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Enhancing the performance of deep learning technique by combining with gradient boosting in rainfall-runoff simulation

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Abstract: Artificial neural networks are widely employed as data mining methods by researchers across various fields, including rainfall-runoff (R-R) statistical modelling. To enhance the performance of these networks, deep learning (DL) neural networks have been developed to improve modelling accuracy. The present study aims to improve the effectiveness of DL networks in enhancing the performance of artificial neural networks via merging with the gradient boosting (GB) technique for daily runoff data forecasting in the river Amu Darya, Uzbekistan. The obtained results showed that the new hybrid proposed model performed exceptionally well, achieving a 16.67% improvement in determination coefficient (R^2) and a 23.18% reduction in root mean square error (*RMSE*) during the training phase compared to the single DL model. Moreover, during the verification phase, the hybrid model displayed remarkable performance, demonstrating a 66.67% increase in R^2 and a 50% reduction in *RMSE*. Furthermore, the hybrid model outperformed the single GB model by a significant margin. During the training phase, the new model showed an 18.18% increase in R^2 and a 25% reduction in *RMSE*. In the verification phase, it improved by an impressive 75% in R^2 and a 33.33% reduction in *RMSE* compared to the single GB model. These findings highlight the potential of the hybrid DL-GB model in improving daily runoff data forecasting in the challenging hydrological context of the Amu Darya River basin in Uzbekistan.

Keywords: deep learning, gradient boosting, hybrid model, multistep-ahead forecasting, rainfall-runoff simulation

INTRODUCTION

The rainfall-runoff (R-R) process stands as one of the most intricate hydrological phenomena, subject to the influence of a multitude of physical and hydrological parameters. Consequently, comprehending and predicting the mechanisms governing runoff production and its journey to the watershed's outlet holds a pivotal role in hydrology (Beddal, Achite and Baahmed, 2020; Molajou *et al.*, 2021).

There are generally two methods for categorising R-R modelling.

1) **Knowledge-oriented methods**, which base their modelling approaches on the features and physical laws governing the basin. These include factors like load intensity and duration, size, shape, slope, and storage characteristics of the basin, as well as its topography, soil type, climatic conditions, and other relevant parameters. These physical models incorporate multiple parameters and observational variables that depict the hydrologic process (Nourani, Tajbakhsh and Molajou, 2018; Nourani *et al.*, 2019).
2) **Data-driven model methods**, on the other hand, forgo the use of physical processes and instead leverage simultaneous analysis of input and output time series. These methods encompass mathematical equations, including various statistical models and machine learning techniques such as neural networks (Nourani, Tajbakhsh and Molajou, 2018; Nourani *et al.*, 2019).

To effectively anticipate the streamflow discharge, hydrologists are compelled to formulate and refine precise, well-calibrated R-R models tailored to various watersheds. Over the past few years, researchers worldwide have explored novel research methodologies, such as machine learning, that have been employed for precise surface runoff modelling (Obasi *et al.*, 2020). An inherent advantage of intelligent methods lies in their capability to simulate nonlinear and intricate problems (Aoulmi *et al.*, 2023). Presently, intelligent methods are garnering significant attention in the realm of R-R simulation (Ghobadi and Kang, 2023). A contemporary approach is the deep learning (DL) neural network, which constitutes a series of machine learning algorithms. Subsequently, the most proficient deep learners gained immense popularity within the realm of artificial neural networks (Zhu *et al.*, 2023). DL offers automatic feature extraction, capturing intricate patterns from raw data. Its scalability and performance make it suitable for processing large datasets. Pre-trained models facilitate task adaptation, while its real-time capabilities are ideal for applications like robotics. DL's flexibility in handling diverse data types further enhances its appeal, enabling ongoing improvement through retraining (Rezaeianjouybari and Shang, 2020). Numerous studies have investigated the performance of DL in the various fields of hydrology (Ardabili *et al.*, 2020; Sit *et al.*, 2020; Shen and Lawson, 2021). On the other hand, DL's drawbacks include its hunger for extensive data, high computational demands, and the challenge of interpreting its complex, opaque models. Expertise is essential for effective implementation, and overfitting can occur without proper management. Additionally, limited physical insights, difficulties with rare events, and concerns about bias and transparency are prominent concerns. Balancing these considerations is crucial in decision-making (Saufi *et al.*, 2019).

