

# **Short-term flood probability density forecasting using a conceptual hydrological model with machine learning techniques**

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## Abstract

1  
2 Making accurate and reliable probability density forecasts of flood processes is  
3 fundamentally challenging for machine learning techniques, especially when prediction  
4 targets are outside the range of training data. Conceptual hydrological models can reduce  
5 rainfall-runoff modelling errors with efficient quasi-physical mechanisms. The Monotone  
6 Composite Quantile Regression Neural Network (MCQRNN) is used for the first time to  
7 make probability density forecasts of flood processes and serves as a benchmark model,  
8 whereas it confronts the drawbacks of overfitting and biased-prediction. Here we propose  
9 an integrated model (i.e. XAJ-MCQRNN) that incorporates Xinanjiang conceptual model  
10 (XAJ) and MCQRNN to overcome the phenomena of error propagation and accumulation  
11 encountered in multi-step-ahead flood probability density forecasts. We consider flood  
12 forecasts as a function of rainfall factors and runoff data. The models are evaluated by long-  
13 term (2009-2015) 3-hour streamflow series of the Jianxi River catchment in China and  
14 rainfall products of the European Centre for Medium-Range Weather Forecasts. Results  
15 demonstrated that the proposed XAJ-MCQRNN model can not only outperform the  
16 MCQRNN model but also prominently enhance the accuracy and reliability of multi-step-  
17 ahead probability density forecasts of flood process. Regarding short-term forecasts in  
18 testing stages at four horizons, the XAJ-MCQRNN model achieved higher Nash-Sutcliffe  
19 Efficiency but lower Root Mean Square Error values, while improving Coverage Ratio and  
20 Relative Bandwidth values in comparison to the MCQRNN model. Consequently, the  
21 improvement can benefit the mitigation of the impacts associated with uncertainties of  
22 extreme flood and rainfall events as well as promote the accuracy and reliability of flood  
23 forecasting and early warning.

24 **Keywords:** Short-term flood forecast; Probability density forecast; Monotone  
25 composite quantile regression; Conceptual model; Machine learning  
26

## 27 **1 Introduction**

28 Floods are among the world's costliest disasters, and climate and anthropogenic  
29 changes have made catastrophic floods much more likely happen. Over the past century,  
30 floods accounted for about 30% of natural disasters, claiming more than 19% of the  
31 total fatalities and more than 48% of the total number of people affected (Adikari and  
32 Yoshitani, 2009; Takeuchi et al., 2018). Flood forecasting and early warning play a  
33 pivotal role in geohazard mitigation, floodplain management, design and management  
34 of infrastructure projects, agricultural cultivation, and human daily life (Liu et al., 2018;  
35 Giuliani et al., 2019). Therefore, accurate and reliable forecasting of flood processes  
36 during rainstorm events is extremely crucial and beneficial for a country or catchment,  
37 whose prosperity is largely dependent on the optimum use of water resources and flood  
38 level control.

39 To date, a wide variety of modelling frameworks have been introduced to model  
40 the complicated nonlinear rainfall-runoff process (Sood and Smakhtin, 2015; Shen,  
41 2018; Kan et al., 2020). In general, these modelling frameworks can be categorized into  
42 three groups: conceptual, physically-based and machine learning models. A conceptual  
43 hydrological model typically includes prior-knowledge as a necessary part of  
44 conceptual components, possessing quasi-physical mechanisms (Li et al., 2020; Tarek  
45 et al., 2020). There are all sorts of spatially lumped and distributed conceptual models  
46 available with deterministic and stochastic parameter values for a given point or region.  
47 A physically-based model usually establishes a simplified catchment system and

48 expresses the internal hydrological processes through several mathematical equations  
49 considering the spatial variability of rainfall and parameters (Li et al., 2019; Li and  
50 Willems, 2020). However, physically-based models encounter a much higher challenge  
51 when trying to achieve the required prediction accuracy due to limited watershed  
52 information. An alternative, the machine learning model, constructs a direct mapping  
53 between rainfall and runoff variables and extracts their relationship according to the  
54 historical observations by machine learning algorithms, without a piece of prior  
55 knowledge in relation to internal hydrological processes (Feng et al., 2020; Kao et al.,  
56 2020; Li et al., 2020; Lin et al., 2020; Nearing et al., 2020; Xiang et al., 2020).

57 To the best of our knowledge, the growth in machine learning for hydrological  
58 sciences is tied to advances in computing power as well as the vast increase of  
59 hydrological observations. However, machine learning models are purely data-driven  
60 and do not have any physical mechanisms, which easily lead to overfitting and biased-  
61 predictions, especially when prediction targets are unobserved and outside the range of  
62 rainfall-runoff data adopted for model training (Hunter et al., 2018; Xie et al., 2021).  
63 Typically, at longer forecast horizons, the non-availability of antecedent streamflow  
64 data makes it fundamentally challenging to maintain the forecast accuracy of data-  
65 driven models. Such weakness imposes limitations on the applicability of data-driven  
66 models in rainfall-runoff studies (Schmidt et al., 2020; Zahura et al., 2020). In  
67 comparison to physically-based models, conceptual models have been widely applied  
68 in rainfall-runoff modelling owing to the practical and simple manner. Formulation of  
69 conceptual models signifies only a partial set of the real hydrological cycle processes.

70 This triggers several constraints like model calibration and parameter transferability  
71 difficulties (Humphrey et al., 2016; Kumanlioglu and Fistikoglu, 2019), in cases where  
72 forecasters and decision-makers usually require prior knowledge for calibrating and  
73 running conceptual models to achieve reasonable accuracy of flood forecasts (Bandai  
74 and Ghezzehei, 2020; Gu et al., 2020). Although conceptual and data-driven models  
75 are derived from different philosophies, they can help remedy and enhance each other  
76 with regard to their inherent limitations and strengths (Tian et al., 2018; Sun et al., 2019;  
77 Chadalawada et al., 2020). Hence, a hybridization of both models is an attractive and  
78 effective approach for rainfall-runoff modelling (Yong et al., 2017; Kurian et al., 2019;  
79 Ghaseminejad and Uddameri, 2020). For instance, Yang et al. (2019) evaluated the  
80 integration of machine learning and conceptual models for flood simulation at 1032  
81 streamflow gauging stations worldwide. Farfan et al. (2020) adopted streamflow series  
82 forecasts made by a conceptual model as input data of back-propagation neural  
83 networks to forecast streamflow data. Hitokoto and Sakuraba (2020) integrated a  
84 rainfall-runoff model and a feed-forward artificial neural network to predict real-time  
85 water level processes. Hosseiny et al. (2020) integrated a two-dimensional hydraulic  
86 model, a random forest classification and a multilayer perceptron for modeling flood  
87 depth of the river segment of the Flaming Gorge Dam in the northeast corner of Utah  
88 in the US. Konapala et al. (2020) verified hybrid models constructed by combining a  
89 conceptual model with a long short-term memory neural network on their capability to  
90 simulate streamflow series in hundreds of catchments across the US. The above-  
91 mentioned studies explored hybrid models for flood prediction in watersheds with

