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Multi-Machine Learning Ensemble Regionalization of Hydrological Parameters for Enhances Flood Prediction in Ungauged Mountainous Catchments

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Abstract:

Machine learning-based parameter regionalization is an important method for flood prediction in ungauged mountainous catchments. However, single machine learning parameter regionalization often exhibits limitations in prediction accuracy and robustness. Therefore, this study proposes a multi-machine learning ensemble regionalization method that integrates Gradient Boosting Machine (GBM), K-Nearest Neighbors (KNN), and Extremely Randomized Trees (ERT) methods (GBM-KNN-ERT) to regionalize the sensitive parameters of the Topography-Based Subsurface Storm Flow (Top-SSF) model. Validated across 80 mountainous catchments in southwestern China, the GBM-KNN-ERT method demonstrates superior performance with 90% of ungauged catchments achieving the Nash-Sutcliffe Efficiency (NSE) above 0.9, representing a 67.44% improvement over single machine learning parameter regionalization. Notably, the GBM-KNN-ERT method shows improved robustness to climate change and changes in the number of donor catchments compared to other regionalization methods. An optimal balance between accuracy and computational efficiency was achieved using 20-40 high quality donor catchments (NSE greater than 0.85). This study provides systematic evidence that multi-machine learning ensemble can effectively address regionalization challenges in ungauged mountainous regions, offering a reliable tool for water resource management and flood disaster mitigation.

Keywords: Flood forecasting; Regionalization; Ungauged mountainous catchments; Top-SSF model;

Highlights:

1. Proposes a novel multi-machine learning ensemble regionalization method
2. The GBM-KNN-ERT method demonstrate superior performance compared to other methods.
3. The GBM-KNN-ERT method exhibits greater stability under climate change.

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

1. Introduction

Floods in mountainous catchments pose a significant threat to human safety and property, particularly in regions lacking sufficient observational data (Luo et al., 2015; Zhai et al., 2018). While hydrological models like the Topography-Based Subsurface Storm Flow (Top-SSF) mode (Li et al., 2024) offer promising simulation capabilities, their application in ungauged catchments is severely limited by the absence of calibration data (Choi et al., 2023; Liu et al., 2018). Effective parameter regionalization methods are therefore essential for transferring hydrological knowledge from gauged to ungauged regions, enabling reliable flood prediction in ungauged mountainous catchment (Garambois et al., 2015; Ragettli et al., 2017; Xu et al., 2018).

Parameter regionalization is a crucial method for flood prediction in ungauged catchments (Arsenault et al., 2022; Guo et al., 2021; Kratzert et al., 2019; Zhang et al., 2020). Compared to purely data-driven methods, parameter regionalization offers enhanced physical interpretability (Nearing et al., 2024; Tang et al., 2023; Zhang et al., 2024). Existing parameter regionalization methods can be broadly classified into three categories: similarity-based, hydrological signatures-based, and regression-based (Arsenault et al., 2019; Wu et al., 2022). Similarity-based methods rely on the assumption that catchments with similar characteristics exhibit similar hydrological responses, considering spatial proximity (Arsenault et al., 2019; Pugliese et al., 2018; Yang et al., 2018) and physical similarity (similar climatic and land cover conditions have similar hydrological characteristics) (Kanishka et al., 2017; Papageorgaki et al., 2016). The hydrological-signatures-based methods forms a regression relationship

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

between hydrological signatures (quantitative metrics that describe statistical or dynamic properties of streamflow) and catchment descriptors (McMillan, 2021; Zhang et al., 2018). Regression-based methods, which directly link hydrological model parameters to catchment descriptors, are widely used due to their simplicity and computational efficiency (Guo et al., 2021; Kratzert et al., 2019; Song et al., 2022; Wu et al., 2022). However, the performance of regression-based methods is frequently constrained by the inherent nonlinearity in the relationships between model parameters and catchment descriptors, coupled with the difficulty in adequately capturing spatial heterogeneity, especially within complex mountainous terrain (Wu et al., 2022).

Recent advances in machine learning offer potential solutions by capturing nonlinear patterns in high-dimensional data. Such as Decision Tree (DT), Extremely Randomized Trees (ERT), Gradient Boosting Machine (GBM), K-Nearest Neighbor (KNN), Random Forest (RF), and Support Vector Machines (SVM) have shown promise in parameter regionalization (Golian et al., 2021; Song et al., 2022). However, existing machine learning-based parameter regionalization studies predominantly focus on runoff prediction at coarser temporal scales (daily or monthly) (Li et al., 2022; Wu et al., 2022), leaving a significant gap in high-resolution (hourly or sub-hourly) flood prediction in ungauged mountainous catchments. Moreover, these studies often rely on single machine learning methods to estimate all hydrological model parameters (Golian et al., 2021; Song et al., 2022; Wu et al., 2022). Given that different machine learning methods operate on distinct principles (Jordan et al., 2015; Zounemat-Kermani et al., 2021) and hydrological model parameters represent diverse hydrological processes (Li

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

et al., 2024), a single machine learning method may not adequately capture the complexity of model parameter estimation (Golian et al., 2021; Wu et al., 2022). Therefore, exploring the multi-machine learning ensemble methods is essential to improve the accuracy of high-resolution flood prediction in ungauged mountainous catchments.

Southwest China's mountainous regions are particularly vulnerable to frequent floods, leading to ecosystem degradation through habitat disruption and biodiversity loss (Gan et al., 2018). The abundance of ungauged catchments in this region poses a significant challenge to reliable flood prediction. To address this critical issue, we systematically evaluate the performance of a novel multi-machine learning ensemble method for regionalizing Top-SSF model parameters across 80 representative catchments (mean area: 1,586 km²) in Southwest China. By assessing ensemble method robustness under climate change and with varying donor catchment configurations, this study aims to significantly enhance flood prediction accuracy in ungauged mountainous catchments, contributing to improved ecosystem resilience, enhanced human safety, and more effective water resource management in the face of escalating climatic pressures.

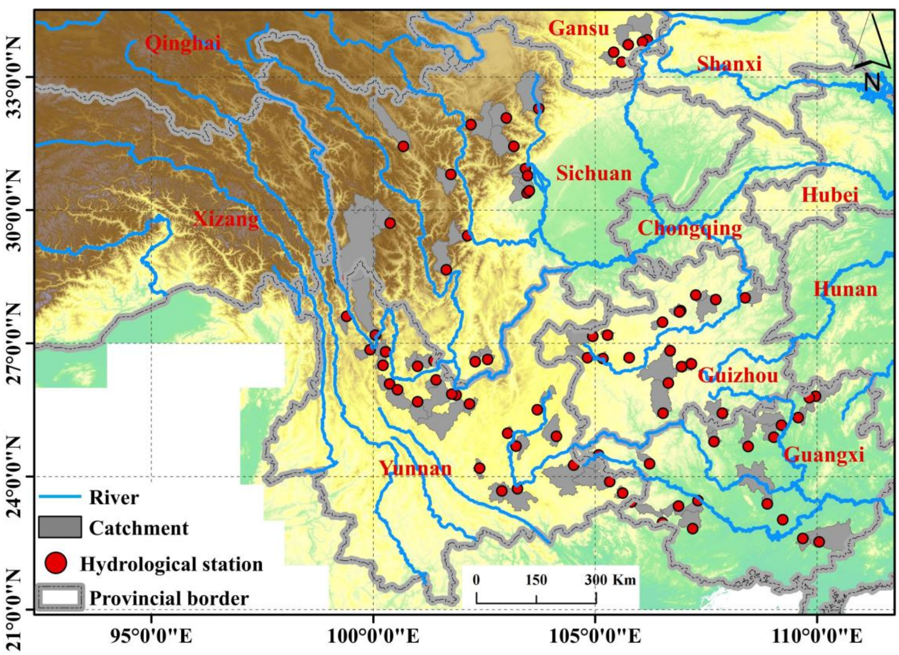
2. Study area and datasets

2.1. Study area

This study investigated 80 mountainous catchments in Southwestern China, encompassing Sichuan, Yunnan, Guangxi, Guizhou, and Chongqing provinces (Fig. 1). This region exhibits diverse climatic zones, including subtropical monsoon, plateau

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

mountain, and tropical monsoon climates. The selected catchments have an average area of 1,586 km², with elevations ranging from 63 to 6,284 meters. Mean annual temperature varies from 15 to 20°C, and annual precipitation ranges from 1,200 to 1,800 mm (Li et al., 2016), with approximately 80% of the annual precipitation occurring during summer and autumn, contributing to frequent flooding events (Cheng et al., 2019). These catchments are situated within a heavily forested region, the second largest in China (Hua et al., 2018), with forest cover ranging from 3% to 92% (mean: 51%), influencing evapotranspiration and runoff generation. Dominant soil types include purple soil (12.20%), yellow soil (11.39%), and red soil (9.52%), each with distinct hydrological properties. Soil data were obtained from the Resource and Environmental Science and Data Center of the Chinese Academy of Sciences (https://www.resdc.cn).



https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

Fig.1. Geographical distribution of the 80 gauged catchments used, with locations of hydrological stations (red points) and major rivers indicated.