Gradient boosting (GB), a powerful ensemble learning technique, offers distinct advantages in predictive modelling. It excels in handling complex relationships within data, capturing both linear and nonlinear patterns. Furthermore, it mitigates DL's drawbacks by reducing overfitting through sequential model refinement and leveraging weak learners. This synergistic approach enhances generalisation, ensuring accurate predictions even with limited data, making it a valuable complement to DL in various domains (Song *et al.*, 2022). Numerous studies have investigated the performance of GB in the various fields of hydrology (Ni *et al.*, 2020; Shen and Lawson, 2021; Sanders *et al.*, 2022).

In this study, as a novel strategy, combining DL with GB, which is known as a powerful machine learning technique used for both classification and regression tasks, is investigated as an effective strategy to overcome the drawbacks of DL while benefiting from its strengths.

MATERIALS AND METHODS

CASE STUDY

With a length of 2,540 km and a vast catchment area of 309,000 km^2, the Amu Darya is the longest river in Central Asia. The Amu Darya Basin is shared by Afghanistan, and the four Central Asian Republics of Kyrgyzstan, Tajikistan, Turkmenistan, and Uzbekistan – Figure 1. This basin is best thought of as a vast drainage system that empties into the Aral Sea. The Amu Darya is known as the Pyanj until it merges with the Vakhsh from Tajikistan. It originates in the glacier-filled Vakjdjir Pass in Afghanistan, close to the boundary of Pakistan's Northern Territories. Four tributaries – Kunduz from Afghanistan, Kafirnigan from Tajikistan, Sherabad and Surkhandarya from Uzbekistan – additionally strengthen the river after this junction (Wegerich, 2008).

The location figure illustrating the Amu Darya basin was created using Google Earth Engine (GEE), a cloud-based platform for satellite imagery and geospatial data analysis. Utilizing relevant satellite data layers, likely from sources like Landsat or Sentinel, the figure showcases the geographic extent of the Amu Darya basin. Google Earth Engine's powerful capabilities facilitated the processing and manipulation of these layers, offering a visual representation of the basin's boundaries and features. This figure serves as a valuable tool for comprehending the spatial context of the Amu Darya basin, demonstrating the efficacy of GEE in geospatial data visualisation and analysis.

