32	ReLU	MSE	Adam	100	32
mBB–06	Past Inflow, Avg. Past Inflow, Rainfall	MinMax	3	2	64/32	ReLU	MSE	Adam	100	64
Monthly Univariate Prediction Models of SK Dam										
mSK–01	Past Inflow,	MinMax	3	2	64/32	ReLU	MSE	Adam	100	16

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Model No.	Input Feature	Standardization Technique	LSTM Parameter in Keras							
			Steps	Number of Layers	Units per Layer	Activation	Loss Function	Optimizer	Epoch	Batch Size
	Avg. Past Inflow									
mSK–02	Past Inflow, Avg. Past Inflow	MinMax	3	2	64/32	ReLU	MSE	Adam	100	32
mSK–03	Past Inflow, Avg. Past Inflow	MinMax	3	2	64/32	ReLU	MSE	Adam	100	64
mSK–04	Past Inflow, Avg. Past Inflow, Rainfall	MinMax	3	2	64/32	ReLU	MSE	Adam	100	16
mSK–05	Past Inflow, Avg. Past Inflow, Rainfall	MinMax	3	2	64/32	ReLU	MSE	Adam	100	32
mSK–06	Past Inflow, Avg. Past Inflow, Rainfall	MinMax	3	2	64/32	ReLU	MSE	Adam	100	64
Daily and Monthly Multivariate Prediction Models of BB–SK Dam										
dBBSK–01, mBBSK–01,	BB Past Inflow, SK Past Inflow, BB Avg. Past Inflow SK Avg. Past Inflow, BB Rainfall, SK Rainfall, BB Humidity, SK Humidity	MinMax	3	2	64	Sigmoid	MSE	Adam	500	64

2.4. Evaluation of predictive performance

The statistical metrics; Coefficient of Determination (R^2), Nash–Sutcliffe Efficiency (NSE), Mean Squared Error (MSE), Root Mean Squared Error (RMSE), were used to evaluate the perfect match between the predicted and observation values of reservoir inflows. R^2 is statistical measures describing the degree of linear correlation between two independent variables which ranges from 0 to 1 (Al–Aqeeli et al., 2015). A higher R^2 value closer to 1 indicates better fit of the prediction model to the observation values making stronger predictive power. NSE is the normalized statistical measure that compares the relative magnitude of the model prediction errors to observed data variance ranging from $-\infty$ to 1 (Brownlee, 2018). The prediction accuracy can be classified into three main classes subject to NSE. When NSE is greater than or equal to 0.90, the prediction accuracy is classified as "Class A–Excellent", NSE ranges between 0.70 and 0.90, it is considered as "Class B–Good), and NSE lies between 0.50 and 0.70, it is classified as "Class C–Moderate" (China National Standardization Management Committee, 2008; Zhang et al., 2021). MSE, and RMSE metrics quantify the absolute and squared differences between the predicted and actual values, respectively. A lower value of MSE, and RMSE indicates better model performance. A prediction model is considered as precise and robust prediction when R^2 and NSE values are relatively approach to 1, MSE and RMSE values are small.

In the last step, the predictability to predict the low, average, and high daily and monthly reservoir inflows of BB and SK dams was assessed to leverage the application of ML–and DL–based prediction model for real–time reservoir operation and planning during the critical periods. The lowest, average, and highest reservoir inflows of the tested results were compared to the observed reservoir inflows. Finally, percentage error in prediction was computed.

3. Results and Discussion

3.1. Predicted one–day and one–month ahead of BB and SK reservoir inflows

In this study, R^2 and NSE were prioritized over MSE and RMSE to identify the optimal predictive model performances on the training and testing datasets. The quantitative and qualitative comparisons between observed and predicted inflows of the optimal daily and monthly univariate and multivariate prediction models for six scenarios are presented in Table 6 and illustrated in Fig. 5 and Fig. 6. The qualitative results from 2000 to 2020 demonstrated that daily and monthly predicted inflows for both BB and SK dams closely matched the observed inflows for both training and testing datasets when univariate and multivariate prediction models were performed. Even the monthly inflow pattern obtained from univariate and multivariate prediction models are likely similar to observed values, however, monthly prediction exhibited larger deviation from the observed values compared to daily prediction particularly the lowest and highest reservoir inflows.