2.2. Datasets

Hourly flood data (2015–2018) for 80 mountainous catchments in China were sourced from the Hydrological Bureau of the Ministry of Water Resources, through China's hydrologic yearbooks. Hourly rainfall data (2015–2018) were obtained from ground meteorological stations across China (http://en.weather.com.cn), providing crucial input for hydrological modelling. Additional meteorological variables, including temperature, wind speed, dewpoint temperature, and surface net solar radiation, were obtained from the ERA5 hourly dataset (1940–present) (Hersbach et al., 2023), ensuring comprehensive atmospheric forcing. Relative humidity was estimated using dewpoint temperature. Historical (1901–2021) and projected future (SSP585, 2022–2100) temperature and precipitation data for China, averaged from the EC-Earth3, GFDL-ESM4, and MRI-ESM2-0 models at 1 km resolution, were obtained from "A Big Earth Data Platform for Three Poles" to assess the impact of climate change (Ding et al., 2020) (http://poles.tpdc.ac.cn). Topographic data, including a 30-m resolution Digital Elevation Model (DEM), used for river network and topographic index derivation, were obtained from EARTHDATA and used for river network delineation and topographic index derivation (https://search.earthdata.nasa.gov/search). Forest cover data (30-m resolution) were sourced from the Global Forest Cover and Forest Change Map (https://www.noda.ac.cn/), providing information on vegetation characteristics. Bulk density (BD) data were derived from the Soil Database of China for Land Surface Modelling (Dai et al., 2013). Soil hydraulic parameters, specifically

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

saturated hydraulic conductivity (Ks_CH) for Clapp and Hornberger functions and the pore-connectivity parameter (L) for van Genuchten and Mualem functions, were acquired from the China Dataset of Soil Hydraulic Parameters Using Pedotransfer Functions for Land Surface Modeling (Shangguan et al., 2013).

Table 1. Model forcing data and catchment descriptors information.

Data type	Name	Unit	Function
Hydro-meteorology	Rainfall	mm	Input for hydrological model
	Flood	m^3/s	Used for model calibration (hourly resolution)
	Temperature	K	Input for hydrological model
	Surface pressure	Pa	
	Dewpoint temperature	K	
	wind speed	m/s	
	Surface net solar radiation	j/m^2	
	Relative humidity	%	
	1 km monthly precipitation (1901-2021)	mm	Multi-year surface average as catchment descriptors
	1 km monthly temperature (1901-2021)	℃	
	1 km monthly temperature (2022-2100, SSP5-8.5, EC-Earth3, GFDL-ESM4, MRI-ESM2-0)	℃	
	1 km monthly precipitation (2022-2100, SSP5-8.5, EC-Earth3, GFDL-ESM4, MRI-ESM2-0)	mm	
Soil characteristics	Soil bulk density (BD)	g/cm^3	Surface average as catchment descriptors
	Pore-connectivity parameter (L) for the van Genuchten and Mualem functions	-	
	Saturated hydraulic conductivity (Ks_CH) of the Clapp and Hornberger Functions	$cm\ d^{-1}$	
Topography	Forest cover (FC)	%	
	DEM	m	
	Topographic index	-	
	Slope	mm^{-1}	
	Catchment area	km^2	

3. Methodology

3.1. Hydrological model

The Top-SSF model, inheriting the straightforward structure, physical interpretability, and ease of parameter transferability from the original TOPMODE (Beven et al., 2021; Gao et al., 2018), consists of 15 parameters representing six key hydrological components: canopy interception, infiltration, evapotranspiration, unsaturated zone moisture transport, subsurface storm flow, and flow routing (Li et al.,

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

2024). In the Top-SSF model, flood can be comprised of four components: infiltration-excess overland flow, saturation-excess overland flow, subsurface storm flow, and groundwater discharge.

Infiltration-excess overland flow occurs when the rainfall intensity exceeds the infiltration capacity. In this study, infiltration is simulated using the Green-Ampt model. When surface ponding occurs, the infiltration rate is determined by solving the Green-Ampt equation iteratively, for which the Newton-Raphson method is employed. The infiltration rate (f_{in}) is given by：

$$f_{in} = -\frac{Ks(CD+F_{satrt})}{Szm(1-e^{(F_{satrt}/Szm)})} \quad (1)$$

where,$f_{in}$is the infiltration rate (m/h)； Ks is surface hydraulic conductivity (m/h)；CD is capillary drive (m);F_{satrt} is the initial cumulative infiltration (m);Szm is the maximum water storage capacity in the unsaturated zone (m).

Saturation excess overland flow occurs at computational cell i when the groundwater table depth, S_i is less than or equal to zero (i.e., $S_i \leq 0$, indicating the water table has reached the surface). It is calculated as:

$$r_{s,i} = max\{Suz_i - \max(S_i, 0)\,, 0\} \quad (2)$$

where, $r_{s,i}$ is the depth of saturation excess overland flow generated at cell i (m); Suz_i is the soil water storage in the unsaturated zone, at cell i (m); $S_i$is the groundwater table depth at cell i (m).

The depth of storm subsurface flow generated at computational cell i , $r_{sf,i}$ is given by:

$$r_{sf,i} = q_{sf0}(1 - S_{sf,i}/S_{fmax}) \quad (3)$$

where, $r_{sf,i}$ is the depth of storm subsurface flow at cell i (m); q_{sf0} is initial subsurface storm flow (m); $S_{sf,i}$ is the water storage deficit in the storm subsurface flow zone at cell i (m).

The depth of groundwater discharge is calculated as:

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

$$r_b = e^{\mathrm{lnTe} - \lambda - \overline{S}_g / Szm} \quad (4)$$

where, r_b is depth of groundwater discharge (m);$lnTe$ is the log of the areal average of $T0$ (m^2/h); is the catchment average topographic index; $\overline{S}_g$ is the catchment average groundwater table depth (m). For the complete set of equations for the Top-SSF model, the reader is referred to the Supplementary Material and (Li et al., 2024).

3.2. Multi-machine learning ensemble method

To improve flood prediction accuracy in ungauged mountainous catchments, we proposed a multi-machine learning ensemble method for regionalizing sensitive parameters of the Top-SSF model. This method leverages the complementary strengths of multi-machine learning methods to estimate model parameters based on catchment descriptors (Fig. 2). The characteristics, strengths, and limitations of each machine learning method are summarized in Table 2. The ensemble method employs a cross-validation procedure to select the best-performing machine learning method for each sensitive parameter. These selections are then integrated into a unified regionalization scheme. By mitigating limitations inherent in single machine learning regionalization, such as model bias and overfitting, and by capturing complex hydrological processes in mountainous catchment, this ensemble method aims to achieve more accurate flood prediction in ungauged catchments.

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

Table.2. Seven machine learning model characteristics, advantages and disadvantages.