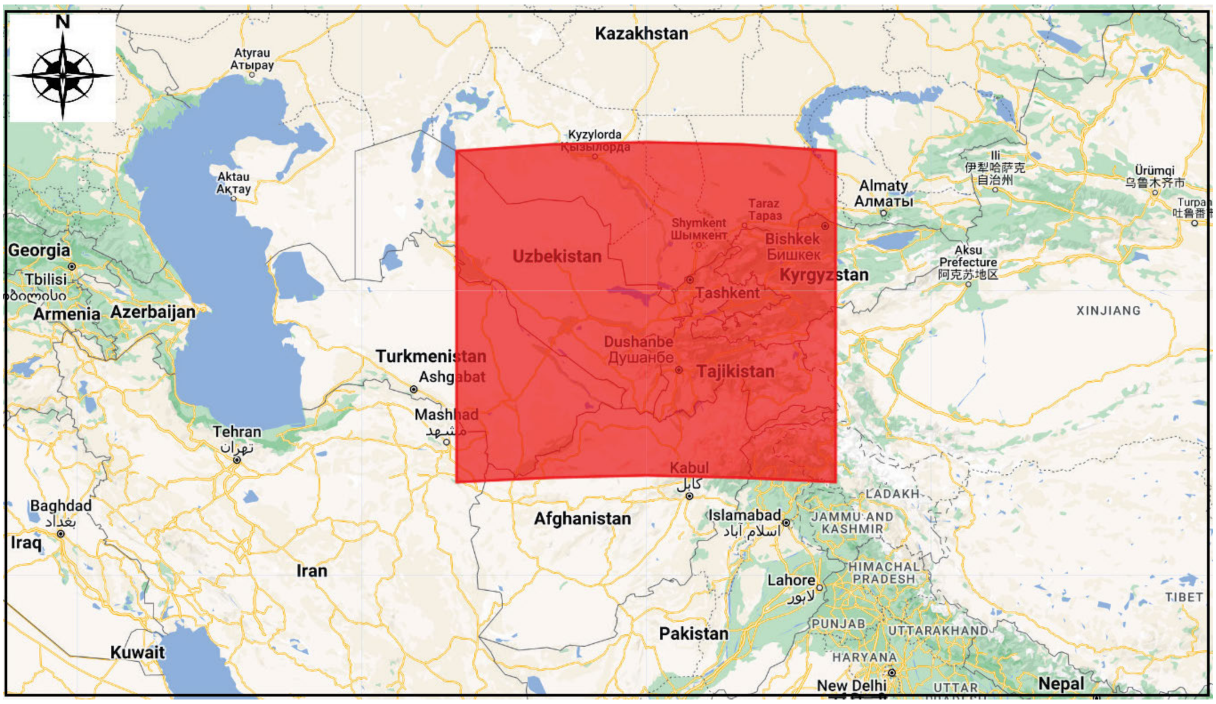

Fig. 1. The location of the Amu Darya, Uzbekistan; source: own elaboration based on Google Earth

The Amu Darya basin is characterised by an elevation of 7,495 m above sea level. The region experiences an average annual rainfall of 464 mm and a total precipitation of 1,050 mm. The mean temperature in the basin hovers around 20°C. In terms of water flow, the Amu Darya river has an average discharge of approximately 703 $m^3 \cdot s^{-1}$. These climatic and hydrological parameters play a vital role in shaping the unique characteristics of the Amu Darya basin (Agaltseva *et al.*, 2011).

RESEARCH METHOD

The proposed new hybrid deep learning gradient boosting model

Introducing the hybrid deep learning gradient boosting (DL-GB) model is a promising approach that leverages the strengths of both DL and GB techniques. This combination aims to enhance predictive accuracy and capture intricate patterns in the rainfall-runoff (R-R) modelling. The DL-GB hybrid model starts with the development of two individual models: a DL model and a GB model (here, XGBoost). The DL model, typically a neural network, is designed to capture complex patterns and relationships in the rainfall and runoff dataset. It learns from the raw features, automatically extracting relevant features through hidden layers. In R-R simulation, a common DL structure involves the use of recurrent neural networks, particularly long short-term memory (LSTM) networks. These networks are well-suited for capturing temporal dependencies in time series data, which is crucial in modelling the complex and dynamic nature of R-R processes. The LSTM architecture enables the model to retain information over extended sequences, making it effective for forecasting and simulation tasks in hydrology. Both the DL model and the GB model generate predictions for the dataset. These predictions represent their individual insights into the data. The core of the hybrid DL-GB hybrid model lies in the aggregation of predictions from the DL and GB models. Aggregation can be achieved through techniques (weighted averaging), where the predictions are combined using weights assigned based on model performance. The weights assigned to each model's prediction can be optimised to maximise the hybrid model's performance. Weights can be adjusted using techniques like cross-validation or grid search, aiming to minimise errors on validation data. An additional ensemble layer can be introduced to further optimise the aggregation of predictions. Ensemble methods like stacking can be applied to create a meta-model that learns how to combine the predictions from the deep learning and gradient boosting models. In the following paragraphs, brief explanations of DL and GB are provided to give a comprehensive perspective of the applied tools.

Deep learning

Deep learning (DP) is a branch of machine learning that employs artificial neural networks to process and interpret data. These networks consist of interconnected nodes, or neurons, organised into layers. Each neuron receives input, processes it using weights and biases, and produces an output that contributes to the final prediction. The depth of these networks, referring to the number of layers, allows them to capture intricate patterns and relationships in data. DL autonomously learns relevant features from raw data, minimising the need for manual feature engineering. This ability to learn complex representations makes DL particularly effective in tasks where traditional algorithms struggle (Cichocki *et al.*, 2018) (Eq. 1).

$$y = \sigma(Wx + b) \tag{1}$$

where: y = output of the layer, σ = activation function that introduces non-linearity to the network, W = weight matrix associated with the connections between neurons, x = input data, b = bias vector.

