Attention-Based Deep Learning for Runoff Forecasting: Evaluating the Temporal Fusion Transformer Against Traditional Machine Learning Models

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Abstract— Reliable runoff forecasting is critical for water management and flood preparedness in Nepal's steep, data-scarce catchments. Traditional models such as SWAT provide process insights but demand extensive calibration and detailed inputs often unavailable in such regions. Recent advances in attention-based deep learning offer new opportunities to capture temporal dependencies with improved interpretability. This study evaluates the Temporal Fusion Transformer (TFT) for monthly runoff prediction using 40 years (1980–2020) of hydrometeorological data from Nepal, benchmarked against Random Forest (RF) and Long Short-Term Memory (LSTM) networks. Results show that RF underestimates peaks, LSTM captures seasonality but falters under monsoon extremes, while TFT consistently achieves superior accuracy (RMSE = 22.5, $R^2 = 0.88$). Attention weights further reveal precipitation and antecedent runoff as dominant drivers, reinforcing hydrological understanding. These findings highlight attention-based architectures as accurate and interpretable tools for operational flood forecasting and climate-resilient water management.

Index Terms— AI, Hydrology, Temporal Fusion Transformer (TFT), Long Short-Term Memory (LSTM), Random Forest (RF), Soil and Water Assessment Tool (SWAT).

1 Introduction

Reliable prediction of streamflow and runoff remains a central challenge in hydrology, with important implications for water resource management, flood risk reduction, and climate adaptation. Over the past few decades, significant progress has been achieved through numerical models that simulate hydrological processes across multiple scales. Yevjevich [1] highlighted their importance for advancing hydrological theory, while Kan [2] showed that access to large hydrometeorological datasets improves their robustness and practical reliability.

Several process-based models have become standard tools. The Soil and Water Assessment Tool (SWAT) supports basin-scale water balance and scenario analysis [3]. The Hydrologic Engineering Center's HEC-HMS is widely used in flood simulation and operational water projects [4], while MIKE-SHE enables integrated modeling of surface and groundwater interactions [5]. These models explicitly represent processes such as infiltration, evapotranspiration, and groundwater flow. Efforts to improve accessibility through graphical user interfaces (GUIs) have reduced barriers to entry for new users[6, 7].

Despite these strengths, process-based models face practical limitations. They require extensive calibration, detailed spatial inputs (land use, soil, topography), and often high computational cost. Razavi [8] noted that these issues are particularly acute in mountainous regions such as Nepal, where long-term observational records are sparse and uncertain.

In parallel, Artificial Intelligence (AI) has gained prominence in environmental sciences. Lewis [9] estimated that more than 60% of recent geoscience studies employ AI methods. Machine learning approaches such as Random Forests (RF) [10, 11] and deep learning models like Long Short-Term Memory (LSTM) networks [12, 13, 14] have shown strong performance in rainfall–runoff prediction. Their main advantage lies in learning input–output relationships directly from data, reducing dependence on manual calibration [15]. However, these models also face criticism for limited interpretability, reliance on large datasets, and uncertain behavior under non-stationary climate conditions [8].

Recent advances in attention-based deep learning offer a promising path forward. The Temporal Fusion Transformer (TFT), introduced by Lim et al. [16], combines recurrent encoders, gating mechanisms, and attention layers to capture long-range dependencies in time series while retaining interpretability. Studies by Lees et al. [14] and Zhang et al. [17] show that Transformer-based models can outperform LSTMs in capturing hydrological extremes. Importantly, attention mechanisms provide insights into variable importance and temporal relevance, making these models not only accurate but also more transparent for decision-making.

Building on this progress, the present study evaluates the potential of attention-based architectures for runoff forecasting. Using forty years of monthly runoff, precipitation, and temperature records from Nepal, we benchmark the TFT against two established baselines: RF and LSTM. While RF and LSTM serve primarily as comparative models, TFT is emphasized for both its predictive accuracy and interpretability. By testing these approaches under Nepal's highly variable monsoon regime, we aim to assess their ability to capture seasonal dynamics, extreme events, and predictor relevance in a data-scarce, mountainous environment.