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Table 6 The optimal predictive performances of daily and monthly reservoir inflow prediction

Univariate Prediction Model					Multivariate Prediction Model				
Scenario Design	Model Building	Statistical Metrics	BB	SK	Scenario Design	Model Building	Statistical Metrics	BB	SK
S1: Daily model using XGBoost algorithm	Training	R^2	0.922	0.884	S5: Daily model using LSTM algorithm	Training	R^2	0.894	0.842
		NSE	0.909	0.871			NSE	0.890	0.841
		MSE	62.919	70.000			MSE	75.698	97.183
		RMSE	7.932	8.367			RMSE	8.700	9.858
	Testing	R^2	0.885	0.836		Testing	R^2	0.873	0.780
		NSE	0.862	0.816			NSE	0.857	0.767
		MSE	31.990	81.308			MSE	36.039	92.455
		RMSE	5.656	9.017			RMSE	6.003	9.615
S2: Daily model using LSTM algorithm	Training	R^2	0.925	0.878	S6: Monthly model using LSTM algorithm	Training	R^2	0.542	0.518
		NSE	0.924	0.878			NSE	0.538	0.512
		MSE	46.898	61.577			MSE	183,353	192,778
		RMSE	6.848	7.847			RMSE	428	439
	Testing	R^2	0.827	0.851		Testing	R^2	0.526	0.487
		NSE	0.818	0.851			NSE	0.397	0.459
		MSE	60.770	67.050			MSE	103,050	130,290
		RMSE	7.800	8.190			RMSE	321	361
S3: Monthly model using XGBoost algorithm	Training	R^2	0.452	0.490					
		NSE	0.411	0.473					
		MSE	217,267	196,562					
		RMSE	466	443					
	Testing	R^2	0.679	0.520					
		NSE	0.675	0.513					
		MSE	65,836	128,363					
		RMSE	257	358					
S4: Monthly model using LSTM algorithm	Training	R^2	0.519	0.678					
		NSE	0.513	0.673					
		MSE	186,719	104,617					
		RMSE	432	323					
	Testing	R^2	0.388	0.434					
		NSE	0.353	0.407					
		MSE	122,597	158,222					
		RMSE	350	398					

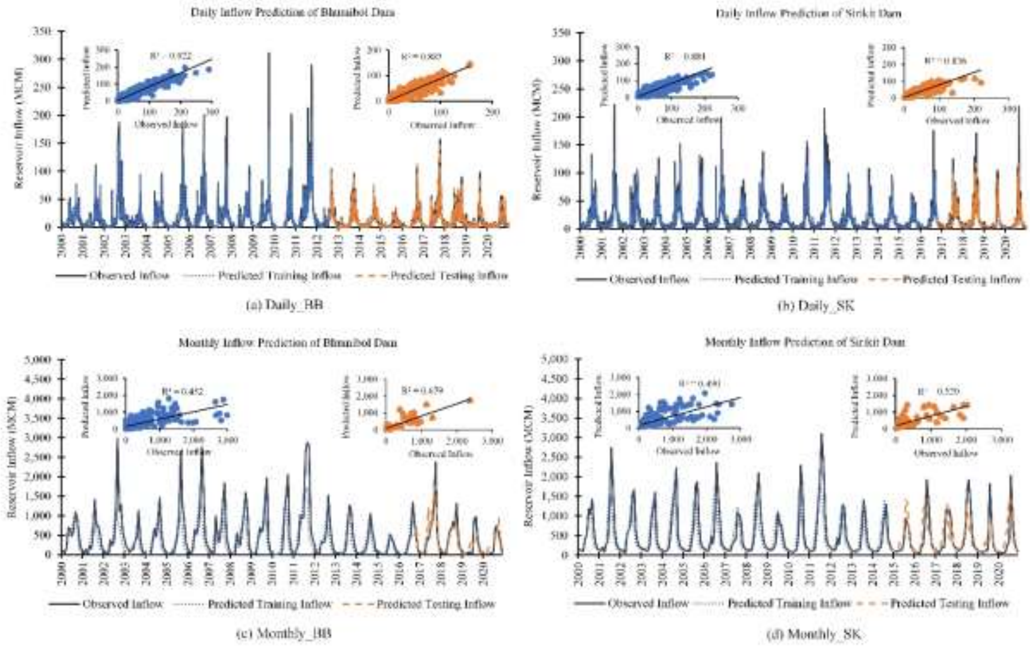

Fig. 5 Optimal predictive performances of one–day and one–month ahead univariate prediction models of BB and SK reservoir inflows