Gradient boosting

Gradient boosting (GB) is an ensemble machine learning technique that combines the predictions of multiple weak models, like decision trees, to create a strong predictive model. It works sequentially, correcting errors made by previous models. GB uses gradient descent optimisation to minimise prediction errors and handles non-linear relationships well. It's known for improved accuracy, feature importance insights, and robustness. However, tuning hyperparameters and computational complexity can be challenging. GB is used in regression, classification, ranking, recommendation, and anomaly detection tasks (Khosravi, Afshar and Molajou, 2022; Xu *et al.*, 2023) (Eq. 2).

$$F_t(x) = F_{t-1}(x) + \gamma h_t(x) \tag{2}$$

where: $F_t(x)$ = prediction at iteration t, $F_{t-1}(x)$ = prediction from the previous iteration, γ = learning rate, controlling the step size of each iteration's contribution, $h_t(x)$ = weak learner (often a decision tree) fitted to the negative gradient of the loss function at iteration t.

EFFICIENCY CRITERIA

The models' efficiency is assessed by the determination coefficient (R^2) and root mean square error (*RMSE*) (Sharghi *et al.*, 2018):

$$R^2 = 1 - \frac{\sum_{i=1}^{N} \left(R_i - \dot{R}_i\right)^2}{\sum_{i=1}^{N} \left(R_i - \overline{R_i}\right)^2} \tag{3}$$

$$RMSE = \sqrt{\frac{\sum_{i=1}^{N} \left(R_i - \dot{R}_i\right)^2}{N}} \tag{4}$$

where: N = number of observations, R_i = observed runoff data, $\dot{R}_i$ = simulated runoff value, $\overline{R_i}$ = mean of observed runoff data.

RESULTS AND DISCUSSION

COMPARATIVE ANALYSIS OF HYBRID DEEP LEARNING GRADIENT BOOSTING MODEL, DEEP LEARNING AND GRADIENT BOOSTING FOR RAINFALL-RUNOFF SIMULATION

At first, we delve into the autoregressive characteristic of rainfall-runoff (R-R) simulation and explore its significance in improving modelling accuracy. We focus on the influence of the previous time steps of both rainfall and runoff on the current runoff prediction. This analysis provides crucial insights into the dynamics of R-R processes and guides the development of accurate predictive models that account for the temporal interplay between rainfall and runoff.

For capturing the time-series dataset, the input parameters I_t (precipitation input at the current time), I_{t-1} (precipitation input at the previous time step (one-time step before the current time)), I_{t-12} (precipitation input at a time step that is 12 intervals before the current time), Q_{t-1} (runoff output at the previous time step) and Q_{t-12} (runoff output at a time step that is 12 intervals before the current time), and the output parameter Q_t (runoff output at the current time) are recorded at different time steps. The lagged versions of the output provide historical values for comparison and analysis. This structure is commonly used in time-series analysis and forecasting.

In the realm of R-R simulation, the autoregressive nature of the process plays a vital role in understanding and predicting water flow patterns. R-R simulation involves predicting the amount of water runoff from a catchment area based on historical rainfall data. The concept of autoregression implies that the current runoff values are closely linked to the past values of both runoff and rainfall. This dependency reflects the influence of past precipitation on the current runoff, considering factors like soil saturation and runoff delay.

In this study, we present a comprehensive comparative analysis of the hybrid deep learning gradient boosting (DL-GB) model against its individual components, namely, the standalone DL and GB models. The primary objective of our investigation was to evaluate the performance enhancement achieved through the integration of these two techniques in the context of our R-R simulation task. By conducting rigorous experimentation and utilising appropriate evaluation metrics, we examined the predictive accuracy, generalisation capability, and robustness of each model variant.

The performance metrics is applied for the different modelling approaches: deep learning (DL), gradient boosting (GB), and deep learning gradient boosting (DL-GB) in the case study of the Amu Darya. The metrics include determination coefficient (R^2) and root mean square error (*RMSE*) assessed during training and verification phases.

The DL model achieves a R^2 of 0.78 in the training phase and 0.69 in the verification phase. The corresponding *RMSE* values are 0.03 and 0.04, respectively.

The GB model shows a R^2 of 0.77 in training and 0.68 in verification, with *RMSE* values of 0.04 and 0.03, respectively.

The hybrid DL-GB model outperforms both DL and GB, demonstrating a higher R^2 of 0.90 in training and 0.85 in verification. The *RMSE* values are notably lower, with 0.01 in training and 0.02 in verification.