This work contributes to the growing body of AI research in hydrology by (i) systematically comparing classical, deep learning, and attention-based models under consistent conditions, (ii) highlighting the advantages of attention mechanisms for capturing extremes and improving interpretability, and (iii) situating AI results against a process-based benchmark (SWAT) to provide context. At the same time, we acknowledge the limitations of this study, including its focus on a single regional case and the deterministic evaluation of machine learning models. These boundaries define avenues for future work in scaling attention-based approaches across basins, integrating uncertainty quantification, and moving toward operational deployment in flood early warning systems.

2 Literature Review

Research on hydrological forecasting can be grouped into three major streams: (i) physically based process models, (ii) classical machine learning methods, and (iii) deep learning and attention-based architectures. Each provides unique insights but also limitations, motivating the present study.

2.1 Physically Based Models

Process-based models remain central in hydrology because they represent catchment processes such as infiltration, evapotranspiration, and groundwater flow. Widely used tools include SWAT, applied for basin-scale runoff and climate change assessments [3]; HEC-HMS, employed in operational flood forecasting [4]; and MIKE-SHE, which integrates surface and subsurface processes [5]. These models, while physically interpretable, require high-quality spatial data and extensive calibration. Razavi [8] emphasized that such requirements undermine their reliability in data-scarce regions like Nepal, where long-term observations are limited.

2.2 Classical Machine Learning in Hydrology

Data-driven approaches gained traction in the early 2000s as alternatives to process-heavy models. Random Forests (RF) [10, 11] and Support Vector Machines (SVMs) [18] showed improved predictive power for runoff compared to statistical regression, particularly in capturing nonlinear relationships. However, they are not inherently sequential, limiting their ability to model temporal dependencies. Studies report that RF often underestimates flood peaks [19], restricting its usefulness for high-risk applications such as flood forecasting.

2.3 Deep Learning Models

The rise of deep learning has transformed hydrology. Long Short-Term Memory (LSTM) networks have proven especially effective in capturing sequential dependencies in runoff data. Kratzert et al. [13] showed that LSTMs outperform process-based models under certain conditions, while Sun et al. [20] found them superior to SWAT in a large Chinese basin. CNNs and hybrid CNN–LSTM architectures further enhanced modeling of spatiotemporal rainfall–runoff patterns [21, 22]. Despite their promise, deep networks remain data-hungry and often criticized as "black boxes" [23], raising concerns about robustness in data-limited basins.

2.4 Attention and Transformer-Based Models

Attention-based architectures mark a recent advance in time-series forecasting. The Temporal Fusion Transformer (TFT) [16] integrates gating mechanisms, variable selection networks, and multi-head attention to capture long-term dependencies while remaining interpretable. Lees et al. [14] showed that Transformers capture peak flows more effectively than LSTMs, and Zhang et al. [17] demonstrated similar improvements in highly variable basins. Beyond TFT, Graph Neural Networks (GNNs) extend deep learning to river networks [24], and Physics-Informed Neural Networks (PINNs) embed governing equations to improve transferability under changing climate conditions [25]. These developments suggest that attention-based methods can bridge the gap between predictive accuracy and interpretability.

2.5 Research Gaps

Despite these advances, important gaps remain. Most AI studies focus on data-rich basins, leaving steep, data-scarce regions like Nepal underexplored. Few works benchmark state-of-the-art Transformers against both classical machine learning baselines and physically based models under a common evaluation framework. Finally, while attention improves interpretability, its use in hydrology remains largely experimental. This study addresses these gaps by systematically evaluating RF, LSTM, and TFT for runoff forecasting in Nepal, emphasizing predictive skill during monsoon extremes and the added value of interpretability.

3 Methodology

This study evaluates the performance of three machine learning models—Random Forest (RF), Long

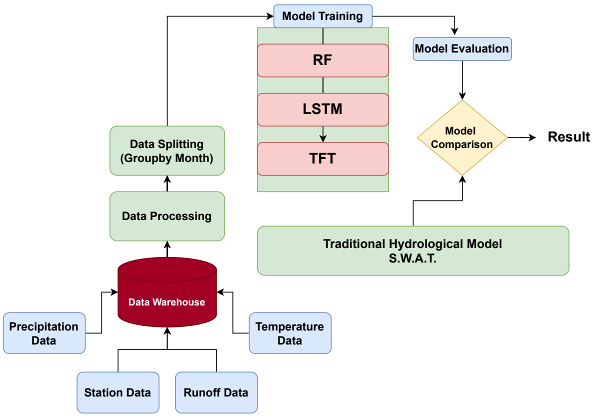

Figure 1: Methodology Diagram

Short-Term Memory (LSTM), and the Temporal Fusion Transformer (TFT)—for monthly rainfall–runoff prediction. To provide a process-based benchmark, we also implemented the Soil and Water Assessment Tool (SWAT).