Machine learning	Characteristic	Advantage	Disadvantages
DT	A single decision tree hierarchically partitions the data space using a tree structure, with internal nodes representing features, branches representing decision rules, and leaf nodes representing class labels.	High interpretability; Minimal data preprocessing.	Unstable; Tends to overfit.
ERT	Construct multiple decision trees with randomly selected feature values and randomly divided nodes (Geurts et al., 2006).	Low overfitting risk; Computational efficiency; Resilient to noise.	Possibility of increased bias; Limited interpretability.
GBM	Construct multiple decision trees. Multiple weak learners are trained iteratively and the loss function is optimised using gradient descent, progressively combined into a robust model through the learning rate (Friedman, 2002).	High accuracy for structured data; Robust to outliers; Minimal data preprocessing.	Limited interpretability; Complex adjustments.
KNN	It is a non-parametric, instance-based supervised learning algorithm. It operates by finding the K nearest data points in the training data to a given data point and making predictions based on these (Wani et al., 2017).	Simple and easy to implement. Learning process is quick.	Sensitivity to noisy and scale of data. Accuracy can be heavily impacted by the choice of K.
RF	A bagging algorithm proposed by Breiman (2001) that uses ensemble learning. Involves training numerous decision trees and aggregating predictions .	Simple and easy to implement; Low computational cost.	Prone to overfitting in noisy regression tasks.
SVM	Identifies hyperplanes in high-dimensional spaces to segregate data. The optimal hyperplane maximizes the margin between it and the nearest data points, termed support vectors (Sain, 1996).	Uses kernel functions to address nonlinear classification issues.	Sensitive to noise

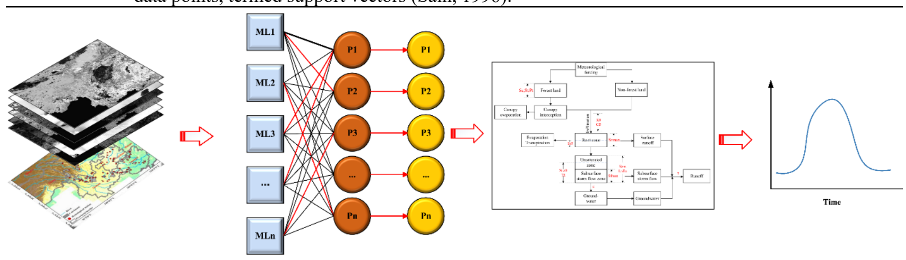


Fig.2. Multi-machine learning ensemble method for regionalization in ungauged mountainous catchments. The red line indicates the machine learning method that yielded the optimal parameter estimates.

3.3. Parameter regionalization process

The parameter regionalization process comprised four key steps: (1) Top-SSF model calibration and parameter sensitivity analysis; (2) selection of relevant catchment descriptors; (3) establishment of regionalization relationships between sensitive model parameters and catchment descriptors using multi-machine learning ensemble methods;

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

and (4) evaluation of parameter regionalization performance.

3.3.1. Top-SSF model calibration and parameter sensitivity analysis

The model was calibrated and validated using two and one flood events each catchment, respectively. The Nash-Sutcliffe Efficiency (NSE) served as the objective function during calibration, with parameter optimization achieved using the Shuffled Complex Evolution (SCE-UA) algorithm (Duan et al., 1994), known for its global convergence and robustness (Dakhlaoui et al., 2012; Qi et al., 2016). Model performance was evaluated using the NSE, Qp, and Tp, following China's Specification for Hydrological Information Forecast (GB/T 22482-2008). These metrics quantify the model's ability to predict flood dynamics, peak flow, and timing. Following calibration, a sensitivity analysis was conducted to identify and exclude insensitive model parameters (Lenhart et al., 2002), which were then used for regionalization. This approach reduces the dimensionality of the regionalization problem and improves the efficiency of the process.

The sensitivity index (Si) of each hydrological model parameter was determined using the method of Lenhart et al. (2002), which assesses the influence of ±10% changes in parameter values (Eq. 1). Table 2 outlines the sensitivity analysis results for the model parameters across the 80 mountainous catchments. The Si values are categorized as follows (Guo et al., 2022): negligible sensitivity ($|Si| < 0.05$), moderate sensitivity ($0.05 < |Si| < 0.2$), high sensitivity ($0.2 < |Si| < 1.00$), and extremely high sensitivity ($|Si| \geq 1.00$). Based on the sensitivity analyses, seven sensitive model parameters were identified: Szm, $lnTe$, $Sfmax$, C, $qsf0$, t (Table 2).

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

$$Si = \frac{1}{N}\sum_t^N \frac{(y_2(t)-y_1(t))/y_0(t)}{2\Delta x/x_0} \quad (5)$$

where $y_0(\mathrm{t})$ is the flood value of the calibrated parameter x_0 at time t; Δx is the adjusted parameter difference，$\Delta x/x_0$=10%；$y_1(\mathrm{t})$ is the flood value of the calibrated parameter $x_0 - \Delta x$ at time t;$y_2(\mathrm{t})$ is the flood value of the calibrated parameter $x_0 + \Delta x$ at time t.

Table 2. Top-SSF model main modules and default range of parameters.

Modular	Parameter	Definition	Unite	Default range	Sensitivity index
Canopy interception	Sc	Canopy storage capacity	m	0.00~0.01	<0.05
	St	Trunk storage capacity	m	0.00~0.01	<0.05
	Pt	Proportion of rain diverted into stemflow per cove	%	0.00~1.00	<0.05
Evapotranspiration	$Sr0$	Initial root zone storage deficit	m	0.00~0.02	<0.05
	$Srmax$	Maximum root zone storage deficit	m	0.00~2	<0.05
Infiltration	Ks	Surface hydraulic conductivity	m/h	0~0.01	<0.05
	CD	Capillary drive (Morel-Seytoux et al., 1974)	m	0~5	<0.05
Unsaturated zone	$Suz0$	Initial baseflow per unit area	m	$0.00\sim10^{-4}$	<0.05
	Szm	Soil maximum water storage capacity	m	0.00~1.00	**0.19**
	td	Unsaturated zone time delay per unit storage deficit	h/m	0~3	**1.07**
	$lnTe$	log of the areal average of T0	m^2/h	-2.00~1.00	**3.4**
Subsurface storm flow zone	$Sfmax$	Maximum subsurface storm flow zone deficit	m	0.00~0.01	**0.16**
	C	Transfer coefficient	m^{-2}/h	0.00~0.1	**0.26**
	$qsf0$	Initial subsurface storm flow per unit area	m	0.00~0.02	**0.18**
Routing	t	Flow routing correction coefficient	-	0.00~5.0	**1.21**

Note, the bolded values in the sensitivity index indicate sensitive model parameters.

3.3.2. Catchment descriptor selection

To mitigate the effects of multicollinearity on the accuracy and reliability of the parameter regionalization methods, catchment descriptors were screened using the variance inflation factor (VIF) and correlation coefficients. A VIF threshold of less than 10 (VIF < 10) was used to indicate acceptably low multicollinearity (Salmeron et al.,

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

2018). Initial analysis revealed strong correlations between specific catchment descriptors, namely L and Ks_CH, and Tem and Elev, indicating potential redundancy. Furthermore, the VIF for Ks_CH and Slope exceeded 10, suggesting substantial multicollinearity, should be removed. Despite this, Tem was retained as a descriptor due to its importance in representing climate change impacts. Fig. 3b illustrates the correlation coefficients between eight catchment descriptors (including Tem) and the sensitive model parameters. These correlations, with the highest reaching only 0.5 (e.g., between $qsf0$ and Pre), suggest that the relationships between the catchment descriptors and sensitive model parameters are complex and nonlinear. The final set of catchment descriptors used for parameter regionalization comprised FC, Elev, Area, L, Tem, Prec, and BD.

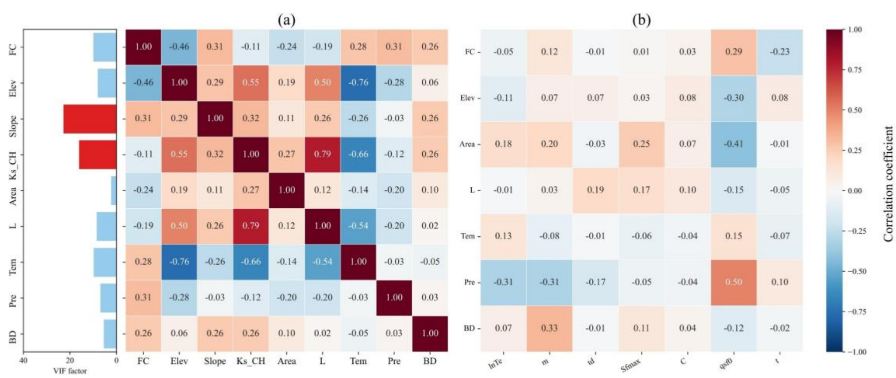


Fig.3. Analysis of catchment descriptor relationships: (a) Correlation coefficients and variance inflation factors (VIF) among all descriptors; (b) Correlation coefficients between sensitivity model parameters and descriptors with VIF values below 10.