92 diverse climate conditions by means of point forecasts. This study is the first to apply  
93 conceptual models with artificial neural networks incorporating flood probability  
94 density (FPD) forecasting for a humid subtropical climate. Exploration of conceptual  
95 and machine learning models for FPD forecasting in this study is owing to the following  
96 reasons: first, conceptual models possess superior operability while machine learning  
97 models possess efficient computation power; and second, physically-based models  
98 usually have bottlenecks of low prediction accuracy and time-consuming due to the  
99 limitation of available data or quality on the physical properties of watersheds (Liu et  
100 al., 2018; Li et al., 2020; Cui et al., 2021; Kao et al., 2021).

101 Previous research regarding hybrid models mainly concentrated on point forecasts  
102 or interval predictions of flood processes by integrating conceptual models with single-  
103 output artificial neural networks, whereas to date no study has involved FPD forecasting.  
104 Point forecasting, the most frequently used approach, can provide a point estimate of  
105 the future flood as precisely as possible for each forecast horizon. Rather than offering  
106 single-valued forecasts, interval prediction approaches attempt to create well-calibrated  
107 lower and upper bounds of each future prediction subject, to a prescribed confidence  
108 level. Furthermore, FPD forecasting can provide flood forecasts in the form of quantile  
109 point forecasts, confidence interval forecasts and probability density functions.  
110 Although it needs extra efforts to calculate the probability for each possible prediction,  
111 additional information gained is highly helpful to promote the full understanding of  
112 flood predictability. FPD forecasting not only effectively quantifies the uncertainties in  
113 input datasets but also has the ability to construct the complete conditional probability

114 density curves of future flood processes. Consequently, there is a noticeable migration  
115 from point forecasts and interval predictions towards FPD forecasts where modelers  
116 seek to characterize the full probability distribution of flood events. Among machine  
117 learning techniques, the Monotone Composite Quantile Regression Neural Network  
118 (MCQRNN) is a special type of multi-output artificial neural networks (ANN) that can  
119 effectively estimate multiple non-crossing and nonlinear quantile functions  
120 simultaneously. It is a novel and appealing approach for probability density forecasting,  
121 as compared with other multi-output ANNs like support vector machine and long short-  
122 term memory (Cannon, 2018). Since MCQRNN applications do not exist in FPD  
123 forecasts, it would be important and interesting to explore in-depth conceptual  
124 hydrological models to decrease the uncertainty of multi-output ANN (e.g. MCQRNN)  
125 for FPD forecasting.

126 The novelty of this study relies on the integration of the Xinanjiang (XAJ)  
127 conceptual model and the innovative MCQRNN with a multi-output task. Meanwhile,  
128 this is the first application of the integrated XAJ-MCQRNN model for FPD forecasting.  
129 There are three main steps in this approach. First, the conceptual hydrological model  
130 for rainfall-runoff simulation was constructed to create point forecasts of flood  
131 processes and the outputs were used as inputs of the machine learning model. Second,  
132 the multi-output machine learning model for FPD forecasting was built to further create  
133 interval forecasts of flood processes after being supplied with point forecasts by the  
134 conceptual model. Third, the training process of the hybrid model was optimized by an  
135 evolutionary optimization algorithm, and the predictability of the hybrid model was

136 tested by using medium-range numeric rainfall forecast products. The Jianxi River  
 137 catchment of China constituted the case study.

138

## 139 **2 Methods**

140 This study aims to integrate the XAJ and MCQRNN models for raising the accuracy  
 141 and reliability of short-term FPD forecasts. Fig. 1 presents the main architectures  
 142 utilized in this study: the MCQRNN (Fig. 1(a)); and the proposed XAJ-MCQRNN  
 143 model that combines XAJ with MCQRNN models (Fig. 1(b)).

### 144 **2.1 Monotone Composite Quantile Regression Neural Network (MCQRNN)**

145 The MCQRNN has been developed to effectively estimate multiple quantile functions  
 146 for making probabilistic density forecasts of time series (Cannon, 2018). In comparison  
 147 to the Quantile Regression Neural Network (QRNN) (Taylor, 2000), the monotone  
 148 QRNN (Cannon, 2011) and the composite QRNN (Xu et al., 2017), the merit of the  
 149 MCQRNN model is that it can estimate multiple non-crossing, non-linear conditional  
 150 quantile functions, can allow for the constraints of optional monotonicity,  
 151 positivity/non-negativity and generalized additive model, and can be applied to  
 152 estimating standard least-squares regression (Cannon, 2018).

153 The structure of the MCQRNN model is composed of input, hidden, and output  
 154 layers (Fig. 1(a)). Regarding the  $k$ th quantile  $\tau_k$ , the outputs of hidden and output layers  
 155 in association with multi-input variables at horizon T are described below.

$$\begin{aligned}
 156 \quad h_j(t + T) = & f \left( \sum_{s=0}^T \hat{P}(t + s) \cdot \exp(w_{sj}^{(h)}) + \sum_{m=0}^p P(t - m) \cdot \exp(w_{mj}^{(h)}) + \right. \\
 157 \quad & \left. \sum_{n=0}^q Q(t - n) \cdot w_{nj}^{(h)} + b_j^{(h)} \right) \quad (1a)
 \end{aligned}$$