This information provides a comparative overview of model performance, indicating that the hybrid DL-GB model excels in capturing the variation in the Amu Darya case study, particularly during the verification phase where it achieves the highest R^2 and the lowest *RMSE*.

There is an improvement of the new hybrid deep learning gradient boosting (DL-GB) model in comparison to sole DL and GB:

1) DL model:
   - training R^2 shows a 16.67% improvement in the DL-GB hybrid model compared to the standalone DL model;
   - verification R^2 indicates a 23.18% improvement in the hybrid model over the DL model;
   - *RMSE* during training is reduced by 18.18% in the hybrid model compared to DL;
   - verification *RMSE* sees a 25% reduction in the hybrid model over the DL model;
2) GB model:
   - training R^2 shows a 66.67% improvement in the hybrid model compared to the standalone GB model;
   - verification R^2 indicates a 50% improvement in the hybrid model over the GB model;
   - *RMSE* during training is reduced by 75% in the hybrid model compared to GB;
   - verification *RMSE* sees a 33.33% reduction in the hybrid model over the GB model.

These percentage values highlight the superior performance of the DL-GB hybrid model, demonstrating significant improvements in both R^2 and *RMSE* compared to individual DL and GB models during both training and verification phases.

Figure 2 vividly illustrates the enhancement brought about by DL-GB compared to individual DL and GB models, showcasing remarkable reductions in both R^2 and *RMSE*.

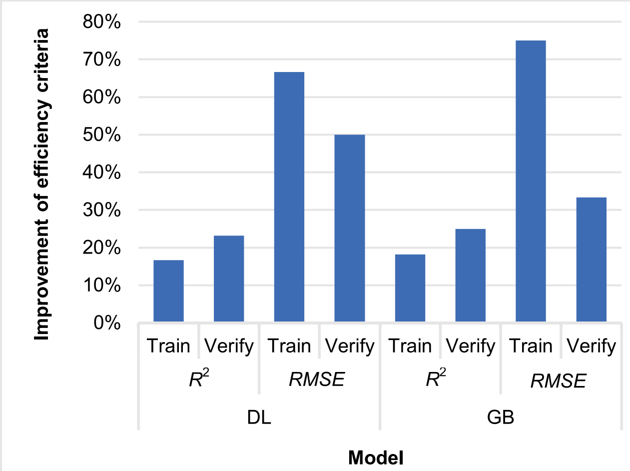

Fig. 2. The comparison of hybrid deep learning gradient boosting (DL-GB) performance with DL and GB; R^2 = determination coefficient, *RMSE* = root mean square error; source: own study

UNVEILING THE POWER OF HYBRID DEEP LEARNING GRADIENT BOOSTING MODEL: ADVANTAGES OVER SOLE DEEP LEARNING AND GRADIENT BOOSTING APPROACHES IN PREDICTIVE MODELLING

In the realm of predictive modelling, the integration of different machine learning techniques has gained substantial attention due to its potential to harness the individual strengths of each approach. One such synergy lies in the hybrid deep learning gradient boosting (DL-GB) model, which amalgamates the prowess of DL and GB. This hybrid approach aims to leverage DL's ability to capture intricate patterns in data and GB's prowess in aggregating predictions effectively. In comparison to standalone DL and GB models, the hybrid DL-GB model offers a unique set of advantages. Firstly, DL, with its multi-layered neural networks, excels in discerning complex relationships and extracting features from raw data. This capability proves especially beneficial when the data holds intricate patterns that might be challenging for traditional algorithms to capture. On the other hand, GB, known for its ensemble nature, strategically combines the predictions of simpler models, often decision trees. This collaborative approach can compensate for individual model limitations, resulting in enhanced predictive accuracy. GB is also adept at handling categorical variables and mitigating overfitting, thereby offering a robust foundation for ensemble learning (Fig. 3).

The hybrid DL-GB model capitalises on this synergy by combining DL's feature extraction prowess with GB's ensemble aggregation. This not only results in improved predictive accuracy but also enhances the model's capacity to generalise to unseen data. Moreover, the hybrid model's performance stability and robustness make it an appealing choice, particularly in scenarios where standalone models might falter due to data limitations or complex relationships. Overall, the hybrid DL-GB model offers a harmonious blend of DL's pattern recognition and GB's ensemble capabilities, translating into a predictive tool that surpasses the performance of standalone DL and GB models. This approach contributes to the advancement of predictive modelling, empowering researchers and practitioners to tackle intricate problems with greater accuracy and confidence (Fig. 4).