3.3.3. Parameter regionalization

To simulate ungauged catchment conditions, each of the 80 catchments was iteratively treated as an ungauged catchment, with the remaining 79 catchments serving as donor catchments. A parameter regionalization method was then constructed using

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

the catchment descriptors and sensitive model parameters of the donor catchments to predict the seven sensitive model parameters for the ungauged catchment based on its catchment descriptors. These predicted model parameters were then input into the Top-SSF model to enable flood prediction in ungauged catchments. To ensure robust and generalizable results, K-fold cross-validation (K = 10) was implemented. This involved randomly partitioning the 79 donor catchments into K subsets, using one subset as a test set and the remaining K-1 subsets for method training in each iteration (Jung, 2018). This approach maximizes data utilization and minimizes bias associated with specific data partitioning. Hyperparameter tuning for each machine learning method was performed using RandomizedSearchCV (Bergstra et al., 2012), with the objective of minimizing the difference between predicted and observed parameter values.

3.3.4. Evaluated metrics

The performance of the parameter regionalization methods was evaluated by considering two key aspects. First, the accuracy of the methods in estimating sensitive model parameters was assessed using three metrics: root mean square error (RMSE), standard deviation (STD), and the coefficient of determination (R^2). The R^2 was used to quantify the agreement between estimated and calibrated parameter sets. Second, to evaluate the impact of parameter regionalization on flood prediction. The resulting flood predictions were then evaluated using the NSE, Qp, and Tp metrics.

$$NSE = 1 - \frac{\sum_{j=1}^{M}(Q_{obs}(j) - Q_{sim}(j))^2}{\sum_{j=1}^{M}(Q_{obs}(j) - \overline{Q}_{obs})^2} \quad (6)$$

$$Q_p = \left| \frac{Q_{obs,p} - Q_{sim,p}}{Q_{obs,p}} \times 100\% \right| \quad (7)$$

$$T_p = \left| T_{obs,p} - T_{sim,p} \right| \quad (8)$$

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

where $Q_{obs}(j)$ is the observed flow rate (m^3/s); $Q_{sim}(j)$ is the simulated flow rate (m^3/s); $\overline{Q}_{obs}$ is the mean value of the observed flow rate (m^3/s); $Q_{obs,p}$ is the observed flood peak flow (m^3/s); $Q_{sim,p}$ is the simulated flood peak flow (m^3/s); $T_{obs,p}$ is the observed flood peak occurrence time (h); and $T_{sim,p}$ is the simulated flood peak occurrence time (h).

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{n}(X_i - Y_i)^2} \quad (9)$$

$$STD = \sqrt{\frac{1}{N-1}\sum_{i=1}^{N}(Y_i - \overline{Y})^2} \quad (10)$$

$$R^2 = \frac{[\sum_{i=1}^{n}(X_i-\bar{X})(Y_i-\bar{Y})]^2}{\sum_{i=1}^{n}(X_i-\bar{X})^2\sum_{i=1}^{n}(Y_i-\bar{Y})^2} \quad (11)$$

where X_i is the Top-SSF calibration model parameter value; Y_i is the model parameter estimated value using the parameter regionalization method; $\overline{X}$ and $\overline{Y}$ are the mean values of X_i and Y_i; N is the sample size equal to 80.

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

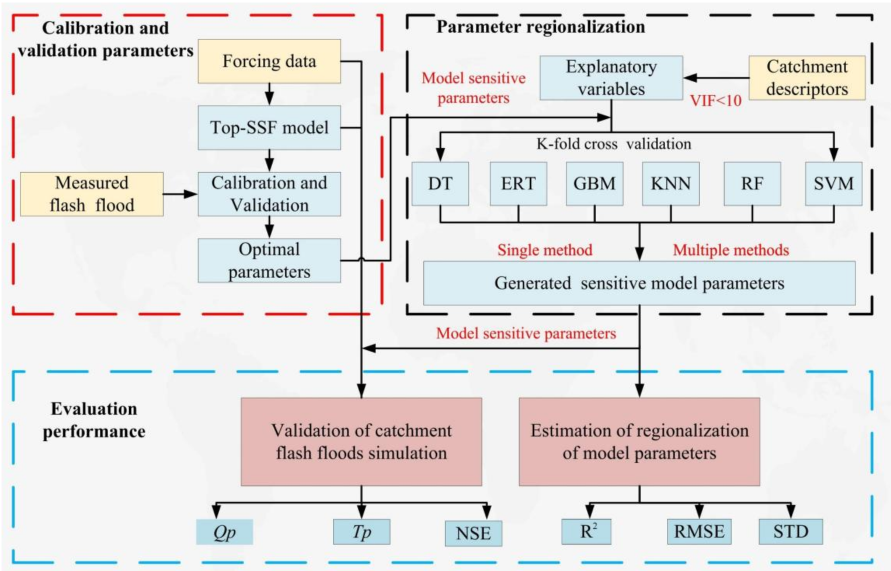


Fig.4. Flowchart illustrating the parameter calibration, validation, and regionalization workflow. Abbreviations: Top-SSF (Topography-Based Subsurface Storm Flow hydrological model), DT (Decision Tree), ERT (Extremely Randomized Trees), GBM (Gradient Boosting Machine), KNN (K-Nearest Neighbor), RF (Random Forest), SVM (Support Vector Machine), NSE (Nash-Sutcliffe efficiency), R^2 (Coefficient of Determination), Qp (Relative error of flood peak flow), Tp (Relative error of flood peak occurrence time), VIF (Variance inflation factor), RMSE (Root mean square error), STD (Standard deviation).

4. Result

4.1. Model performance

The Top-SSF model demonstrated good flood simulation performance across the 80 gauged catchments, as quantified by NSE, Qp, and Tp. During the calibration period, 50% of the catchments achieved NSE values exceeding 0.78 (Fig. 5a), the median Qp value was below 10% (Fig. 5b), and the median Tp value was within 2 hours (Fig. 5c). The average NSE value was approximately 0.8, with a maximum of 0.96. The majority of Qp values were around 8%, and the majority of Tp values were below 2 hours. During the validation period, the median NSE value was 0.76 (Fig. 5a), the median Qp

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

value was below 10% (Fig. 5b), and the median Tp value was within 4 hours (Fig.5c). Model performance also exhibited some dependence on catchment characteristics. For instance, NSE generally improved with increasing forest cover (Fig. 6a), potentially due to the model's explicit representation of forest canopy interception and subsurface storm flow generation mechanisms. The relationship between NSE, Qp, Tp and elevation was more complex, suggesting a nonlinear influence of elevation on model performance (Fig. 6a-c). The demonstrated robust performance of the Top-SSF model provides a strong foundation for its application in subsequent parameter regionalization analyses.

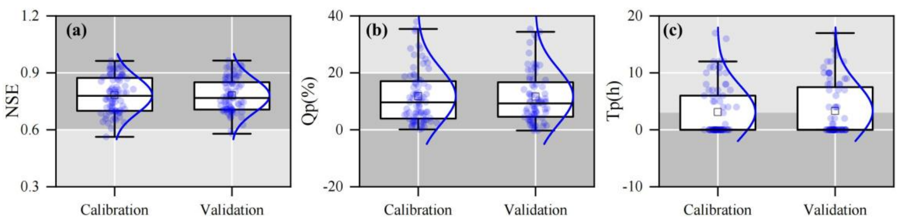


Fig. 5. Boxplots of (a) NSE, (b) Qp, and (c) Tp during the calibration and validation periods for 80 gauged catchments. The box represents the interquartile range, with the middle line indicating the median (50th percentile). The whiskers represent the minimum and maximum values. "□" represents the mean value. Dark grey indicates the range of flood prediction criteria (i.e., NSE> 0.75, Qp< 20%, and Tp < 2 hours).