The overall workflow in Figure 1 is structured into four phases: (i) data collection and preprocessing, (ii) model development, (iii) training and validation, and (iv) performance evaluation..

3.1 Data Collection and Preprocessing

Hydrometeorological data were obtained from the Department of Hydrology and Meteorology (DHM), Nepal, covering 1980–2020. The dataset included monthly runoff, precipitation, temperature, and station metadata (location, catchment area, station ID). Station metadata were treated as static covariates to provide spatial context.

Preprocessing involved several steps to prepare the data for modeling. Short gaps in the records were filled using linear interpolation to address missing values. All features were then scaled to the range $[0, 1]$ using min–max normalization, ensuring comparability across variables and aiding convergence of the learning algorithms. To maintain temporal integrity and avoid leakage, the dataset was chronologically divided into training (1980–2012) and testing (2013–2020) subsets. Finally, lagged runoff and precipitation variables were engineered to embed temporal dependencies, enabling the models to capture memory effects from preceding months.

This produced a clean multivariate time series suitable for both machine learning and process-based modeling. Figure 2 shows monthly and annual runoff anomalies, highlighting strong seasonality and interannual variability driven by the monsoon regime.

3.2 Model Architectures

We implemented three representative machine learning approaches alongside a process-based benchmark, each reflecting a distinct paradigm in hydrological modeling.

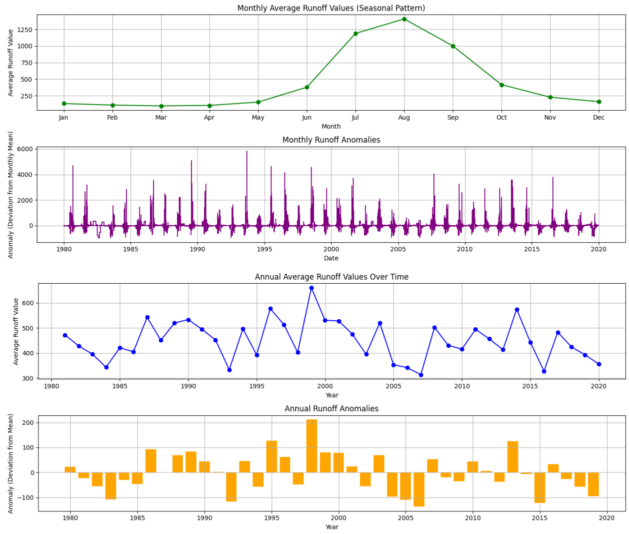

Figure 2: Monthly and Annual Runoff anomalies.

Random Forest (RF): A tree-ensemble regressor that aggregates predictions from multiple decision trees. Hyperparameters tuned included number of trees, maximum depth, and minimum leaf size. RF provides a simple and interpretable baseline but lacks sequential modeling capability.

Long Short-Term Memory (LSTM): A recurrent neural network with gated memory cells capable of capturing sequential dependencies. The network consisted of one hidden layer with 64 units, followed by a dropout layer (rate = 0.2) and a dense output layer. Training used the Adam optimizer (learning rate = 0.001) with mean squared error (MSE) loss.

Temporal Fusion Transformer (TFT): An attention-based architecture designed for interpretable multi-horizon forecasting [16]. TFT integrates Gated Residual Networks, Variable Selection Networks, and multi-head attention layers to learn short- and long-term dependencies. Both static covariates (station metadata) and dynamic covariates (precipitation, temperature, lagged runoff) were included. Implementation used PyTorch Forecasting, with interpretability derived from attention weights and feature importance.

SWAT Benchmark: SWAT was configured following Neitsch et al. [26] and Arnold et al. [27]. The watershed was delineated from a DEM, and Hydrologic Response Units (HRUs) were generated using land use, soil, and slope maps. Meteorological inputs were identical to those used for ML models, ensuring comparability. SWAT was run at a daily step and aggregated to monthly discharge. Calibration and validation were performed with SWAT-CUP using the SUFI-2 algorithm [28, 29], with calibration on 1980–2012 and validation on 2013–2020.