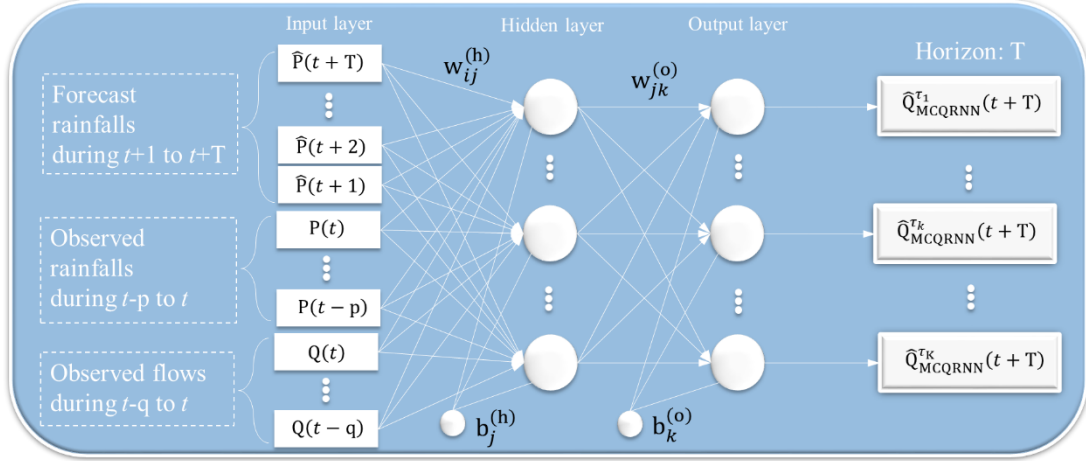


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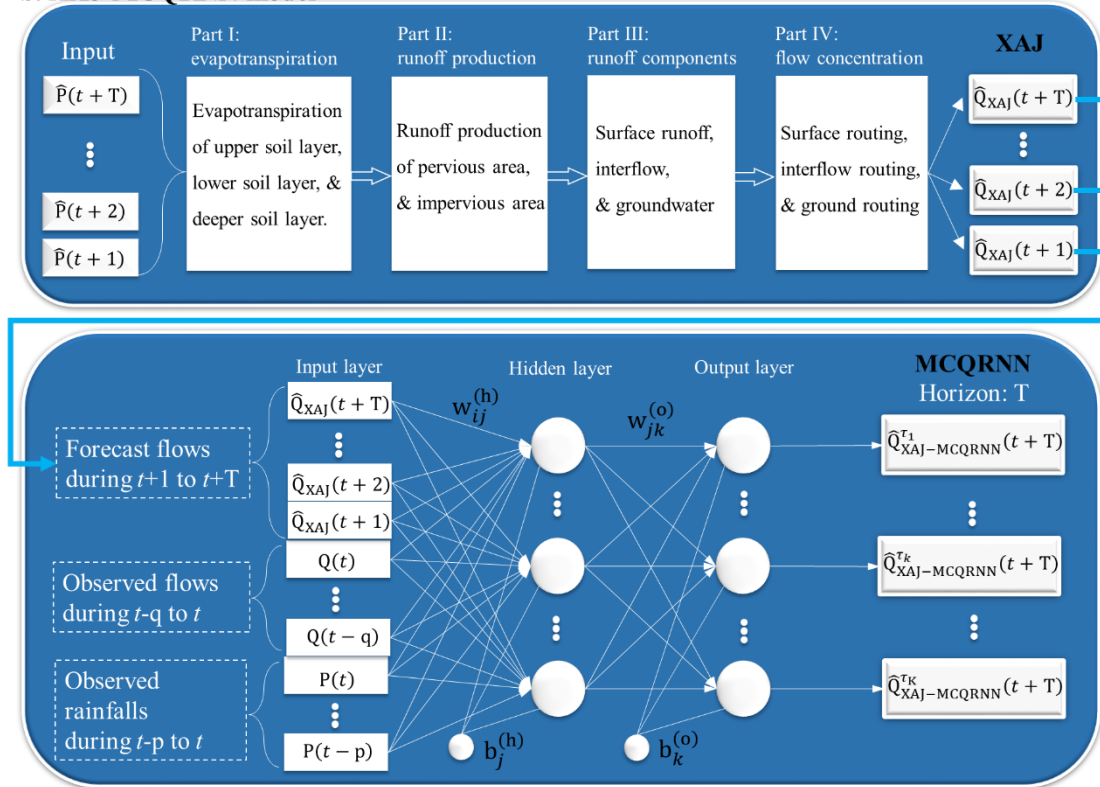
$$\widehat{Q}_{MCQRNN}^{\tau_k}(t+T) = g \left[ \sum_{j=1}^J h_j(t+T) \cdot \exp(w_{jk}^{(o)}) + b_k^{(o)} \right] \quad (1b)$$

159

### a. MCQRNN model



### b. XAJ-MCQRNN model



160

161 **Fig. 1** Main architectures adopted in this study. a. Monotone composite QRNN model162 (MCQRNN). b. Proposed XAJ-MCQRNN model.  $w_{ij}^{(h)}$ ,  $b_j^{(h)}$ ,  $w_{jk}^{(o)}$  and  $b_k^{(o)}$  are the163 parameters in hidden and output layers of MCQRNN model.  $\widehat{Q}_{MCQRNN}(t+T)$  is the164 forecast streamflow of MCQRNN model at horizon  $t+T$ .  $\widehat{Q}_{XAJ}(t+1), \dots, \widehat{Q}_{XAJ}(t+T)$ 165 are the forecast streamflows of XAJ model during horizons  $t+1$  up to  $t+T$ .166  $\widehat{Q}_{XAJ-MCQRNN}^{\tau_k}(t+T)$  is the forecast streamflow of XAJ-MCQRNN model with  $\tau_k$ 167 quantile at horizon  $t+T$ .  $t$  and  $T$  are the current time and forecast horizon, respectively.

168

169 where  $h_j(t + T)$  and  $\widehat{Q}_{\text{MCQRNN}}^{\tau_k}(t + T)$  are the  $j$ th node's output transformed from  
 170 input variables in the hidden layer and the model output with the  $\tau_k$  quantile ( $1 \leq k \leq K$ )  
 171 in the output layer at horizon  $T$ , respectively.  $\widehat{P}(t + s)$  is the forecast rainfall at  
 172 horizon  $s$  ( $1 \leq s \leq T$ ).  $P(t - m)$  and  $Q(t - n)$  are the  $m$ th antecedent rainfall and the  
 173  $n$ th antecedent streamflow, respectively.  $f(\cdot)$  is the hyperbolic tangent function in the  
 174 hidden layer.  $g(\cdot)$  is the sigmoid transfer function in the output layer.  $k$  and  $j$  are the  
 175 indexes of quantile and node, respectively.  $p$  and  $q$  are the numbers of antecedent  
 176 rainfall and antecedent streamflow variables at horizon  $T$ , respectively.  $w_{sj}^{(h)}$  is the  
 177 weight parameter which connects the  $s$ th forecast rainfall and the  $j$ th node in the  
 178 hidden layer, where the superscript (h) represents the hidden layer.  $w_{mj}^{(h)}$  and  $w_{nj}^{(h)}$   
 179 are the weight parameters which connects the  $m$ th ( $n$ th) antecedent rainfall  
 180 (streamflow) input variable and the  $j$ th node in the hidden layer, respectively.  $b_j^{(h)}$  is  
 181 the intercept parameter of the  $j$ th node in the hidden layer.  $w_{jk}^{(o)}$  and  $b_k^{(o)}$  are the  $j$ th  
 182 weight and the intercept parameter of the  $k$ th quantile in the output layer, respectively,  
 183 where the superscript (o) represents the output layer.  $J$  is the number of nodes.