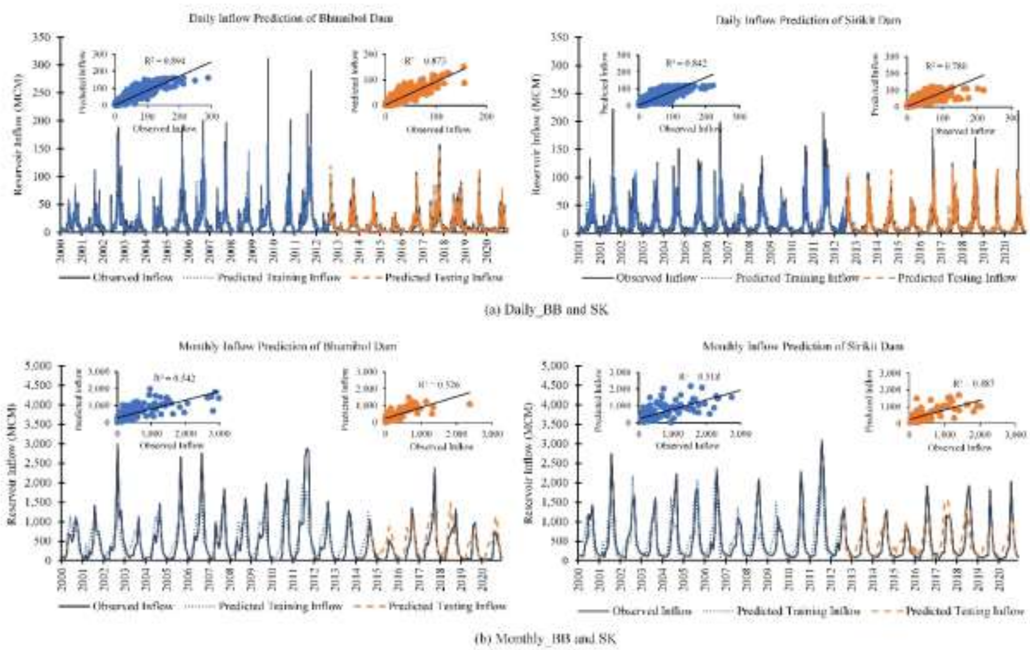

Fig. 6 Optimal predictive performances of one–day and one–month ahead multivariate prediction models of BB and SK reservoir inflows

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Fig. 7 and Fig. 8 quantitatively illustrate the performance metrics of all scenarios of 1–day ahead and 1–month ahead reservoir inflow predictions for both univariate and multivariate predictions. For the daily univariate prediction using XGBoost on the training dataset, Scenario 1 (S1) achieved R^2 and NSE values of 0.922 and 0.909 for BB dam and 0.884 and 0.871 for SK dam, respectively. However, R^2 and NSE values were slightly lower on the testing dataset with the values of 0.885 and 0.862 for BB dam and 0.836 and 0.816 for SK dam, respectively. MSE and RMSE values for BB dam were likely lower by –49.16% and –28.68% when 20% of dataset was accordingly tested. In contrast, these two values were slightly increased on the testing dataset for SK dam by +16.15% and +7.77%. It is revealed that the daily univariate prediction using LSTM (Scenario 2, S2) on the training dataset mostly demonstrated higher R^2 and NSE values of 0.925 and 0.924 for BB dam and 0.878 and 0.878 for SK dam, respectively indicating slightly higher predictive performances than XGBoost. Similar to XGBoost, R^2 and NSE values slightly decreased on the testing dataset achieving 0.827 and 818 for BB dam. For SK dam, these two statistical metrics considerably increased to 0.851 and 0.851 for SK dam, respectively. However, MSE and RMSE values performed by LSTM were +29.58% and +13.90% for BB dam and +8.89% and +4.37% for SK dam which were lower than XGBoost, respectively. For the Scenario 5 (S5) when daily multivariate prediction model was executed using LSTM to predict reservoir inflow for both BB and SK dams, R^2 and NSE values of training dataset were 0.894 and 0.890 for BB dam and 0.842 and 0.841 for SK dam, respectively. These values were slightly lower than those trained by daily univariate prediction model using both XGBoost and LSTM. On the testing dataset with daily multivariate prediction model, R^2 and NSE values for BB dam were slightly higher than those obtained by daily univariate prediction model for both XGBoost and LSTM, reaching 0.873 and 0.857, respectively. However, these values decreased considerably to 0.780 and 0.767, respectively for SK dam. In terms of MSE and RMSE, there was an insubstantial difference between univariate and multivariate prediction models.

The predictive results exhibited that the predictability of daily univariate prediction models is slightly superior than multivariate models, as they were developed independently to extract the specific input features of each dam. However, the daily multivariate prediction model could provide two predictive outputs relatively closer to daily univariate prediction model which is beneficial for real–time operational applications in the river basin. Due to the high complexity of all input features and larger dataset used in the daily multivariate prediction model, however, DL–based prediction model with LSTM algorithm could perform well in learning and capturing the input–output relation and features, resulting in providing predictive performance closer to those achieved by the daily univariate prediction model. Training larger datasets with LSTM for both daily univariate and multivariate prediction models gave the better predictive performances than XGBoost. However, when smaller testing datasets were tested by LSTM, statistical performance was slightly decreased compared to training dataset as obviously presented in Scenario 2 and Scenario 5. It is also revealed that daily reservoir inflow predictions for BB dam demonstrated higher performance compared to SK dam, for both daily univariate and multivariate models. In comparison between XGBoost and LSTM for daily reservoir inflow prediction on tested datasets, individual XGBoost model outperformed LSTM models across both univariate and multivariate predictions for BB dam. For SK dam, the individual LSTM prediction model could predict better results than the individual XGBoost model and the LSTM multivariate prediction model.