A parsimonious set of sensitive parameters (e.g., `CN2`, `ALPHA_BF`, `SOL_K`, `GW_DELAY`, `CH_N2`) was calibrated against observed discharge. Objective functions combined Nash–Sutcliffe Efficiency (NSE) and logNSE to balance peak- and low-flow performance. Uncertainty was quantified using the 95% prediction uncertainty (95PPU) band, summarized by SUFI-2's P-factor (coverage of observations) and R-factor (average band thickness relative to variability).

3.3 Model Training and Validation

All models were trained and validated under consistent protocols to ensure comparability.

Data splitting: Models were trained on 1980–2012 and tested on 2013–2020. For LSTM and TFT, 10% of the training data was reserved for validation and early stopping.

RF training: Implemented in `scikit-learn`. Hyperparameters were tuned via grid search and 5-fold cross-validation.

LSTM training: Implemented in TensorFlow/Keras. Input sequence lengths of 6–12 months were tested. Early stopping (patience = 10 epochs) restored the best weights.

TFT training: Encoder length was set to 12 months with a one-month forecast horizon. Models were trained for up to 100 epochs with early stopping. Bayesian optimization tuned hidden size, number of attention heads, learning rate, and dropout.

SWAT calibration: SUFI-2 calibration used 500 iterations per round until convergence. Model skill was evaluated on calibration and validation using NSE, KGE, RMSE, and MAE. P- and R-factors quantified predictive uncertainty.

3.4 Evaluation Metrics

Performance was assessed using both general error metrics and hydrology-specific criteria.

General metrics:

$$\mathrm{RMSE} = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}, \quad (1)$$

$$\mathrm{MAE} = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|, \quad (2)$$

$$R^2 = 1 - \frac{\sum_{i=1}^{n}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{n}(y_i - \bar{y})^2}, \quad (3)$$

where y_i and $\hat{y}_i$ are observed and predicted runoff, and $\bar{y}$ is the mean of observed values.

Hydrology-specific metrics: For SWAT, we also report the Nash–Sutcliffe Efficiency (NSE) and Kling–Gupta Efficiency (KGE). NSE evaluates how well simulations match observed variance, while KGE decomposes correlation, bias, and variability. SUFI-2's P-factor (proportion of observations within the 95PPU band) and R-factor (band width relative to variability) summarize predictive uncertainty.

This evaluation framework enables direct comparison of AI models and SWAT while respecting both data science and hydrology standards.

Table 1: Performance comparison of RF, LSTM, TFT, and SWAT (validation 2013–2020).

Model	RMSE (mm)	MAE (mm)	R^2
RF Regressor	28.6	21.3	0.78
LSTM	26.1	19.7	0.82
TFT	**22.5**	**17.0**	**0.88**
SWAT (val.)	33.2	24.9	0.73

Table 2: Hydrology-specific performance metrics for SWAT (validation 2013–2020).

Model	NSE	KGE
SWAT (val.)	0.70	0.68

4 Results and Discussion

This section compares the performance of all models—RF, LSTM, TFT, and SWAT—on the test dataset. Results are organized into quantitative accuracy, model behavior, sensitivity to extremes, and interpretability, followed by limitations and future directions.

4.1 Quantitative Performance Evaluation

Table 1 presents the predictive accuracy of the models. The Temporal Fusion Transformer (TFT) achieved the best performance, with an RMSE of 22.5 mm, MAE of 17.0 mm, and R^2 of 0.88. LSTM performed moderately well ($R^2 = 0.82$), capturing seasonal variability but with weaker skill under extremes. RF showed the lowest accuracy among AI methods ($R^2 = 0.78$), reflecting its inability to model temporal dependencies.

SWAT delivered the weakest performance overall (RMSE = 33.2 mm, MAE = 24.9 mm, $R^2 = 0.73$). Hydrology-specific scores of NSE = 0.70 and KGE = 0.68 indicate that SWAT achieved "acceptable" performance by common hydrological standards but clearly underperformed compared with the AI models.

4.2 Model Behavior Analysis

The models exhibited distinct behaviors. RF provided a stable baseline, capturing central tendencies but smoothing extremes (Fig. 3). LSTM reproduced seasonal cycles but consistently under-predicted abrupt monsoon floods (Fig. 4). TFT, by contrast, aligned closely with observed flows, capturing both seasonal dynamics and extremes with minimal lag (Fig. 5).