184 To enhance the stability of model training, regularization terms are integrated into  
 185 the error function to penalize the magnitude of the weight parameters within hidden and  
 186 output layers, as described below.

$$187 \quad \rho_{\tau_k}(\varepsilon) = \begin{cases} \tau_k \cdot \varphi(\varepsilon) & \varepsilon \geq 0 \\ (\tau_k - 1) \cdot \varphi(\varepsilon) & \varepsilon < 0 \end{cases} \quad (2a)$$

$$188 \quad \varphi(\varepsilon) = \begin{cases} \frac{\varepsilon^2}{2\alpha} & 0 \leq |\varepsilon| \leq \alpha \\ |\varepsilon| - \frac{\alpha}{2} & |\varepsilon| > \alpha \end{cases} \quad (2b)$$

$$189 \quad E = \sum_{k=1}^K \omega_{\tau_k} \cdot \sum_{t=1}^D \rho_{\tau_k} \left( Q(t + T) - \widehat{Q}_{\text{MCQRNN}}^{\tau_k}(t + T) \right) \quad (2c)$$

190 
$$\tilde{E} = E + \lambda^{(h)} \cdot \frac{1}{(T+p+q) \cdot J} \sum_{i=1}^{(T+p+q)} \sum_{j=1}^J \left( w_{ij}^{(h)} \right)^2 + \lambda^{(o)} \cdot \frac{1}{J} \sum_{j=1}^J \left( w_{jk}^{(o)} \right)^2 \quad (2d)$$

191 where  $\rho_{\tau_k}(\varepsilon)$  and  $\varphi(\varepsilon)$  are the Huber-norm function (Chen, 2007) with the  $\tau_k$   
 192 quantile and the Huber function (Huber, 1964) with the variable  $\varepsilon$ , respectively.  $|\varepsilon|$   
 193 and  $\alpha$  are the absolute error and the given positive value, respectively. The Huber  
 194 function transforms smoothly from the squared error, which is applied around the  
 195 origin ( $\alpha$ ) to accomplish differentiability, and the absolute error.  $\omega_{\tau_k}$  is the weight  
 196 that represents the contribution of the forecast streamflow with the  $\tau_k$  quantile to the  
 197 total error.  $Q(t + T)$  is the observed streamflow.  $K$  is the number of quantiles.  $\lambda^{(h)}$   
 198 and  $\lambda^{(o)}$  are the coefficients (i.e., regularization items) that denote the penalties  
 199 applied to the weight parameters in hidden and output layers, respectively.  $i$  is the  
 200 index of input variable.  $w_{ij}^{(h)}$  is the weight parameter for connecting the  $i$ th input  
 201 variable and the  $j$ th node in the hidden layer.  $D$  is the number of input data.  $E$  and  
 202  $\tilde{E}$  are the error functions without (the former) and with (the latter) regularization items  
 203 considering the Huber-norm approximation, respectively.

204 In the case of the specified model architecture (i.e. three layers, shown in Fig. 1(a))  
 205 with the numbers of input variables ( $V$ ), hidden nodes ( $J$ ), and output variables ( $O$ ),  
 206 the total number of weight and intercept parameters in the MCQRNN model is the  
 207 sum of  $(V \times J + J \times O)$  weight parameters and  $(J + O)$  intercept parameters.

## 208 **2.2 Xinanjiang (XAJ) conceptual hydrological model**

209 The XAJ model is a conceptual rainfall-runoff model suitable for flood forecasts of  
 210 humid and semi-humid catchments (Zhao, 1992). From the viewpoint of model  
 211 architecture, the XAJ model has four implementation phases (Fig. 1(b)). Part I is to

212 compute evapotranspiration by three representative soil layers. Part II is to calculate  
 213 runoff production under runoff formation on repletion of storage. Part III is to separate  
 214 total runoff into the components of surface runoff, interflow and groundwater. Part IV  
 215 is to compute flow concentrations by means of the Nash Unit Hydrograph and  
 216 Muskingum routing. The advantage of the XAJ model is that the model has not only  
 217 the explicit physical meaning of rainfall-runoff processes but also a simple manner for  
 218 flood forecasting. The mathematical equation of the rainfall-runoff process in the XAJ  
 219 model during horizons  $t+1$  up to  $t+T$  is depicted as follows.

$$220 \quad \widehat{\mathbf{Q}}_{\text{XAJ}}^T = \phi[\widehat{P}(t+1), \widehat{P}(t+2), \dots, \widehat{P}(t+T)] \quad (3a)$$

$$221 \quad \widehat{\mathbf{Q}}_{\text{XAJ}}^T = [\widehat{Q}_{\text{XAJ}}(t+1), \widehat{Q}_{\text{XAJ}}(t+2), \dots, \widehat{Q}_{\text{XAJ}}(t+T)] \quad (3b)$$

222 where  $\widehat{\mathbf{Q}}_{\text{XAJ}}^T$  is the vector of the XAJ model output with lead time  $T$ .  $\widehat{P}(t+T)$  and  
 223  $\widehat{Q}_{\text{XAJ}}(t+T)$  are the forecast rainfall (i.e., model input) and flow (i.e., model output) at  
 224 horizon  $t+T$ , respectively.  $\phi[\cdot]$  is the transformation function of rainfall-runoff  
 225 processes including four parts (Fig. 1(b)).

226 The XAJ model has 15 parameters, including 4 evapotranspiration parameters, 3  
 227 runoff production parameters, 4 runoff separation parameters, and 4 flow concentration  
 228 parameters. Owing to the effectiveness and practicality, the Shuffled Complex  
 229 Evolution method developed at The University of Arizona (SCE-UA) (Duan et al., 1994)  
 230 was adopted to optimize the XAJ model parameters in this study. More details on the  
 231 XAJ model can be found in Zhao (1992).