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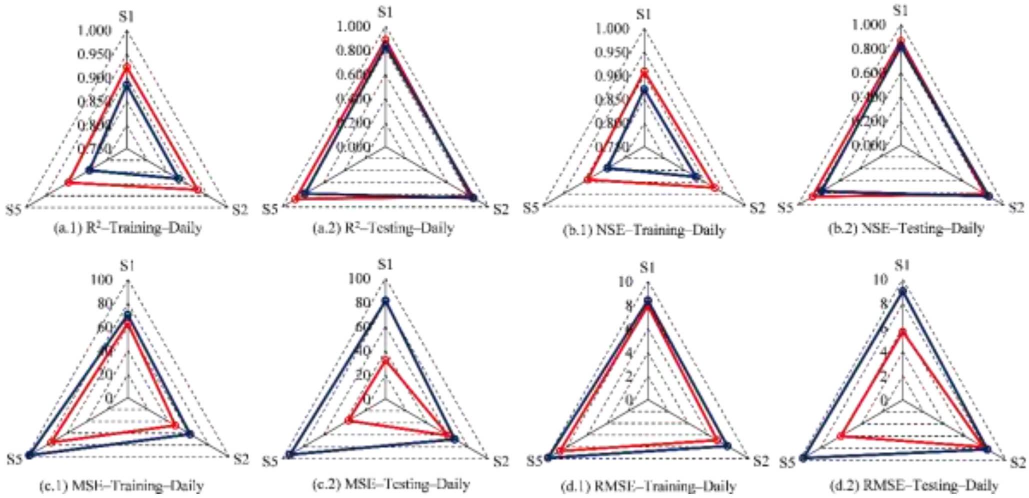

Fig. 7 Radar chart illustrating the performance metrics of all scenarios of 1–day ahead reservoir inflow prediction (Legend: Red–BB, Blue–SK)

For ML–based monthly univariate prediction using XGBoost, Scenario 3 (S3) achieved R^2 and NSE values of 0.452 and 0.411 for BB dam and 0.490 and 0.473 for SK dam, respectively on the training dataset. In contrast to daily prediction models with XGBoost, R^2 and NSE values were slightly higher on the testing dataset with the values of 0.679 and 0.675 for BB dam and 0.520 and 0.513 for SK dam, respectively. However, MSE and RMSE values were significantly decreased by –69.70% and –44.85% for BB dam and –34.70% and –19.19% for SK dam when testing dataset was accordingly employed. DL–based monthly univariate prediction using LSTM in Scenario 4 (S4) exhibited higher statistical performances in terms of R^2 and NSE values of 0.519 and 0.513 for BB dam and 0.678 and 0.673 for SK dam, respectively. However, these performance metrics considerably decreased to 0.388 and 0.353 for BB dam and 0.434 and 0.407 for SK dam when the testing datasets were investigated. The MSE and RMSE values performed by monthly prediction model with LSTM were significantly decreased by –34.34% and –18.98% for BB dam. In contrast, it showed the substantial increase in MSE and RMSE values by +53.24% and +23.23% for SK dam when testing dataset was accordingly employed. Compared to the individual monthly prediction by LSTM on testing datasets, LSTM–based monthly multivariate prediction in Scenario 6 (S6) could predict better results achieving R^2 and NSE values of 0.526 and 0.397 for BB dam and 0.487 and 0.459 for SK dam, respectively. However, it showed lower R^2 and NSE values compared to those obtained by individual monthly prediction using XGBoost.

In comparison between daily and monthly prediction models, the results demonstrated that ML– and DL–based prediction models achieved higher statistical metrics in predicting daily reservoir inflow compared to monthly predictions. This is because prediction modeling with ML and DL algorithms can handle and leverage larger datasets available in daily prediction model, enabling them to learn and capture patterns more effectively. Similarly, training larger datasets with LSTM for both daily and monthly univariate and multivariate prediction models mostly outperformed XGBoost. However, slight decrease in statistical metrics is found when dealing with the smaller testing datasets. To improve the robustness and precision of LSTM–based forecasts for both univariate and multivariate predictions, it is recommended to increase the testing dataset size during model validation. Importantly, cross–validation should be conducted to assess model overfitting and ensure its generalizability.