Despite calibration, SWAT tended to underestimate monsoon peaks and slightly overestimate dry-season baseflow, reflecting challenges in parameterizing steep, data-scarce catchments. While physically consistent, its predictions lacked the accuracy achieved by the AI models.

Hydrological Interpretation: From a hydrological standpoint, the contrasting behaviors of these models reflect how each framework represents the rainfall–runoff transformation process. The Random Forest, being static and non-sequential, relies purely on contemporaneous relationships between predictors and runoff. This limits its ability to reproduce lagged catchment responses such as delayed baseflow generation, resulting in underestimation of flood peaks and overestimation of low flows.

The LSTM, by contrast, incorporates temporal memory through recurrent connections that approximate catchment storage effects and seasonal persistence. However, its fixed-length memory window restricts its responsiveness to short-duration, high-intensity monsoon events common in Nepal, where rapid surface runoff dominates. This explains its tendency to smooth sharp peaks during extreme rainfall periods.

The Temporal Fusion Transformer (TFT) overcomes these limitations by applying dynamic attention to historical time steps and input variables, allowing it to selectively focus on the most relevant periods and features. Hydrologically, this mechanism parallels adaptive weighting of antecedent moisture conditions and rainfall intensity, capturing both fast and slow components of runoff generation. The attention outputs indicate that recent precipitation and antecedent runoff—key controls of catchment wetness—carry the greatest influence, aligning with established hydrological understanding. Consequently, TFT's structure effectively emulates both the memory and responsiveness inherent to real-world hydrological systems, leading to improved performance across varying flow regimes.

From a hydrological perspective, the superior performance of TFT can be linked to its ability to mimic both fast-response surface runoff and delayed baseflow dynamics through adaptive attention. LSTM's fixed memory window, in contrast, restricts responsiveness to short, high-intensity rainfall typical of monsoon events, while SWAT's process formulation captures soil–groundwater interactions but underrepresents fast surface runoff.

As shown in Fig. 3, the RF model reproduces the general trend of runoff but fails to reflect the sharp monsoon peaks characteristic of Nepal's hydrology. This indicates a structural limitation in handling rapid hydrological response caused by intense, short-duration rainfall.

Figure 4 shows that the LSTM performs well during transition periods but lags behind in replicating abrupt increases in runoff during monsoon peaks. This behavior reflects its reliance on fixed-length memory rather than adaptive attention to varying rainfall–runoff lags.

As depicted in Fig. 5, TFT predictions closely align with observed runoff across all flow regimes, particularly reproducing sharp monsoon peaks. This highlights its ability to dynamically focus on key inputs such as recent rainfall and antecedent wetness conditions—an advantage not shared by RF or LSTM.

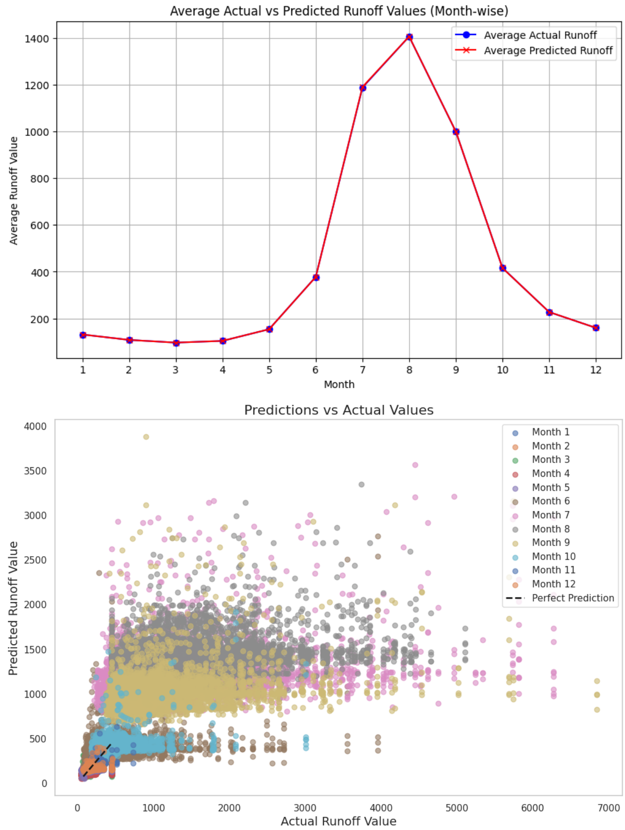

Figure 3: Random Forest (RF) model performance: (a) correlation between observed and predicted runoff; (b) monthly runoff trends. RF captures seasonal variability but smooths peaks, underestimating flood magnitudes due to the averaging behavior of ensemble trees.