### 232 ***2.3 Hybridization of the XAJ and MCQRNN (XAJ-MCQRNN)***

233 The comparison between MCQRNN (Fig. 1(a)) and XAJ-MCQRNN (Fig. 1(b)) models

234 established in this study is summarized as follows: when making FPD forecasts, the  
 235 former adopts the forecast rainfall data ( $\hat{P}(t + 1), \hat{P}(t + 2), \dots, \hat{P}(t + T)$ ) provided by  
 236 available numerical forecast products as input variables to test the model during  
 237 horizons  $t+1$  up to  $t+T$ , while the latter adopts the forecast streamflow data  
 238  $\hat{Q}_{XAJ}(t + 1), \hat{Q}_{XAJ}(t + 2), \dots, \hat{Q}_{XAJ}(t + T)$  made by the XAJ model during horizons  
 239  $t+1$  up to  $t+T$  as input variables to test the model.

240 From the perspective of model complementarity, the XAJ model can produce stable  
 241 point forecasts of flood hydrographs so that the MCQRNN model can create more  
 242 accurate and reliable FPD forecasts after being supplied with point forecasts by the XAJ  
 243 model. The general equation of the proposed hybrid model for the quantile  $\tau_k$  is  
 244 described below.

$$245 \quad \hat{Q}_{XAJ-MCQRNN}^{\tau_k}(t + T) = \psi[\hat{Q}_{XAJ}(t + T), \dots, \hat{Q}_{XAJ}(t + 2), \hat{Q}_{XAJ}(t + 1), Q(t),$$

$$246 \quad Q(t - 1), \dots, Q(t - q), P(t), P(t - 1), \dots, P(t - p)] \quad (4)$$

247 where  $\hat{Q}_{XAJ-MCQRNN}^{\tau_k}(t + T)$  is the forecast streamflow of the XAJ-MCQRNN model  
 248 with the quantile  $\tau_k$  at horizon  $t+T$ .  $\psi[\cdot]$  is the quantile regression function that is the  
 249 combination of the hyperbolic tangent function  $f(\cdot)$  in the hidden layer and the sigmoid  
 250 transfer function  $g(\cdot)$  in the output layer.

#### 251 ***2.4 Training process of the MCQRNN model***

252 The gradient-based nonlinear optimization algorithm (Kingma and Ba, 2015; Cannon,  
 253 2018) was used to optimize the weight ( $w_{sj}^{(h)}$ ,  $w_{mj}^{(h)}$ ,  $w_{nj}^{(h)}$  and  $w_{jk}^{(o)}$  in Eqs. 1(a) and  
 254 1(b)) and intercept ( $b_j^{(h)}$  and  $b_k^{(o)}$  in Eqs. 1(a) and 1(b)) parameters of the MCQRNN  
 255 while the training process of the XAJ-MCQRNN was performed after being supplied

256 with point forecasts by the XAJ at the same time. Furthermore, the Genetic Algorithm  
257 (GA) (Goldberg and Deb, 1991; Zhou et al., 2019) was used to optimize the  
258 hyperparameters (the maximal iteration  $I_{\max}$ , the number of nodes  $J$ , the regulation  
259 coefficients  $\lambda^{(h)}$  and  $\lambda^{(o)}$ , and the learning rate  $\eta$ ). Fig. 2 illustrates the flow chart of  
260 the XAJ-MCQRNN training process. The implementation procedure is described as  
261 follows.

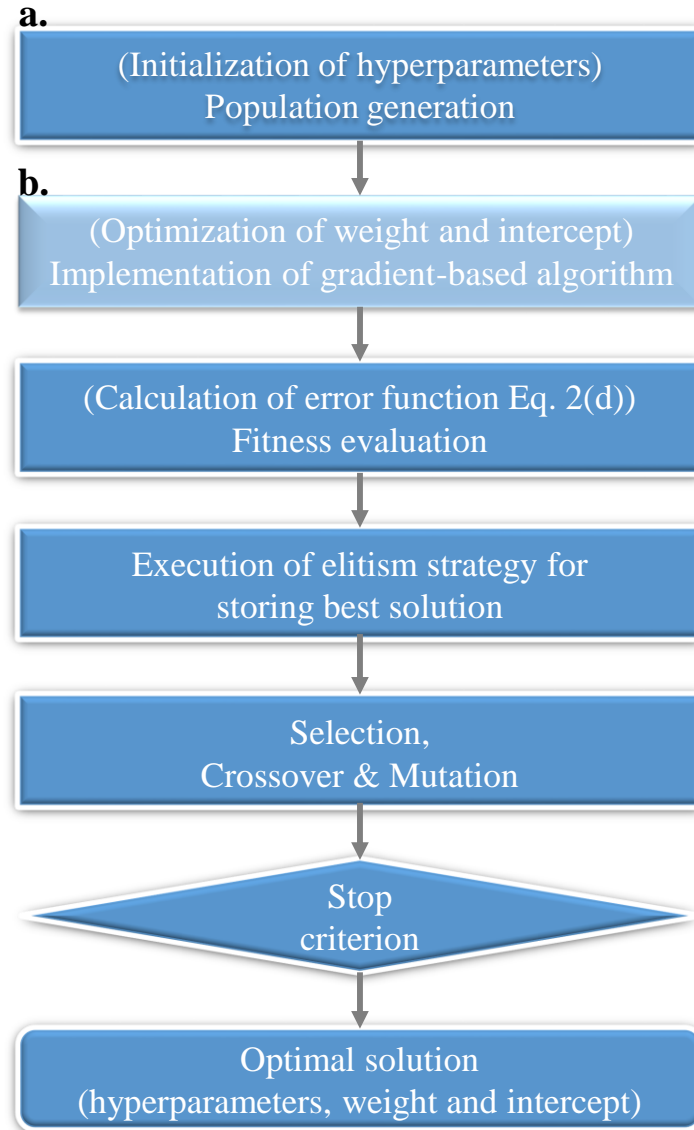
262 Step 1: Randomly generate an initial population  $X_0$  of size  $I_{\text{pop}}$  with respect to the  
263 hyperparameters. Integer-coded and real-coded solutions are adopted for  
264 hyperparameters  $I_{\max}$  and  $J$  as well as for hyperparameters  $\lambda^{(h)}$ ,  $\lambda^{(o)}$  and  $\eta$ ,  
265 respectively. The search spaces of  $I_{\max}$ ,  $J$ ,  $\lambda^{(h)}$ ,  $\lambda^{(o)}$  and  $\alpha$  are set to be [200,  
266 500], [1, 30], [0.001, 0.01], [0.001, 0.01] and [0.001, 0.05], respectively.

267 Step 2: Perform the gradient-based nonlinear optimization algorithm for optimizing  
268 weight and intercept parameters of the MCQRNN model, and execute the  
269 tournament selection, the crossover operator with probability ( $P_c$ ) and the mutation  
270 operator with probability ( $P_m$ ) to create an offspring population  $Y_0$  of size  $I_{\text{pop}}$ .