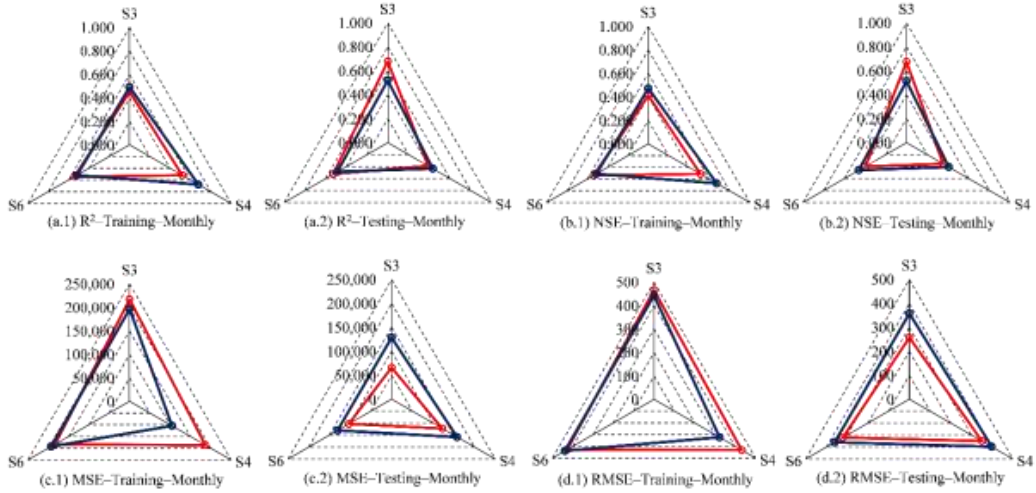

Fig. 8 Radar chart illustrating the performance metrics of all scenarios of 1–month ahead reservoir inflow prediction (Legend: Red–BB, Blue–SK)

3.2. Optimal model configuration for univariate and multivariate reservoir inflow prediction models

Based on the optimization criteria of maximizing R^2 and NSE values as optimal prediction model, accordingly the optimal input features, training and testing dataset ratio, and optimal hyperparameter of prediction models were explored. The results of optimal model configuration are summarized in Table 7.

Table 7 Optimal model configuration for reservoir inflow prediction models

Input Features & Training:Testing Ratio & Hyperparameter	S1: Daily Univariate Model_XGBoost		S2: Daily Univariate Model_LSTM		S3: Monthly Univariate Model_XGBoost		S4: Monthly Univariate Model_LSTM		S5: Daily Multivariate Model_LSTM	S6: Monthly multivariate Model_LSTM
	BB	SK	BB	SK	BB	SK	BB	SK	BB–SK	BB–SK
Past Inflow at Time t	✓	✓	✓	✓	✓	✓	✓	✓	✓	✓
Avg. Past Inflow at t–3	✓	✓	–	–	✓	–	✓	✓	✓	✓
Avg. Past Inflow at t–7	–	–	✓	✓	–	✓	–	–	–	–
Rainfall at Time t	–	–	–	–	✓	✓	–	–	✓	✓
Humidity at Time t	–	–	–	–	✓	–	–	–	✓	✓
Training:Testing Ratio	80:20	80:20	**70:30**	**70:30**	80:20	70:30	**60:40**	**60:40**	**70:30**	**60:40**
XGBoost: Learning Rate	0.1	0.1	–	–	0.001	0.001	–	–	–	–
XGBoost: Nrounds	10,000	10,000	–	–	10,000	10,000	–	–	–	–
XGBoost: Max Depth	6	6	–	–	6	6	–	–	–	–
LSTM: Learning Rate	–	–	0.1	0.1	–	–	0.1	0.1	0.1	0.1
LSTM: No. of Layers	–	–	2	2	–	–	2	2	2	2
LSTM: No. of Units	–	–	64	64	–	–	64	64	64	64

It is emphasized that information on past reservoir inflow including the previous time step and its moving average was observed to be a significant predictor to predict future inflow for all prediction scenarios. For daily and monthly multivariate predictions by LSTM, rainfall and humidity data was incorporated as input features which demonstrated a substantial impact on predictive performances. Since XGBoost can work effectively with smaller datasets compared to LSTM for both univariate and multivariate prediction models, it is crucial to select key predictors that are highly correlated with reservoir inflow for the model development. Conversely, LSTM is specifically designed for larger sequential datasets, a broad range of potential input features can be included in the prediction models. Moreover, altering optimal training and testing ratios by increasing the testing datasets into 70:30 and 60:40 can significantly enhance the predictive performances of optimal LSTM–based prediction models. However, handling the larger datasets require more computational resource to capture relevant data features making LSTM–based prediction models computationally expensive than XGBoost. Furthermore, multivariate prediction models generally consume more computational resources than univariate prediction models.

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It is revealed from the model configuration experiment that learning rate of 0.1 and 0.001 significantly impacts stability and convergence of both XGBoost and LSTM algorithms during model training. The number of boosting rounds (nrounds) of 10,000 in all scenarios of XGBoost–based prediction models can improve the statistical performance metrics substantially. However, overfitting risk due to increased number of boosting rounds should be carefully investigated through model validation. In this study, to control complexity of individual tree and capture complex data pattern from deeper tress, maximum depth was set to 6 for all scenarios of univariate prediction. For the LSTM–based prediction models, learning rate of 0.1 of both univariate and multivariate prediction models is a significant hyperparameter in achieving model stability and convergence. Number of layers was set to 2 across all prediction scenarios to identify model complexity. Furthermore, the optimal number of LSTM units was observed to be 64 across all scenarios exhibiting increased predictive performances.