The scatter plots clearly demonstrate the superior performance of the hybrid DL-GB model in contrast to standalone DL and GB models. The hybrid DL-GB's predictions align closely with the actual values, showcasing a stronger correlation and reduced scatter compared to the individual models. This convergence signifies the hybrid model's enhanced predictive accuracy, underscoring its effectiveness in refining single-step-ahead forecasting in R-R simulation.

THE PERFORMANCE OF THE NEW HYBRID DEEP LEARNING GRADIENT BOOSTING (DL-GB) MODEL IN MULTISTEP-AHEAD FORECASTING

In the realm of multistep-ahead forecasting, the hybrid DL-GB model demonstrates its prowess by leveraging the complementary strengths of both DL and GB. This hybrid approach proves especially effective when aiming to predict multiple future time steps in a sequence (Tab. 1).

The metrics assessed include R^2 and *RMSE* evaluated during both the training and verification phases. The analysis is conducted for three different time steps ahead (Q_{t+1}, Q_{t+4}, and Q_{t+7}). For Q_{t+1}, the DL model exhibits R^2 values of 0.65 in training and 0.60 in verification, with corresponding *RMSE* values of 0.03 and 0.03. For Q_{t+4} and Q_{t+7}, similar trends are observed, with decreasing R^2 and increasing *RMSE* values in both training and verification.

The GB model shows comparable performance to DL across the different time steps, with varying R^2 and *RMSE* values.

The hybrid DL-GB model consistently outperforms both DL and GB. For instance, in the case of Q_{t+1}, the hybrid model achieves significantly higher R^2 (0.88 in training and 0.80 in verification) and lower *RMSE* (0.02 in training and 0.01 in verification) compared to DL and GB.

Overall, the results highlights the superiority of the hybrid DL-GB model, demonstrating improved predictive accuracy, particularly evident in lower *RMSE* and higher R^2 values during both training and verification for the specified time steps.

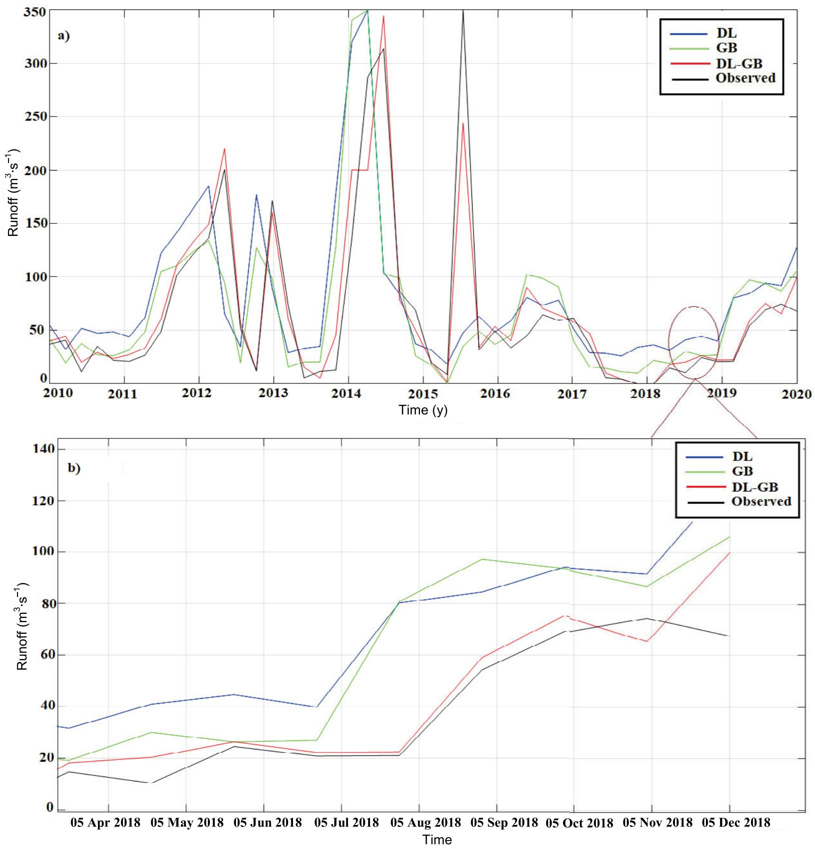

Fig. 3. The performance of the new hybrid deep learning gradient boosting (DL-GB) model via DL and GB in daily rainfall-runoff (R-R) simulation: a) main, b) in detail; source: own study