271 Step 3: Evaluate the fitness values of  $Y_u$  for the  $u$ th generation, combine  $Y_{u-1}$  and  $Y_u$   
272 into an intermediate population  $X_u$  of size  $2 * I_{\text{pop}}$ , partition this combined  
273 population into different ranks according to fitness values, and store the best  
274 solution using the elitism strategy.

275 Step 4: Implement the tournament selection to select a new parent population  $X_{u+1}$  of  
276 size  $I_{\text{pop}}$  from  $X_u$ , create an offspring population  $Y_{u+1}$  using crossover and mutation  
277 operators, and evaluate their fitness values.

278 Step 5: Repeat Steps 3 and 4 when the generation number  $u$  is smaller than the maximal  
 279 generation ( $G_{\max}$ ). Otherwise, output the optimal results after stopping iteration.



280  
 281 **Fig. 2** Flow diagram of the XAJ-MCQRNN model trained simultaneously by: a. the  
 282 Genetic Algorithm applied to the optimization of hyperparameters; b. the gradient-  
 283 based nonlinear optimization algorithm applied to the optimization of weight and  
 284 intercept parameters.

285

286 In this study, the population size ( $I_{\text{pop}}$ ), the maximal generation ( $G_{\max}$ ), the  
 287 crossover probability ( $P_c$ ) and the mutation probability ( $P_m$ ) of GA were set to be 200,  
 288 100, 0.85 and 0.1, respectively. The aforementioned computations regarding the GA,

289 XAJ model and MCQRNN model are conducted in R software ([https://www.r-](https://www.r-project.org/)  
 290 [project.org/](https://www.r-project.org/)), where the computation of the MCQRNN is based on the freely available  
 291 QRNN package (<https://CRAN.R-project.org/package=qrnn>).

292 As river streamflow data are time series, this study applied the Root Mean Square  
 293 Error (RMSE), the Nash-Sutcliffe Efficiency (NSE) and the Mutual Information (MI)  
 294 to evaluate the point forecast results of the two MCQRNN models. The RMSE value  
 295 indicates the error between forecasts and observations, and its value ranges from 0 to  
 296 infinity (Legates and McCabe, 1999). The NSE is commonly employed to evaluate the  
 297 forecast accuracy of hydrological models and its value ranges from negative infinity to  
 298 1 (Nash and Sutcliffe, 1970). Considering that the upper bound (=1) of the NSE doesn't  
 299 leave much room for improvement, a logarithm conversion for the NSE (LNSE) is used  
 300 instead of an unbounded quality indicator to evaluate model accuracy. The MI value  
 301 suggests the goodness-of-fit between forecasts and observations, and its value ranges  
 302 from 0 to infinity (Shannon, 1948). A model with low RMSE and high LNSE and MI  
 303 values suggests it can produce high forecast accuracy. The computations of RMSE,  
 304 LNSE and MI values are described below.

$$305 \quad \text{RMSE} = \sqrt{\frac{1}{D} \sum_{t=1}^D \left( Q(t+T) - \widehat{Q}_{\text{Model}}^{\tau_k}(t+T) \right)^2} \quad (5)$$

$$306 \quad \text{LNSE} = -\ln(1 - \text{NSE}) = -\ln\left(\frac{\sum_{t=1}^D \left( Q(t+T) - \widehat{Q}_{\text{Model}}^{\tau_k}(t+T) \right)^2}{\sum_{t=1}^D (Q(t+T) - \bar{Q}_T)^2}\right) \quad (6)$$

$$307 \quad \text{MI} = \sum_{t=1}^D \sum_{t=1}^D p\left(Q(t+T), \widehat{Q}_{\text{Model}}^{\tau_k}(t+T)\right) \log_2 \left( \frac{p\left(Q(t+T), \widehat{Q}_{\text{Model}}^{\tau_k}(t+T)\right)}{p(Q(t+T))f\left(\widehat{Q}_{\text{Model}}^{\tau_k}(t+T)\right)} \right) \quad (7)$$

308 where  $\widehat{Q}_{\text{Model}}^{\tau_k}(t+T)$  is the forecast value of a model (MCQRNN or XAJ-MCQRNN)  
 309 with the  $\tau_k$  quantile at horizon T.  $\bar{Q}_T$  is the average of observed values at horizon T.



310  $p(\cdot, \cdot)$  is the joint probability density function of observations and forecasts.  $p(\cdot)$  is the  
 311 probability density function of observations or forecasts. The median (i.e.,  $\tau_k=0.5$ )  
 312 forecasts of a model are commonly employed to evaluate the prediction accuracy of  
 313 point forecast results (Zhou et al., 2020).

314 The Coverage Ratio (CR) of the forecast interval relative to observations and the  
 315 Relative Bandwidth (RB) of the forecast interval (Xiong and O'Connor, 2008) were  
 316 used to evaluate the accuracy of the forecast interval results in this study. The CR  
 317 represents the coverage interval of the forecasts and its value ranges from 0 to 100%.  
 318 The RB represents the width of the forecast interval and its value ranges from 0 to  
 319 infinity. A model with its CR value closer to 100% and its RB closer to 0 implies it can  
 320 forecast more accurately. The computations of CR and RB values are depicted as  
 321 follows.

$$322 \quad CR = \frac{1}{D} \times \sum_{t=1}^D \theta_t \times 100\%, \quad \theta_t = \begin{cases} 1, & Q(t+T) \in [\hat{Q}_L(t+T), \hat{Q}_U(t+T)] \\ 0, & Q(t+T) \notin [\hat{Q}_L(t+T), \hat{Q}_U(t+T)] \end{cases} \quad (8)$$

$$323 \quad RB = \frac{1}{D} \times \sum_{t=1}^D \left( \frac{\hat{Q}_U(t+T) - \hat{Q}_L(t+T)}{Q(t+T)} \right) \times 100\% \quad (9)$$