3.3. Evaluation of Percentage Error of Low, Average and High Reservoir Inflow Prediction

The percentage error of low, average and high reservoir inflow prediction, was computed to diagnose the predictability of ML– and DL–based prediction models as summarized the results in Table 8. It is revealed that the daily minimum and average reservoir inflows performed by XGBoost univariate model (S1) on the training and testing datasets were very close to the observed values. On the training datasets, a small discrepancy of daily minimum and average reservoir inflows was +0.17 MCM and –0.81 MCM (–4.62% error), respectively for BB dam and +3.03 MCM and –0.62 MCM or –3.58%, respectively for SK dam. Similarly, it showed small discrepancy of daily minimum and average reservoir inflows on the testing datasets was +0.17 MCM and +0.03 MCM (+0.27% error), respectively for BB dam and +3.03 MCM and –0.34 MCM or –2.38%, respectively for SK dam. Importantly, this analysis exhibited a consistent overprediction of minimum reservoir inflows for these two dams on both training and testing datasets. In contrast, larger percentage error in underprediction of maximum reservoir inflows on both training and testing datasets were observed ranging –36.73% and –6.93%, respectively for BB dam and –33.77% and –46.78%, respectively for SK dam. While, the small percentage error of average reservoir inflows predicted by XGBoost univariate model varied positively and negatively relative to observed values indicating both under–and overprediction.

Similar to XGBoost, the predictive results performed using LSTM (S2) for daily univariate prediction showed the small discrepancy in minimum and average reservoir inflows of BB and SK dams. However, bigger discrepancy was observed in maximum inflow prediction for these two dams. On the training datasets, discrepancy error in minimum, average, and maximum reservoir inflows were +0.27 MCM, +0.26 MCM (+1.74% error), and –9.87 MCM (–3.17% error), respectively, for BB dam, and +1.62 MCM, –0.05 MCM (–0.32% error), and –11.71 MCM (–5.46%), respectively, for SK dam. On testing datasets, LSTM model exhibited small discrepancy error in minimum, average, and maximum reservoir inflows by +0.27 MCM, +0.65 MCM (+6.00% error), and +18.05 MCM (+9.63% error), respectively, for BB dam, and +1.14 MCM, +0.04 MCM (+0.30% error), and –11.14 MCM (–5.09%), respectively, for SK dam.

For the daily multivariate prediction model using LSTM (S5), the discrepancy of minimum, average, and maximum reservoir inflows of two dams were definitely close to those obtained from univariate prediction models using two algorithms; XGBoost and LSTM. The daily minimum reservoir inflows performed by multivariate prediction model for BB and SK dams were +0.20 MCM and +2.65 MCM, respectively on training datasets, and +0.21 MCM and +2.65 MCM, respectively on testing datasets. These predictive results were slightly overpredicted compared to the minimum observed values. In addition, the daily average inflows for BB and SK dams on the training datasets, were slightly underpredicted by –2.74% and –2.50%, respectively. On the testing datasets, overprediction was observed, with values of +4.37% and +6.48%, respectively. Similar to the univariate models, multivariate prediction models consistently underpredicted maximum reservoir inflows for both BB and SK dams, as obviously found in both training and testing datasets.

All in all, the LSTM univariate model (S2) exhibited the smallest percentage errors in predicting minimum, average, and maximum reservoir inflows for daily predictions compared to the XGBoost model (S1) and multivariate prediction using LSTM (S5). Among all ML– and DL–based prediction models (S1, S2, and S5) for daily prediction, underprediction of low reservoir inflows and overprediction of high reservoir inflows by both univariate and multivariate prediction models were consistently emerged. However, LSTM–based individual prediction model is recommended for high inflow prediction.

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Table 8 Percentage error of low, average and high reservoir inflow prediction