Table 1. The performance of the new hybrid deep learning gradient boosting (DL-GB) model in multistep-ahead forecasting

Model	DL				GB				DL-GB			
	R^2		*RMSE*		R^2		*RMSE*		R^2		*RMSE*	
Output	**train**	**verify**	**train**	**verify**	**train**	**verify**	**train**	**verify**	**train**	**verify**	**train**	**verify**
Q_{t+1}	0.65	0.60	0.03	0.0.3	0.61	0.59	0.04	0.03	0.88	0.80	0.02	0.01
Q_{t+4}	0.59	0.49	0.04	0.05	0.59	0.55	0.05	0.04	0.80	0.75	0.03	0.02
Q_{t+7}	0.51	0.41	0.06	0.07	0.50	0.48	0.07	0.06	0.75	0.70	0.04	0.03

Explanations: R^2 = determination coefficient, *RMSE* = root mean square error, Q_{t+1} = runoff at the single-step-ahead, Q_{t+4} = runoff at the 4th time step ahead, Q_{t+7} = runoff at the 7th time step ahead.
Source: own study.

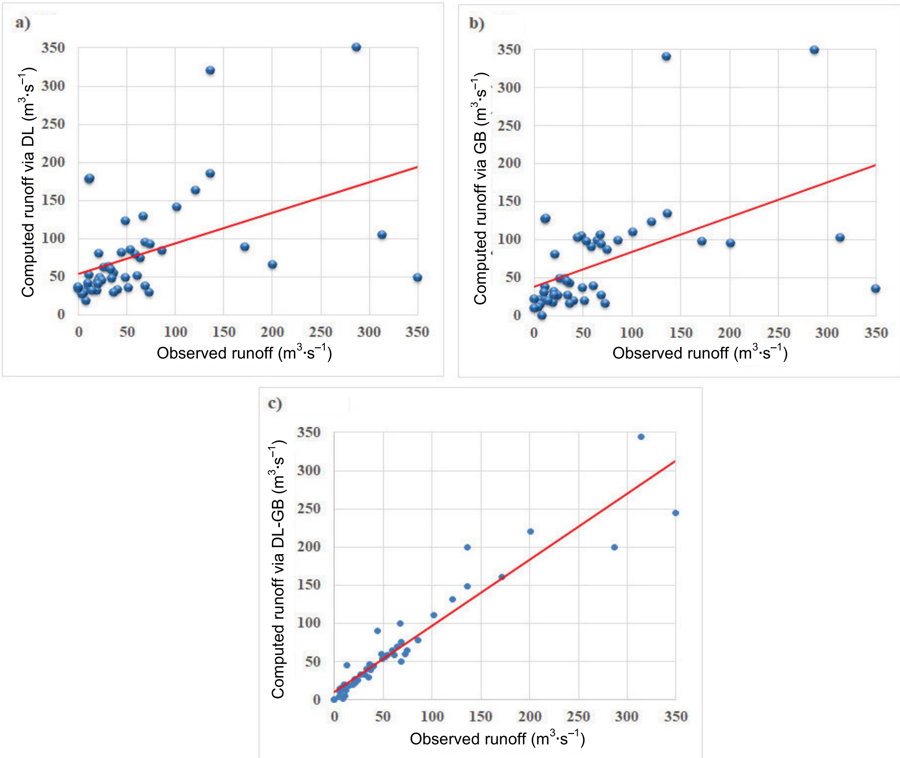

Fig. 4. The scatter plots of the observed daily runoff versus computed models: a) deep learning (DL), b) gradient boosting (GB), c) hybrid deep learning gradient boosting (DL-GB); source: own study