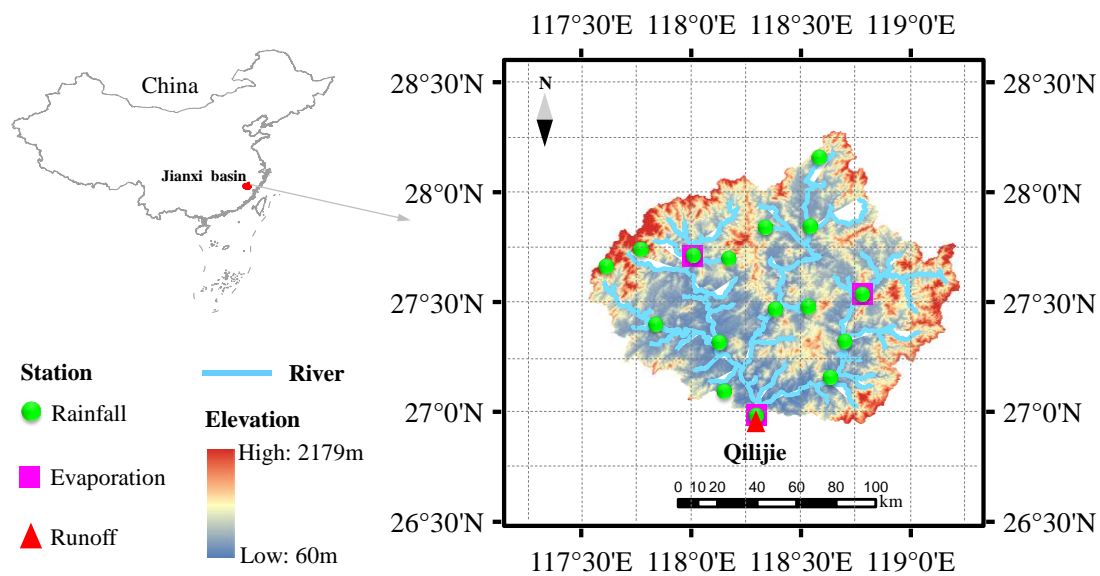
324 where  $\hat{Q}_L(t+T)$  and  $\hat{Q}_U(t+T)$  are the lower and upper boundaries of forecast  
 325 interval results at horizon T with respect to a given confidence level (e.g. 90%),  
 326 respectively (e.g. L=5%, U=95%). The  $\theta_t$  values are either one or zero, in which one  
 327 implies the observed data fall within its forecast intervals while zero implies the  
 328 observed data fall outside of its forecast intervals at  $t$  time.

329

### 330 **3 Study area and materials**

#### 331 **3.1 Study area**

332 The Jianxi River catchment with an area of 14787 km<sup>2</sup> is located in southern China (Fig.  
 333 3). The catchment climate is affected by the southwest Indian Ocean and southeast  
 334 Pacific Ocean subtropical monsoons and regional landforms (Lin et al., 2020). The  
 335 annual rainfall ranges from 1800 mm to 2200 mm and the annual runoff ranges from  
 336 950 to 1700 mm, the highest amount (74%) of which occurs within six months  
 337 (April–September). Due to the moist and rainy features as well as red, yellow, and  
 338 paddy soils, runoff production of this catchment is dominated by the runoff generation  
 339 on repletion of storage, which is in line with the typical rainfall-runoff characteristics  
 340 in southern China.



341  
 342 **Fig. 3** Locations of the Jianxi River catchment and hydro-meteorological (rainfall,  
 343 evaporation and runoff) gauge stations.

### 345 **3.2 Materials**

346 This study collected the data associated with flood events during the flood season  
 347 (April 1st–September 30th), including the 3-hour (time step) rainfall data of 16 gauge  
 348 stations, the 3-hour evaporation of 3 gauge stations and the 3-hour streamflow data of

349 the Qilijie hydrological station from 2009 to 2015, and the 3-hour forecast rainfall of  
350 ERA-Interim datasets of the European Centre for Medium-Range Weather Forecasts  
351 (ECMWF) from 2014 to 2015. The spatial resolution of each grid in ERA-Interim is  
352  $0.125^{\circ}\text{E}\times 0.125^{\circ}\text{N}$ , while 32 grid points are required to fully cover the Jianxi River  
353 catchment (Fig. 3). More details on the ERA-Interim datasets of the ECMWF can be  
354 found in Berrisford et al. (2011). The areal mean value of observed rainfall data was  
355 calculated by using the datasets of 16 gauge stations colored in green (Fig. 3), the areal  
356 mean value of observed evaporation data was calculated by using the datasets of 3  
357 gauge stations colored in purple (Fig. 3), and the areal mean value of forecast rainfall  
358 data was calculated by using the datasets of 32 grid points through the Thiessen polygon  
359 method (Thiessen, 1911).

360 A total of 20448 ( $=8 \text{ time step} \times 365 \text{ days} \times 6 \text{ non-leap years} + 8 \text{ time step} \times 366$   
361  $\text{days} \times 1 \text{ leap year}$ ) time series values were divided into three datasets for model training  
362 (8760 from 2009-2011), validation (5848 from 2012-2013), and testing (5840 from  
363 2014-2015). The training dataset was applied to adjusting the parameters (weights and  
364 intercepts) of the XAJ model (the MCQRNN model). The validation dataset was  
365 applied to checking whether a prediction model is overfitted or undertrained. The test  
366 dataset was applied to evaluating the model prediction accuracy.

### 367 ***3.3 Model construction***

368 A 12-hour forecast horizon has been considered in this study since the longest transform  
369 time in the rainfall-runoff processes is 12 hours in this catchment. Besides, the current  
370 forecast horizon at the Qilijie station is only 6 hours, inducing the demand for

371 improving the lead time and forecast accuracy. In the light of the observed 3-hour  
 372 rainfall-runoff datasets of the Jianxi River catchment, the model output was set to be  
 373  $t+1$  (Horizon=3 hours) up to  $t+4$  (Horizon=12 hours) time-step-ahead streamflow,  
 374 where  $t$  is the current time.

375 As aforementioned, the GA was performed to determine the optimal  
 376 hyperparameters in association with MCQRNN models at four horizons. The optimal  
 377 values of the maximal iteration ( $I_{\max}$ ), the number of nodes ( $J$ ), the regulation  
 378 coefficients ( $\lambda^{(h)}$  and  $\lambda^{(o)}$ ) and the learning rate ( $\eta$ ) were 300, 12, 0.006, 0.004 and  
 379 0.009, respectively, while the weight and intercept parameters optimized by the  
 380 gradient-based nonlinear optimization algorithm within the QRNN package were  
 381 adopted in this study.

382 This study adopted the Partial Mutual Information and Partial Weights (PMI-PW)  
 383 method (Sharma et al., 2016) to quantify the contribution of input combination to model  
 384 performance (Table 1). To estimate the input variables weights for constructing the  
 385 MCQRNN and XAJ-MCQRNN models, the following framework was adopted. Apart  
 386 from the observed streamflow and rainfall data (traced back to the previous 12 hours),  
 387 the rainfall of the ERA-Interim during horizon  $t+1$  up to  $t+4$  was used to train, validate  
 388 and test the former, while the forecast streamflow of the XAJ model during horizon  $t+1$   
 389 up to  $t+4$  was used to train, validate and test the latter.