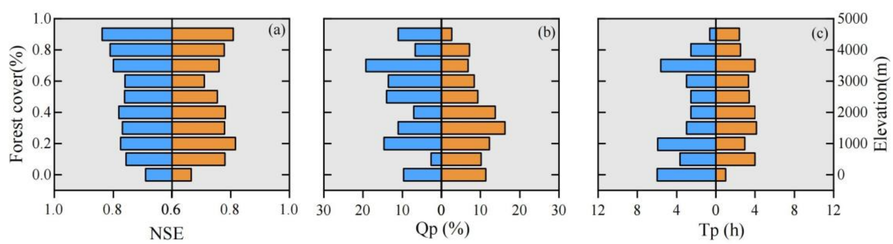


Fig.6. Influence of environmental factors on Top-SSF model performance in flood simulation. The graphs illustrate the relationship between model evaluation metrics and forest cover (left) and elevation (right)."

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Preprint. Discussion started: 10 June 2025

4.2. Results of parameter regionalization

4.2.1. Comparison of sensitive model parameter estimates

The six single machine learning parameters regionalization methods exhibited varying performance in estimating sensitive model parameters (Fig. 7), likely due to differences in catchment descriptor characteristics and the underlying principles of each method. GBM demonstrated the highest accuracy in estimating Szm, td, and C (R^2 = 0.90, 0.86, and 0.87, respectively,), with its estimates also exhibiting a STD that closely matched the distribution of the calibrated parameter values. KNN provided the most accurate estimates for $lnTe$, $qsf0$, and t (R^2 = 0.87, 0.89, and 0.90, respectively), also with STD closely resembling the calibrated parameter distributions. RT performed best in estimating $Sfmax$ (R^2 = 0.87), but its performance was generally poorer for other parameters. DT, SVM, and RF methods generally showed lower performance across all sensitive model parameters. These differences in performance highlight the potential benefits of multi-machine learning ensemble methods for improving flood prediction in ungauged mountainous catchments.

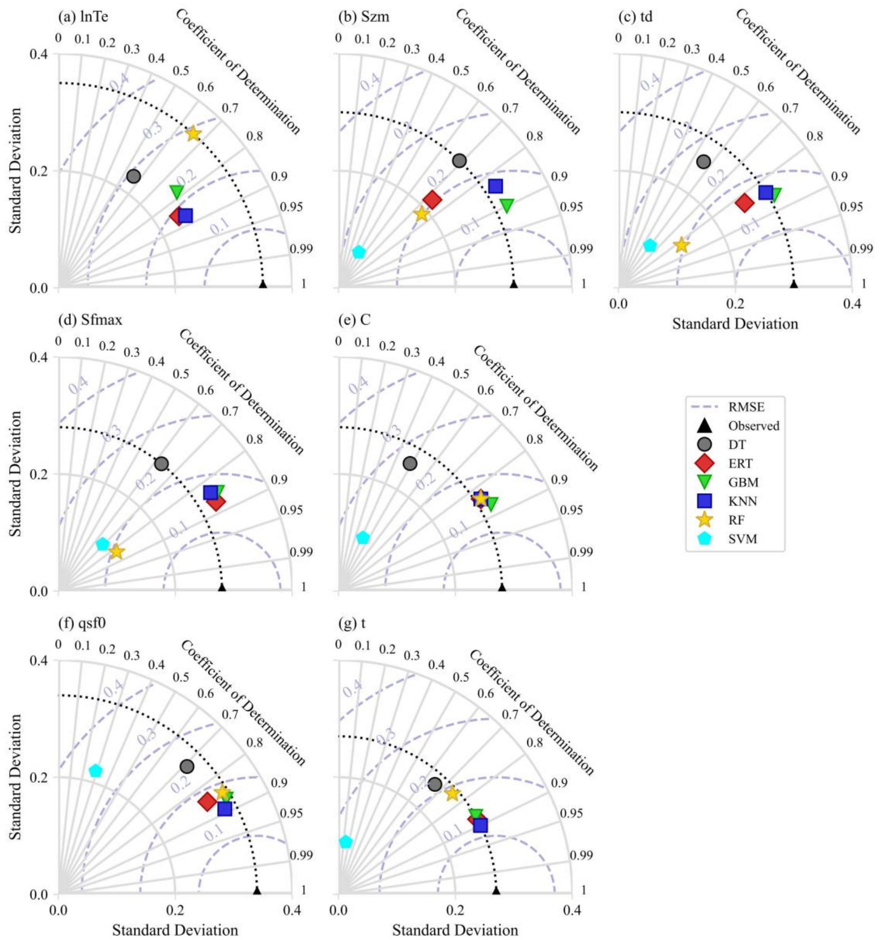

Fig.7. Performance of parameter regionalization methods assessed using Taylor diagrams. The diagrams show the accuracy of sensitive model parameter estimates, with the coefficient of determination (R^2) indicated by the radial axis, standard deviation (STD) by the horizontal and vertical axes, root mean square error (RMSE) by the grey-blue dotted lines, and the standard deviation of observations by the black dotted line."

4.2.2. Comparison of flood forecasting results

The flood prediction performance of the Top-SSF model, integrated with different parameter regionalization methods, was compared across 80 mountainous catchments in southwestern China. The methods included single machine learning methods and a multi-machine learning ensemble method (GBM-KNN-ERT), where GBM estimated

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

Szm, td, and C; KNN estimated $lnTe$, $qsf0$, and t; and ERT estimated $Sfmax$. The performance of these parameter regionalization methods was then evaluated against the performance of the Top-SSF model using calibrated parameter. Among the single machine learning methods, GBM performed best. Approximately 75% of the catchments achieved NSE greater than 0.9 (Fig. 8a), Qp less than 5% (Fig. 8b), and Tp less than 1 hour (Fig. 8c). These results surpass the flood prediction standards outlined in the Specification for Hydrological Information Forecast of China (GB/T 22482-2008; NSE > 0.75, Qp < 20%, Tp < 2 hours). The GBM-KNN-ERT method yielded even better results than the GBM. With GBM-KNN-ERT, 75 of the catchments had NSE > 0, and 90% of the catchments had NSE > 0.9. The Qp values were also more concentrated near 0, and while the Tp values exhibited a slightly broader distribution, 90% of the catchments still had Tp values near 0. These results strongly suggest the potential of multi-machine learning ensembles for improving flood prediction in ungauged catchments.

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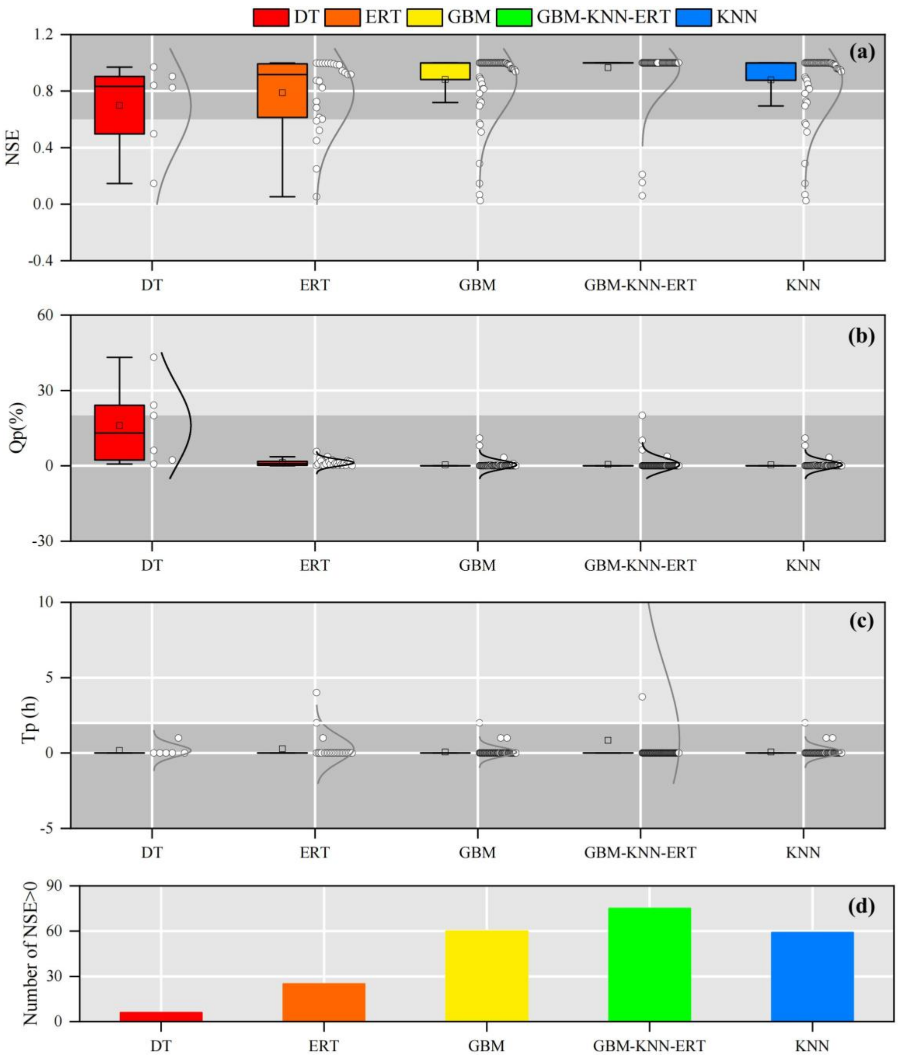