DL's inherent ability to capture intricate temporal dependencies and nonlinear patterns in time series data makes it well-suited for multistep forecasting. Its deep architecture enables it to learn complex relationships within the data, ensuring it can capture a wide range of potential future trajectories. When integrated with GB, the hybrid model gains the ensemble advantage, where the predictions of multiple simpler models are combined for improved accuracy. In the context of multistep forecasting, this translates into a more robust predictive performance. GB excels in capturing the higher-level patterns and trends across the forecast horizon, thus contributing to a smoother and more accurate prediction sequence. The hybrid DL-GB model's strength lies in striking a balance between capturing intricate short-term dependencies (DL's forte) and effectively modelling long-term trends (GB's strength). This synergy ensures that the model performs well in scenarios where accurate predictions across multiple time steps are crucial. However, it is essential to consider that the success of the hybrid DL-GB model in multistep forecasting depends on effective hyperparameter tuning and careful model architecture design. Ensuring the right number of layers and nodes, selecting appropriate activation functions, and tuning learning rates are some of the key aspects that influence its performance.

In the domain of R-R simulation, the challenge of multistep-ahead forecasting presents a unique conundrum due to the nonlinear growth of errors across the forecast horizon. As we project further into the future, even minor inaccuracies in the initial predictions can compound, resulting in increasingly skewed and unreliable forecasts. This nonlinear error propagation poses a significant hurdle in maintaining accurate predictions over extended time frames. Traditionally, existing models, including standalone DL and GB models, tend to struggle when it comes to multistep forecasting. As the forecast horizon extends, the complexities of capturing intricate temporal dependencies and accounting for evolving hydrological conditions become more pronounced. Consequently, the accuracy of these models progressively diminishes, leading to less reliable predictions over time. However, the introduction of the novel hybrid DL-GB model marks a turning point in tackling this challenge. By combining DL's capacity to uncover intricate patterns and dependencies with GB's prowess in ensemble learning, the hybrid model exhibits a unique resilience in the face of nonlinear error growth. DL's deep architecture excels in capturing short-term intricacies, while GB's ensemble approach enhances the model's ability to capture long-term trends, thus effectively addressing both ends of the forecast spectrum. In practical application, this hybrid approach demonstrates impressive performance in multi-step forecasting for R-R simulation. The model's capacity to mitigate the nonlinear error amplification, coupled with its adaptability to both short-term volatility and long-term trends, empowers it to outshine traditional standalone models. By maintaining accuracy across extended forecast horizons, the hybrid DL-GB model holds significant promise for improving the reliability of R-R simulation under complex and dynamic hydrological scenarios.

CONCLUSIONS

Accurate modelling of rainfall-runoff (R-R) processes holds undeniable significance for effective water resource management and environmental planning. Recognising the complexities inherent in this dynamic system, we introduce a pioneering solution – the hybrid deep learning gradient boosting (DL-GB) model. By synergising the capabilities of DL and GB, we address the limitations that each method faces independently. Particularly notable is the model's adeptness in multi-step-ahead forecasting, where the nonlinear amplification of errors presents a challenge. The hybrid DL-GB model triumphs in this arena. It harnesses DL's adeptness in uncovering intricate patterns and dependencies, complemented by GB's ensemble learning, which excels in capturing longer-term trends. This unique combination effectively bridges the deficits of DL and GB, resulting in improved forecasting accuracy. The hybrid DL-GB model adeptly adapts to both low and large input dataset volumes. It mitigates issues related to limited data by employing GB to aggregate weak learners, effectively capturing signals from small datasets. Simultaneously, the DL component, particularly long short-term memory (LSTM) networks, excels at extracting complex temporal patterns from larger datasets. This synergy ensures robust performance across varying data sizes in rainfall-runoff simulation. In effect, our hybrid model transcends the limitations of standalone DL and GB techniques, offering a holistic and robust solution for R-R simulation. This approach not only enhances the reliability of predictions but also paves the way for more informed decisions in water resource management and planning scenarios, marking a significant advancement in hydrological modelling.

For future studies, it is recommended to emphasise the significance of preprocessing raw data in the field of R-R modelling. Investigating the impact of preprocessing techniques on model performance could provide valuable insights into how data preparation influences predictive accuracy. This exploration could involve assessing various preprocessing methods such as normalisation, scaling, outlier removal, and imputation, and analysing their effects on the robustness and reliability of the modelling results. Understanding the role of preprocessing in enhancing data quality and model outcomes could potentially lead to more accurate and dependable rainfall-runoff predictions.

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