Model Type	Optimal Prediction Model					Min. Reservoir Inflow (MCM)			Avg. Reservoir Inflow (MCM)			Max. Reservoir Inflow (MCM)		
	Algorithm	Training: Testing	Learning Rate	Dam	Dataset	Obs.	Pred.	Δ (%)	Obs.	Pred.	Δ (%)	Obs.	Pred.	Δ (%)
S1: Daily Univariate Prediction	XGBoost	80:20	0.1	BB	Training	0.00	0.17	+0.17	17.52	16.71	–0.81 **(–4.62)**	311.46	197.05	–114.41 **(–36.73)**
				BB	Testing	0.00	0.17	+0.17	10.99	11.02	+0.03 **(+0.27)**	156.57	145.71	–10.86 **(–6.94)**
	XGBoost	80:20	0.1	SK	Training	0.00	3.03	+3.03	17.32	16.70	–0.62 **(–3.58)**	221.87	146.95	–74.92 **(–33.77)**
				SK	Testing	0.00	3.03	+3.03	14.26	13.92	–0.34 **(–2.38)**	218.70	116.39	–102.31 **(–46.78)**
S2: Daily Univariate Prediction	LSTM	70:30	0.1	BB	Training	0.00	0.27	+0.27	14.90	15.16	+0.26 **(+1.74)**	311.46	301.59	–9.87 **(–3.17)**
				BB	Testing	0.00	0.27	+0.27	10.83	11.48	+0.65 **(+6.00)**	187.34	205.39	+18.05 **(+9.63)**
	LSTM	70:30	0.1	SK	Training	0.00	1.62	+1.62	15.81	15.76	–0.05 **(–0.32)**	214.42	202.71	–11.71 **(–5.46)**
				SK	Testing	0.00	1.14	+1.14	13.25	13.29	+0.04 **(+0.30)**	218.70	207.56	–11.14 **(–5.09)**
S3: Monthly Univariate Prediction	XGBoost	80:20	0.001	BB	Training	0.00	8.05	+8.05	476.49	360.10	–116.39 **(–24.43)**	2,990.21	1,811.99	–1,178.22 **(–39.40)**
				BB	Testing	12.99	10.87	–2.12 **(–16.32)**	370.31	359.75	–10.56 **(–2.85)**	2,373.51	1,740.76	–632.75 **(–26.66)**
		70:30	0.001	SK	Training	61.48	78.04	+16.56 **(+26.94)**	543.94	479.97	–63.97 **(–11.76)**	3,095.97	2,076.67	–1,019.30 **(–32.92)**
				SK	Testing	40.30	83.60	+43.30 **(+107.44)**	429.62	437.75	+8.123 **(+1.89)**	2,026.29	1,432.32	–593.97 **(–29.31)**
S4: Monthly Univariate Prediction	LSTM	70:30	0.1	BB	Training	0.00	56.53	+56.53	460.61	479.25	+18.64 **(+4.05)**	2,877.23	2,373.81	–503.42 **(–17.50)**
				BB	Testing	9.03	116.48	+107.45 **(+1,190)**	336.64	410.65	+74.01 **(+21.98)**	1,944.38	1,469.24	–475.14 **(–24.44)**
		70:30	0.1	SK	Training	46.50	110.20	+63.70 **(+136.99)**	486.21	495.34	+9.14 **(+1.88)**	3,095.97	2,477.07	–618.90 **(–19.99)**
				SK	Testing	40.30	112.55	+72.25 **(+179.28)**	410.14	460.03	+49.89 **(+12.17)**	2,026.29	1,845.41	–180.88 **(–8.93)**
S5: Daily Multivariate Prediction	LSTM	60:40	0.1	BB	Training	0.00	–0.20	–0.20	17.52	17.04	–0.48 **(–2.74)**	311.46	161.51	–149.95 **(–48.14)**
				BB	Testing	0.00	–0.21	–0.21	10.99	11.47	+0.48 **(+4.37)**	156.57	151.09	–5.48 **(–3.50)**
		60:40	0.1	SK	Training	0.00	2.65	+2.65	18.38	17.92	–0.46 **(–2.50)**	221.87	121.05	–100.82 **(–45.44)**
				SK	Testing	0.00	2.65	+2.65	14.20	15.12	+0.92 **(+6.48)**	218.70	118.95	–99.75 **(–45.61)**
S6: Monthly Multivariate Prediction	LSTM	70:30	0.1	BB	Training	0.00	17.92	+17.92	510.59	551.76	+41.17 **(+8.06)**	2,990.21	1,984.74	–1,005.47 **(–33.63)**
				BB	Testing	1.57	16.09	+14.52 **(+924.84)**	323.19	455.97	+132.78 **(+41.08)**	2,373.51	1,481.92	–891.59 **(–37.56)**
		60:40	0.1	SK	Training	61.48	38.49	–22.99 (–37.39)	563.63	551.53	–12.097 **(–2.15)**	3,095.97	2,258.06	–837.91 **(–27.06)**
				SK	Testing	40.30	54.61	+14.309 (+35.51)	428.26	485.17	+56.91 **(+13.29)**	2,026.29	1,688.66	–337.631 **(–16.66)**

In view of the crucial role of accurate long–term reservoir inflow predictions in effective reservoir management planning, this study focuses on developing robust monthly inflow prediction models. Even both monthly univariate and multivariate prediction models efficiently learned and captured the inflow patterns, exhibiting similarities to observed values, monthly prediction models (S3, S4, and S6) demonstrated larger deviations from observed values with higher percentage errors compared to daily predictions (S1, S2, and S5). On the training datasets of S3, a bigger discrepancy of monthly minimum reservoir inflows was +8.05 MCM and +16.56 MCM for BB and SK dams, respectively. While, the monthly average and maximum reservoir inflows were –24.43% and –39.40%, respectively for BB dam and –11.76% and –39.92%, respectively for SK dam. Base on the testing datasets, the percentage errors particularly in monthly minimum and maximum inflows were found to be underpredicted by –16.32% for BB dam and overpredicted by +107.44% for SK dam. The maximum reservoir inflows of both BB and SK dams were underpredicted with the errors of –26.66% and –29.31%, respectively. Analysis of monthly minimum

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and average inflows for both training and testing datasets of S4 and S6 revealed overprediction primarily for BB and SK dams. Conversely, monthly maximum reservoir inflows were consistently underpredicted, exhibiting larger percentage errors.