Fig.8. Evaluation of flood prediction performance achieved by different parameter regionalization methods, relative to the calibrated Top-SSF model. Boxplots and normal distribution curves illustrate the distribution of (a) NSE, (b) Qp, (c) Tp, and (d) the number of catchments exceeding NSE > 0. Shaded regions highlight where flood prediction standards were met (NSE > 0.75, Qp < 20%, Tp < 2 hours).

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Preprint. Discussion started: 10 June 2025

5. Discussion

5.1. Reliability of multi-machine learning ensemble in parameter regionalization

In this study, the GBM-KNN-ERT method demonstrated superior parameter regionalization performance in ungauged mountainous catchments, highlighting the potential of multi-machine learning methods for improving hydrological predictions in ungauged mountainous catchments. The GBM method exhibited distinct parameter-specific sensitivities to hyperparameters (Fig. 9a-c). For parameter C, the negative correlation between R^2 and n_estimators (>500 trees) indicates overfitting risks when modeling complex rainfall-runoff interactions in heterogeneous mountainous terrain (Fig. 9a). This aligns with previous findings emphasizing the need for complexity control in hydrological generalization (Schoups et al., 2008). Conversely, the improved R^2 for parameter td with increased n_estimators highlights the capacity of ensemble learning to capture complex, nonlinear relationships between catchment descriptors and hydrological parameters (Hastie et al., 2009). The contrasting optimal max_depth of 5 layers for parameter C, compared to shallower optimal depths (3 layers) for Szm and td, suggests that parameters governing more complex hydrological processes in mountainous catchments may require deeper decision trees to effectively capture the interactions between climate, topography, and soil properties (Wainwright et al., 2013).

KNN performance exhibited pronounced sensitivity to neighborhood size (n_neighbors) and distance metric (p), highlighting the spatial heterogeneity of catchment descriptors. For parameters $lnTe$ and $qsf0$, optimal performance was observed at n_neighbors=20 (Fig. 9d). This aligns with the hypothesis that meaningful

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

hydrological similarities can emerge even in topographically complex mountainous regions when considered at broader spatial scales (Li et al., 2022). Conversely, parameter t achieved peak accuracy at n_neighbors=5, suggesting that localized, short-term weather events and fine-scale topographic similarities in adjacent mountainous areas can significantly influence local runoff processes (Garambois et al., 2015).The Manhattan distance metric (p=1) outperformed Euclidean distance across all parameters (Fig. 9e). This superiority stems from its ability to mitigate the "curse of dimensionality" (Bellman, 1961) in high-dimensional datasets, a common characteristic of mountainous catchments. In such datasets, sparse data distributions and the presence of mixed variable types (e.g., topographic indices, land cover) can significantly degrade the discriminative power of Euclidean distance (Rockström et al., 2023). The robustness of the Manhattan distance arises from its axis-aligned sensitivity, which provides a more effective means of handling feature scaling and integrating categorical descriptors compared to the radial symmetry of Euclidean distance.

ERT performance was maximized at max_features = 0.15 (Fig. 9f). By restricting the random sampling of features during node splits (using only 15% of the features), both the diversity of the trees was enhanced and the effects of multicollinearity between topographic and soil attributes were reduced. This finding aligns with the theory proposed by Geurts et al. (2006), which suggests that random feature selection can significantly improve model generalization, a particularly important consideration in ungauged mountainous catchments characterized by high levels of inter-correlation among predictor variables.

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Preprint. Discussion started: 10 June 2025

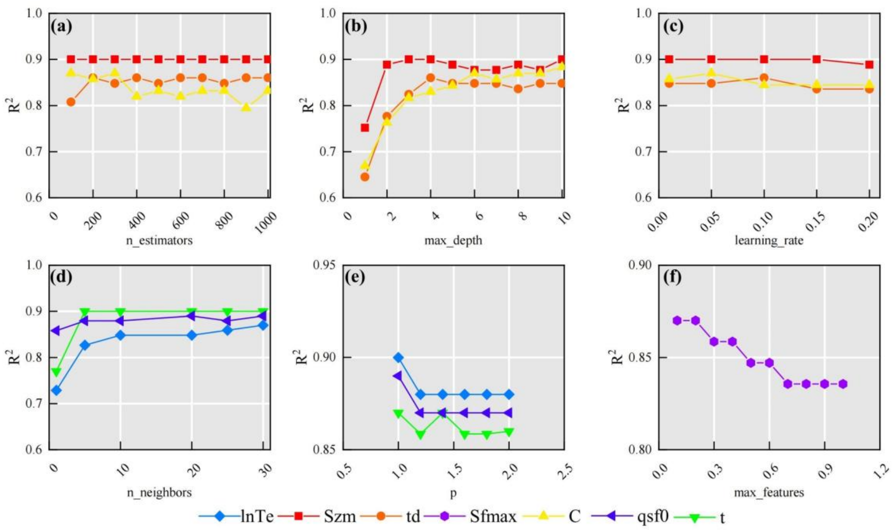

Fig.9. Sensitivity of parameter estimation performance to key hyperparameters in (a-c) GBM, (d-e) KNN method, and (f) ERT. (a) n_estimators (number of decision trees in GBM), (b) max_depth (maximum depth of decision trees in GBM), (c) learning rate (GBM), (d) n_neighbors (number of neighbors in KNN), (e) p-value of Minkowski distance (KNN; p=1: Manhattan distance, p=2: Euclidean distance), and (f) max_features (ERT).

5.2. Combining multiple machine learning methods for parameter regionalization

Machine learning methods exhibit distinct strengths in hydrological parameter estimation due to fundamental differences in data processing mechanisms, pattern recognition strategies, and prediction generation (Bishop et al., 2006). This suggests that multi-machine learning ensemble methods have the potential to synergistically integrate advantages while effectively compensating for individual limitations, leading to more robust and accurate parameter estimates. As demonstrated in Fig. 10, the GBM-KNN-ERT method achieved notable improvements over single machine learning method, particularly for sensitive parameters $lnTe$, $Sfmax$, $qsf0$ and t, with R^2 increases ranging from 0.02 to 0.03 compared to the best-performing GBM method (Fig.10e). Interestingly, a comparison of GBM4-KNN3 (where $Sfmax$ is estimated by GBM) and GBM3-KNN4 (where $Sfmax$ is estimated by KNN) revealed critical

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

insights into model parameter compatibility. Despite achieving identical $Sfmax$ estimation accuracy (R^2 = 0.85), GBM4-KNN3 exhibited superior flood prediction performance, with 72 catchments achieving NSE > 0 compared to only 68 catchments for GBM3-KNN4. This suggests that GBM possesses an enhanced capability to resolve the complex coupling between soil moisture dynamics and topographic, leading to more accurate representation of subsurface storm flow processes (Gupta et al., 2023). The wider distribution of flood prediction performance observed for GBM3-KNN4 (Fig. 10a–c) further suggests that uncertainties introduced by KNN in the estimation of $Sfmax$ may propagate nonlinearly during flood simulations, potentially amplifying errors. This observation aligns with theoretical expectations that distance-based methods may tend to over smooth critical thresholds or sharp transitions in heterogeneous environments, leading to a less accurate representation of hydrological responses (Bellman, 1961).