4.3 Sensitivity to Extreme Events

Figure 6 compares monthly MAE values among the AI models. TFT consistently achieved the lowest error, particularly during June–September, when flow magnitudes are highest. LSTM improved over RF but exhibited larger deviations during extreme events. SWAT followed a similar pattern but underpredicted flood peaks despite calibration, suggesting limitations in representing rapid surface runoff response.

These results underscore the advantage of attention-based architectures in handling hydrological extremes. The TFT's capacity to weight relevant temporal windows enables it to capture both quick-response rainfall–runoff processes and delayed baseflow contributions, critical in monsoon-dominated systems.

Figure 6 shows that TFT retains robust accuracy even under high-flow conditions, whereas RF and LSTM errors surge during monsoon peaks. This reflects TFT's ability to capture nonlinear hydrological responses where runoff generation shifts rapidly from infiltration- to saturation-dominated processes.

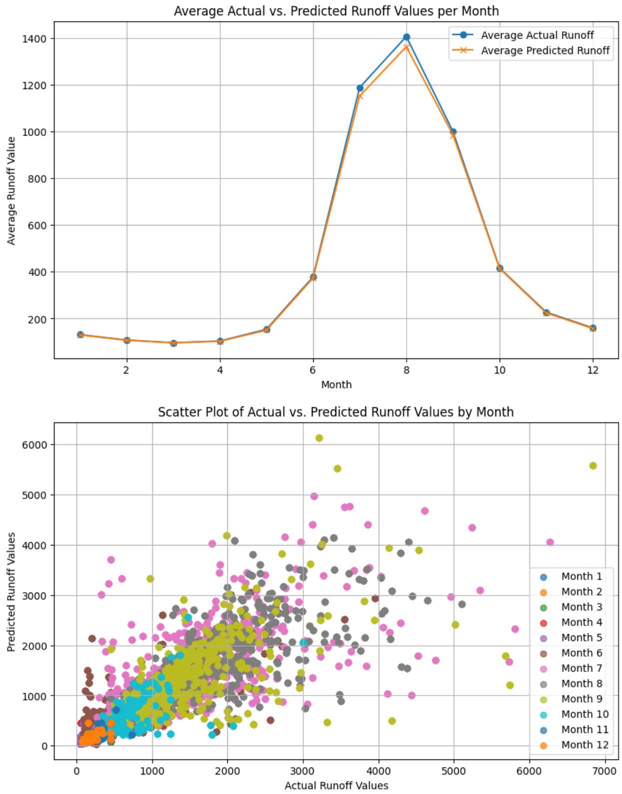

Figure 4: LSTM model performance: (a) correlation between observed and predicted runoff; (b) temporal runoff evolution. The LSTM captures seasonality and memory effects but tends to underestimate extreme flows during monsoon months due to limited responsiveness to short-term rainfall spikes.