4. Conclusion

This study demonstrated the ability of ML–and DL–based univariate and multivariate prediction models to predict daily and monthly reservoir inflows of BB and SK dams. Due to a wide range of successful applications of ML and DL algorithms for hydrological prediction, XGBoost, a tree–based ensemble method, and LSTM, a deep neural network, were selected for this study. To support real–time reservoir operation for the BB and SK dams, two short–term prediction scenarios (S1 and S2) of daily univariate models and one scenario (S5) of daily multivariate models were developed. In addition, two long–term prediction scenarios (S3 and S4) of monthly univariate models and one scenario (S6) of monthly multivariate models were developed to support reservoir management planning. For univariate prediction, the inflows of the BB and SK dams were predicted separately using two individual models. In contrast, for multivariate prediction, a single model was developed to simultaneously predict the inflows of both the BB and SK dams facilitating the integrated decision–making processes in the river basin. The results of all prediction scenarios demonstrated that ML– and DL–based prediction models achieved higher statistical metrics evaluated in terms of R^2, NSE, MSE, and RMSE in predicting daily reservoir inflow compared to monthly predictions. This is because prediction modeling with ML and DL algorithms can handle and leverage larger datasets available in daily prediction model, enabling them to learn and capture patterns more effectively. Based on a number of model configuration experiments, individual XGBoost models mostly outperformed LSTM when tested on the datasets for both daily and monthly univariate predictions. LSTM models consistently outperformed XGBoost when mostly trained on larger datasets for both daily and monthly univariate and multivariate predictions. However, a slight decrease in statistical metrics was apparently observed with smaller testing datasets. To enhance the robustness and precision of LSTM–based forecasts, it is recommended to increase the testing dataset size during model validation and employ cross-validation techniques to check for model overfitting. For input feature selection, the information on past reservoir inflow including the previous time step and its moving average was considered as a significant predictor to predict future inflow for all prediction scenarios. As LSTM can handle large datasets effectively, consequently, rainfall and humidity data were also incorporated as additional input features indicating a substantial impact on improved predictive performance. Ability to predict low, average, and high reservoir inflow by ML– and DL–based prediction models were also assessed. Overall, LSTM–based univariate model distinctively exhibited the smallest percentage errors in predicting minimum, average, and maximum reservoir inflows for daily and monthly predictions compared to the XGBoost model and multivariate prediction using LSTM. Consequently, LSTM–based individual daily and monthly prediction models are recommended for predicting low and high values of reservoir inflow during critical events. In addition, monthly prediction models demonstrated larger discrepancy from observed values with higher percentage errors compared to daily predictions. Among all ML– and DL–based prediction models for daily and monthly predictions, underprediction of low reservoir inflows and overprediction of high reservoir inflows by both univariate and multivariate prediction models were consistently existed. Therefore, extracting specific and informative insights from the results of each prediction model and forecasting horizon can significantly enhance decision–making support for both real–time reservoir operation and long–term reservoir management planning.

Code and data availability statement

The data and code are available upon request from the corresponding author.

Interactive computing environment

An R–based environment utilizing the Dplyr, ggplot2, imputeTS, Matrix, Metrics, RcppRoll, and Xgboost libraries was used for developing XGBoost–based prediction models. A custom Python–based environment leveraging RNN, Reticulate, Modeler, Keras, and other relevant Python libraries was employed for the development of LSTM–based prediction models.

Author contribution

All authors contributed to the study conception and design. Material preparation, data collection and analysis were performed by Areeya Rittima, Jidapa Kraisangka, and Pheeranat Dornpunya. The first draft of the manuscript was written and reviewed by Areeya Rittima, Jidapa Kraisangka, Pheeranat Dornpunya and all authors commented on previous versions of the manuscript. All authors read and approved the final manuscript.

Completing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Review statement

This study demonstrated the predictability of Machine Learning (ML)– and Deep Learning (DL)–based univariate and multivariate predictions of reservoir inflows of Bhumibol (BB) and Sirikit (SK), two major dams in the Chao Phraya River Basin. XGBoost, tree–based ensemble–, and LSTM, deep neural network–based algorithms were selected for development of daily and monthly prediction models. Input features selection and configuration design of two different types of daily and monthly reservoir inflow prediction models; (1) univariate prediction with XGBoost and LSTM algorithms and (2) multivariate prediction with LSTM algorithm, were definitely highlighted. In the last step, predictability of predicting low and high reservoir inflow values of these models were accordingly explored to assess their statistical performances.

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