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Preprint. Discussion started: 10 June 2025

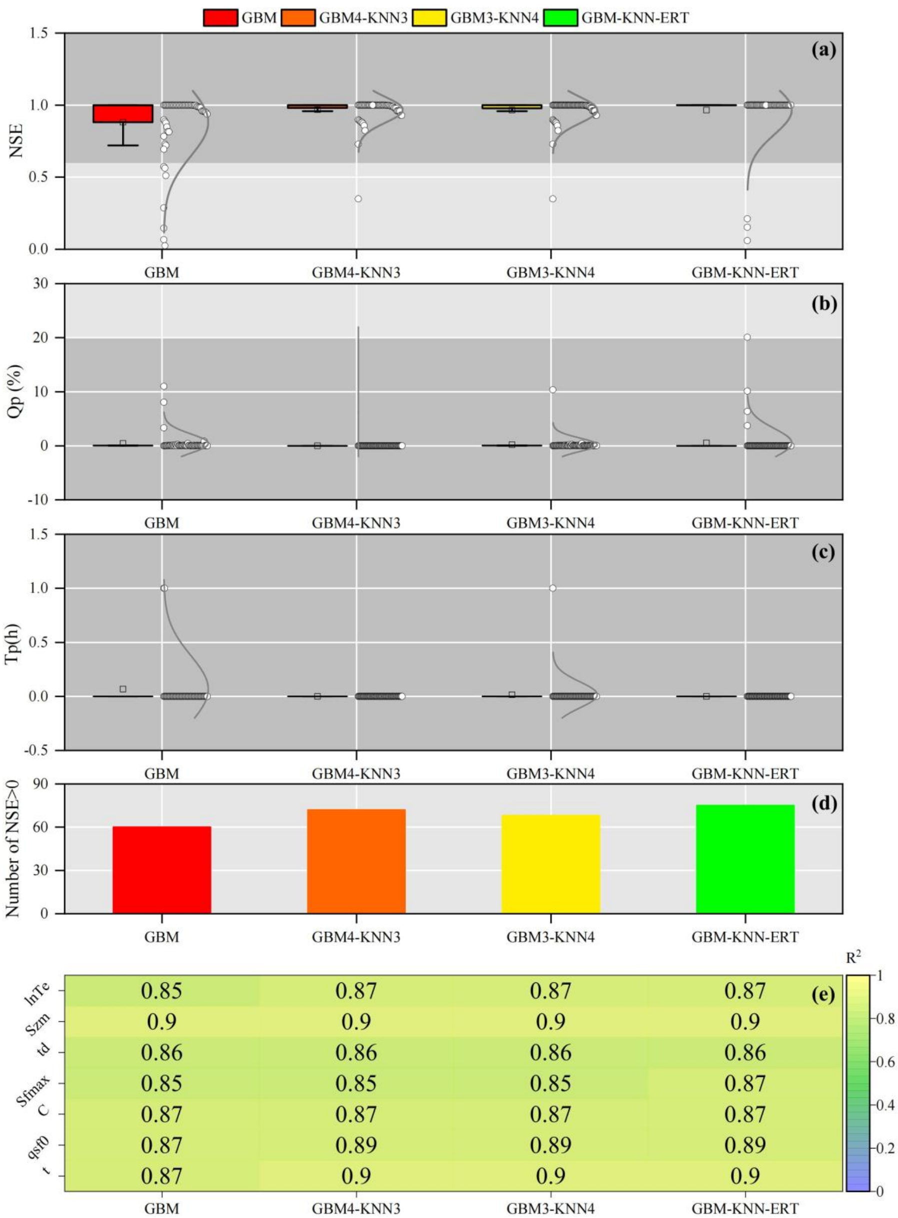

Fig.10. Assessment of combined machine learning methods for improved parameter regionalization in ungauged mountainous catchments. Performance is evaluated against the GBM method, showing (a) NSE, (b) Qp, (c) Tp, (d) Number of catchments with NSE > 0, and (e) the difference in R^2.

5.3. The influence of donor catchment quantity on machine-learning parameter regionalization

The number of donor catchments used in machine learning-based parameter regionalization methods is a critical factor influencing the accuracy and robustness of hydrological predictions in ungauged catchments (Gauch et al., 2021; Song et al., 2022; Zhang et al., 2022). In this study, we investigated the influence of donor catchment quantity (ranging from 20 to 80) on the flood prediction performance of the two best-performing parameter regionalization methods (GBM4-KNN3 and GBM-KNN-ERT) across the 80 mountainous catchments (Fig 11). To systematically investigate the influence of donor catchment quantity on parameter regionalization, two distinct sampling strategies were employed across the 80 mountainous catchments. In Mode 1 (selection of donor catchments based on decreasing NSE), a non-monotonic relationship between donor catchment quantity and regionalization performance was observed, indicating that simply increasing the number of donor catchments does not guarantee improved model performance. Specifically, in Mode 1, regionalization performance exhibited a significant decrease when the number of donor catchments exceeded 40 (particularly within the 40-60 range, and below 70 for GBM4-KNN3) (Fig. 11a-c). This performance decline likely arises from the increasing dissimilarity in hydrological behavior between the added donor catchments and the target catchment as the donor pool expands, potentially introducing irrelevant or misleading information into the regionalization process (Gauch et al., 2021; Zhang et al., 2022). However, for the GBM-KNN-ERT method in Mode 1, regionalization performance tended to stabilize when the number of donor catchments exceeded 70, suggesting a potential saturation point beyond which additional donor catchments contribute little to improving model accuracy. In contrast, Mode 2 (random selection of donor catchments)

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

demonstrated a consistent improvement in regionalization performance for both NSE and Tp as the number of donor catchments increased (Fig. 11d-f). However, it's important to acknowledge that the potential for bias may also increase with the inclusion of more randomly selected donor catchments, potentially leading to overfitting or reduced generalizability. Notably, under both modes, the GBM-KNN-ERT method consistently exhibited significantly greater performance stability compared to the simpler combined strategy, GBM4-KNN3. This enhanced robustness likely arises from its more effective suppression of data heterogeneity and noise interference, indicating that more complex ensemble methods possess a greater capacity to balance the benefits of increased data quantity with the potential drawbacks of reduced data quality.

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Preprint. Discussion started: 10 June 2025

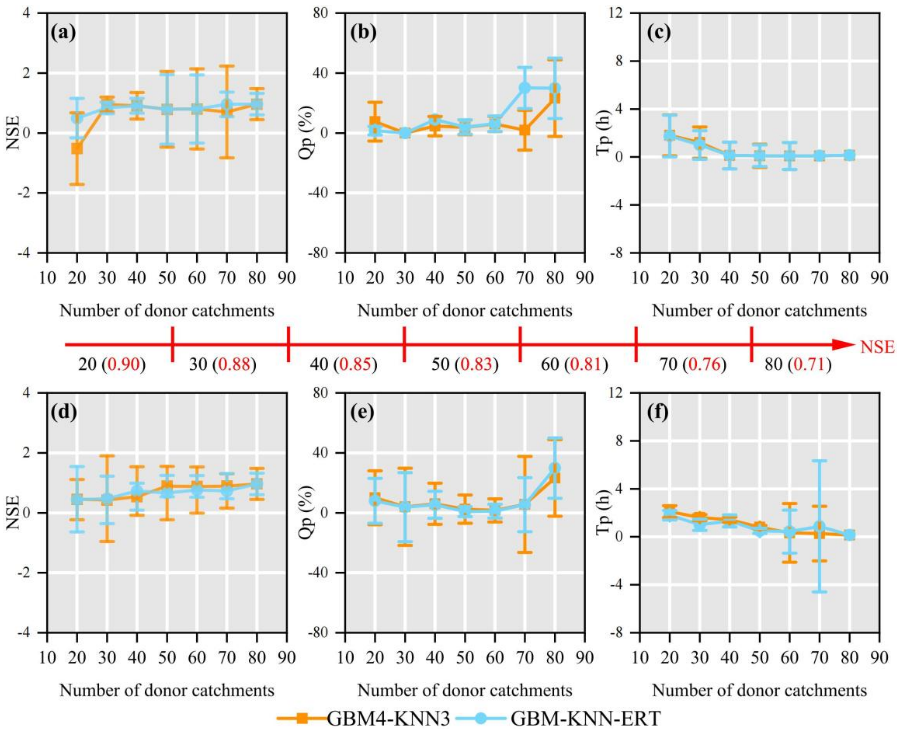

Fig. 11. Performance comparison of two donor catchment selection methods for parameter regionalization as a function of donor catchment quantity. Mode1 (a-c) selects donor catchments in order of decreasing NSE, while Mode 2 (d-f) selects them randomly. Flood prediction accuracy is assessed using NSE, Qp, and Tp.