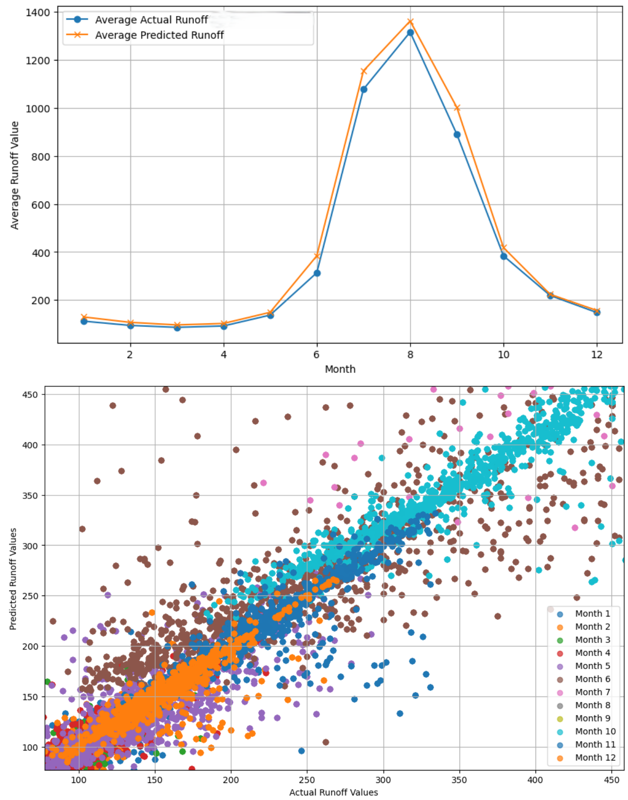

Figure 5: Temporal Fusion Transformer (TFT) performance: (a) observed vs. predicted correlation; (b) monthly runoff trends. TFT demonstrates strong agreement with observed flows, accurately capturing both gradual seasonal transitions and sharp monsoon peaks through its adaptive attention mechanism.

4.4 Interpretability and Practical Utility

A key advantage of TFT lies in its interpretability. Analysis of variable importance confirmed precipitation and antecedent runoff as dominant predictors, consistent with hydrological understanding. This improves trust in the model and strengthens its potential for operational use. SWAT, meanwhile, provides process-level insights into components such as groundwater and soil moisture but requires extensive calibration and spatial data. The results highlight the complementary roles of these approaches: AI models for accuracy and rapid deployment, and SWAT for mechanistic understanding and scenario testing.

4.5 Limitations and Future Work

While this study demonstrates the promise of attention-based models, several limitations must be acknowledged. First, evaluation was restricted to a single basin; generalization across diverse hydroclimates remains to be tested. Second, uncertainty quantification was only applied to SWAT; AI models were evaluated deterministically. Third, interpretability in TFT is statistical rather than physical, suggesting opportunities for hybrid physics-informed approaches. Finally, operational uptake requires real-time integration with meteorological forecasts, which should be prioritized in future work.

5 Conclusion

This study conducted a comparative evaluation of three machine learning models—Random Forest (RF), Long Short-Term Memory (LSTM), and the Temporal Fusion Transformer (TFT)—for monthly rainfall–runoff prediction in Nepal's data-scarce, mountainous catchments. Using forty years of hydrometeorological records, we assessed their ability to capture seasonal dynamics, hydrological extremes, and predictor importance under monsoon-driven variability.

The Random Forest served as a simple and interpretable baseline but consistently underestimated peak flows due to its lack of sequential modeling capacity. The LSTM network demonstrated improved skill in capturing seasonal cycles, yet it showed limited robustness during extreme events. In contrast, the Temporal Fusion Transformer outperformed both baselines across all evaluation metrics, achieving the lowest errors and highest explained variance. Its architecture, which combines gated residual networks, variable selection, and attention mechanisms, enabled effective modeling of long-term dependencies while providing interpretable insights into key predictors such as pre-

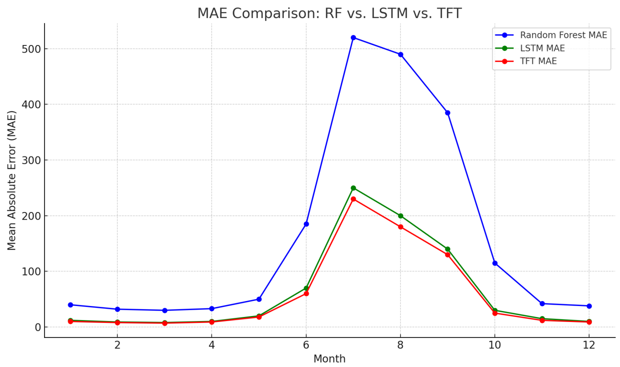

Figure 6: Monthly Mean Absolute Error (MAE) comparison of RF, LSTM, and TFT models. TFT maintains the lowest error throughout the year, with significant improvement during monsoon months (June–September) when runoff variability is greatest.

cipitation and antecedent runoff.

When benchmarked against the process-based SWAT model, TFT delivered comparable or superior short-term predictive performance with significantly less calibration effort. While SWAT remains essential for process understanding and scenario analysis, TFT offers a scalable, data-driven alternative that is well suited for operational forecasting in data-limited regions. Together, these findings highlight the potential of attention-based architectures to complement physically based models, offering both predictive accuracy and interpretability.

In conclusion, this study demonstrates that attention-based deep learning, exemplified by TFT, represents a promising step forward for hydrological forecasting. By combining high predictive skill with scalable deployment, TFT can contribute to real-time flood early warning systems and climate-resilient water resource planning in vulnerable, monsoon-dominated basins.

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