5.4. The impact of climate change on parameter regionalization methods

The hydrological cycle within catchments is fundamentally governed by complex interactions between climate and environmental factors. The Intergovernmental Panel on Climate Change (IPCC) has consistently documented a continuous and accelerating transition in global climatic patterns, characterized by increased variability and extreme events (Pachauri et al., 2014). Consequently, future flood predictions derived from parameter regionalization methods are expected to exhibit increased uncertainty and variability, highlighting the substantial influence of climate change on the reliability and precision of flood predictions in ungauged mountainous catchments (Yang et al.,

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

2019). Therefore, the stability and robustness of parameter regionalization methods under changing climatic conditions are paramount for their practical application in long-term flood risk assessment and management. To quantitatively assess the impact of climate change on the performance of the parameter regionalization methods, cumulative distribution functions (CDFs) were employed to illustrate the discrepancies between the parameter regionalization simulations and the reference simulations (derived from calibrated model parameters) across the historical (1901-2021) and projected future (2021-2100) periods for the 80 catchments (Fig 12). A comparative analysis of Fig. 12a and 12b reveals a clear amplification of the absolute differences in predicted flood peaks (quantified as the error in runoff modulus) between the two parameter regionalization methods and the reference Top-SSF model simulations during the transition from the historical period to the projected future period. Specifically, the maximum error in runoff modulus for the GBM4-KNN3 method increased by 67.26 m3 s-1 km-2 from the historical period to the projected future period, while the equivalent maximum error for the GBM-KNN-ERT method increased by a smaller margin of 57.75 m3 s-1 km-2 over the same period. These results underscore the increased sensitivity of parameter regionalization methods to changing climatic forcing conditions. However, they also provide compelling evidence that the GBM-KNN-ERT method exhibits superior stability and resilience under climate change, demonstrating its potential for more reliable long-term flood risk assessment in ungauged mountainous regions.

Exploring the effects of climate change on parameter regionalization methods

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

provides valuable insights for advancing flood prediction research in PUBs. Additionally, the combination of multiple machine learning methods, as demonstrated by the GBM-KNN-ERT method, shows increased stability under climate change, offering promising directions for future development of parameter regionalization methods.

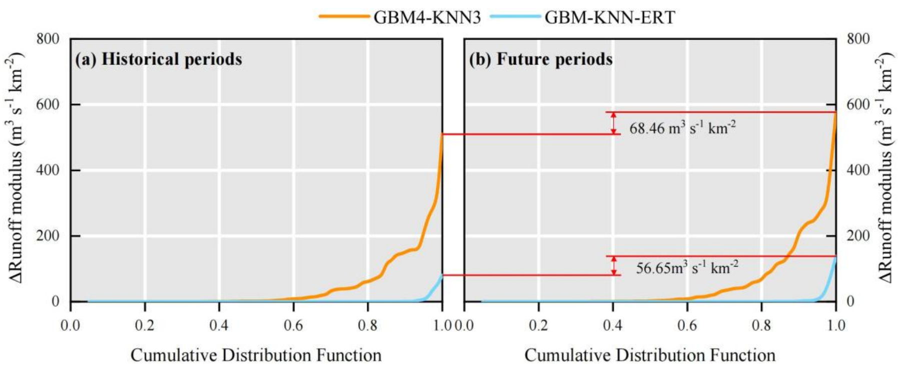

Fig.12. Comparison of flood peak runoff modulus between parameter regionalization and calibrated Top-SSF model results, showing cumulative distribution functions (CDFs) of absolute differences for 80 catchments during (a) historical and (b) future periods.

5.5. Uncertainty and limitation

The uncertainty in parameter regionalization within this study primarily originated from the hydrological model and the parameter regionalization methods. Although the Top-SSF model demonstrated satisfactory performance in flood prediction across the study catchments, inherent uncertainties associated with model parameters remained. To mitigate these uncertainties and enhance the reliability of the hydrological model, we employed the SCE-UA algorithm for parameter optimization and conducted comprehensive sensitivity analyses to identify and focus on the most influential parameters. The training data used in the machine learning-based parameter

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

regionalization methods, derived from the donor catchments, are susceptible to various sources of error, including noise, labeling inconsistencies, and missing values, all of which can contribute to increased estimation uncertainty (Mosavi et al., 2018; Xu et al., 2021).

Furthermore, the inherent stochasticity present in certain machine learning methods, such as ERT, can lead to outcome variations across different algorithm iterations, potentially influencing the stability and reproducibility of the results (Breiman, 2001; Geurts et al., 2006). To address the potential for overfitting and to obtain a more robust assessment of model performance, we employed K-fold cross-validation, a widely used technique that partitions the data into K subsets and iteratively evaluates model performance across different folds. This approach maximizes data utilization, improves the reliability of model performance evaluation by averaging results across multiple folds, and reduces the sensitivity to specific data partitioning schemes, thereby minimizing the overall uncertainty associated with the parameter regionalization methods. For hyperparameter tuning, we utilized the RandomizedSearchCV approach implemented in Python (Bergstra and Bengio, 2012). This method involves random sampling from a predefined hyperparameter space to identify the optimal hyperparameter combination for each machine learning method, thereby minimizing the potential for overfitting and improving the generalization performance of the models. The RandomizedSearchCV approach allows for a more comprehensive exploration of the hyperparameter space compared to grid search methods, even with a limited number of search iterations, and provides multiple

https://doi.org/10.5194/egusphere-2025-1795
Preprint. Discussion started: 10 June 2025

performance evaluations for a diverse range of model configurations. This random sampling strategy mitigates the uncertainty arising from fixed partitioning or manual parameter selection, ultimately enhancing the model's stability and its ability to generalize to unseen data (Bergstra and Bengio, 2012). During the assessment of parameter regionalization methods performance, the results were compared with the Top-SSF model simulation results (estimated model parameters and simulated flood process) rather than directly with measured flood data. Consequently, uncertainties related to the parameter regionalization methods may be significantly reduced.

6. Conclusions

This study introduces a novel multi-machine learning ensemble method (GBM-KNN-ERT) to enhance model parameter transferability and improve flood prediction in ungauged mountainous catchments. The proposed GBM-KNN-ERT method demonstrated a substantial advancement in both flood prediction accuracy and model robustness, achieving exceptional performance with 90% of ungauged catchments exhibiting a NSE exceeding 0.9, a significant 67.44% improvement compared to traditional single machine learning methods. Importantly, the GBM-KNN-ERT method exhibited remarkable stability under simulated climate change, thereby highlighting its potential for reliable application in non-stationary hydrological environments. Furthermore, the method demonstrated notable adaptability to varying donor-catchment configurations, achieving an optimal balance between predictive accuracy and computational efficiency with a relatively limited set of 20–40 high-quality donor catchments (NSE >0.85). By integrating the diverse strengths of multiple machine learning with hydrological model, the proposed methodology significantly advances the field of flood prediction in ungauged catchments, offering a reliable tool for water resource management and flood disaster mitigation.

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Competing 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.

Author contributions

In this study, K L, G W, and J G were responsible for the conceptualization of the research. Data curation was carried out by K L, L G, and X S, while formal analysis was performed by K L, J G, and J M. The methodology was developed by K L, L G, P H, and J L. Project administration was overseen by G W and J G. K L took the lead in writing the original draft, and the writing, review, and editing process involved contributions from K L, G W, J L, P H, J M, X Z, and J G.

Code and data availability

The code used in this study is available upon request from the authors. The meteorological, soil characteristics, and topography datasets are publicly accessible online, as detailed in Table 1. The hourly flood data for the 80 catchments were sourced from China's Hydrological Yearbook. These data are not publicly available due to

https://doi.org/10.5194/egusphere-2025-1795
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governmental restrictions but can be accessed by contacting the corresponding author for further information.

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