390  
 391 **Table 1** Weights of input variables for constructing models by the Partial Mutual  
 392 Information and Partial Weights (PMI-PW) method

Variable	Input combination	Contribution			
		Horizon $t+1$	Horizon $t+2$	Horizon $t+3$	Horizon $t+4$

		MCQRNN	XAJ- MCQRNN	MCQRNN	XAJ- MCQRNN	MCQRNN	XAJ- MCQRNN	MCQRNN	XAJ- MCQRNN
Rainfall	P( $t+4$ )							0.03	
	P( $t+3$ )					0.04		0.06	
	P( $t+2$ )			0.05		0.06		0.08	
	P( $t+1$ )	0.05		0.06		0.09		0.10	
	P( $t$ )	0.07	0.07	0.09	0.08	0.11	0.09	0.17	0.15
	P( $t-1$ )	0.09	0.09	0.11	0.11	0.15	0.14	0.09	0.10
	P( $t-2$ )	0.12	0.10	0.17	0.13	0.08	0.09	0.06	0.06
	P( $t-3$ )	0.18	0.14	0.08	0.09	0.04	0.04	0.02	0.05
Forecast	$\widehat{Q}_{XAJ}(t+4)$								0.25
streamflow of XAJ model	$\widehat{Q}_{XAJ}(t+3)$						0.23		0.19
	$\widehat{Q}_{XAJ}(t+2)$				0.22		0.17		0.10
	$\widehat{Q}_{XAJ}(t+1)$		0.20		0.14		0.11		0.06
Observed streamflow	Q( $t$ )	0.20	0.18	0.21	0.11	0.24	0.09	0.25	0.04
	Q( $t-1$ )	0.15	0.09	0.13	0.08	0.12	0.04	0.09	
	Q( $t-2$ )	0.09	0.07	0.07	0.04	0.05		0.04	
	Q( $t-3$ )	0.05	0.06	0.03		0.02		0.01	
	Sum	1	1	1	1	1	1	1	1

393

## 394 4 Results

395 To improve the predictability and reliability of FPD forecasts, this study intends to  
396 explore and evaluate the accuracy of the XAJ model coupled with the MCQRNN on  
397 short-term (12 hours) flood forecasts at different horizons. The results, findings and  
398 discussion were as follows.

### 399 4.1 Reliability of XAJ and MCQRNN models on point forecasts of flood processes

400 The point forecasts of floods under the circumstance of the quantile  $\tau_k=0.5$  (i.e. median  
401 forecasts) were specified to test the reliability of the constructed models. Table 2  
402 summarizes the RMSE, LNSE and MI values of the XAJ, MCQRNN and XAJ-  
403 MCQRNN models in training, validation and testing stages at four horizons. It is  
404 apparent from this table that the XAJ-MCQRNN model performs better than the XAJ  
405 and MCQRNN models in the three stages at four horizons. Take the testing stage for

406 example, the LNSE and MI values of the XAJ-MCQRNN model exceed 0.90 and 22  
 407 respectively while the RMSE values are less than 140 m<sup>3</sup>/s.

408 Two main results are acquired from the Table 2. Firstly, the comparison of the XAJ-  
 409 MCQRNN and XAJ models in the testing stage reveals that there are significant  
 410 differences in the improvement rates of RMSE and NSE values at four horizons. The  
 411 improvement rates of RMSE (LNSE & MI) for median flood forecasting reach 4.7%  
 412 (9.0% & 4.3%) and 5.2% (17.0% & 6.1%) at horizons  $t+1$  and  $t+2$ , respectively, while  
 413 they increased to 6.6% (22.2% & 8.8%) and 8.1% (28.4% & 11.2%) at horizons  $t+3$   
 414 and  $t+4$ , respectively. Secondly, the comparison of the XAJ-MCQRNN and MCQRNN  
 415 models in the testing stage points out that the former can provide stable forecast results  
 416 after being supplied with point forecasts by the XAJ model either at shorter horizons  
 417 ( $t+1$  and  $t+2$ ) or at longer horizons ( $t+3$  and  $t+4$ ). That is to say, the XAJ-MCQRNN  
 418 model can effectively extract the dependence between rainfall and runoff processes  
 419 even in the case of the 12-hour forecast horizon. The fluctuations of forecast rainfalls  
 420 are stronger at long horizons ( $t+3$  and  $t+4$ ) than at short horizons ( $t+1$  and  $t+2$ ). Higher  
 421 fluctuations of forecast rainfall data are easy to induce overfitting problems, which  
 422 would demand more complex models to mimic the relationship between rainfall and  
 423 runoff. This is considered as a driver to improve the forecast of the XAJ-MCQRNN  
 424 model.

425  
 426

427 **Table 2** Results of Root Mean Square Error (RMSE), Nash-Sutcliffe Efficiency (NSE)  
 428 and Mutual Information (MI) values acquired from the XAJ, MCQRNN and XAJ-  
 429 MCQRNN models in training, validation and testing stages

Stage	Horizon	RMSE (m <sup>3</sup> /s)	LNSE	MI
-------	---------	--------------------------	------	----

		XAJ	MCQRNN	XAJ- MCQRNN	XAJ	MCQRNN	XAJ- MCQRNN	XAJ	MCQRNN	XAJ- MCQRNN
Training	$t+1$		71	68		3.91	3.91		1.87	1.94
	$t+2$		89	84		3.51	3.51		1.79	1.90
	$t+3$	91	115	106	3.22	3.00	3.22	1.75	1.68	1.85
	$t+4$		137	124		2.53	2.81		1.54	1.78
Validation	$t+1$		77	73		3.51	3.51		1.85	1.93
	$t+2$		94	88		3.22	3.51		1.78	1.91
	$t+3$	102	121	111	3.00	2.66	3.00	1.72	1.69	1.84
	$t+4$		146	130		2.41	2.81		1.60	1.77
Testing	$t+1$	84	90	80 (4.7)*	3.22	3.22	3.51 (9.0)	1.85	1.85	1.93 (4.3)
	$t+2$	96	103	91 (5.2)	3.00	3.00	3.51 (17.0)	1.79	1.74	1.90 (6.1)
	$t+3$	122	131	114 (6.6)	2.41	2.30	2.81 (22.2)	1.70	1.67	1.85 (8.8)
	$t+4$	149	168	137 (8.1)	2.12	1.97	2.53 (28.4)	1.61	1.56	1.79 (11.2)

430 \* The number in the bracket is the improvement rate of the XAJ-MCQRNN model over the XAJ  
431 model.

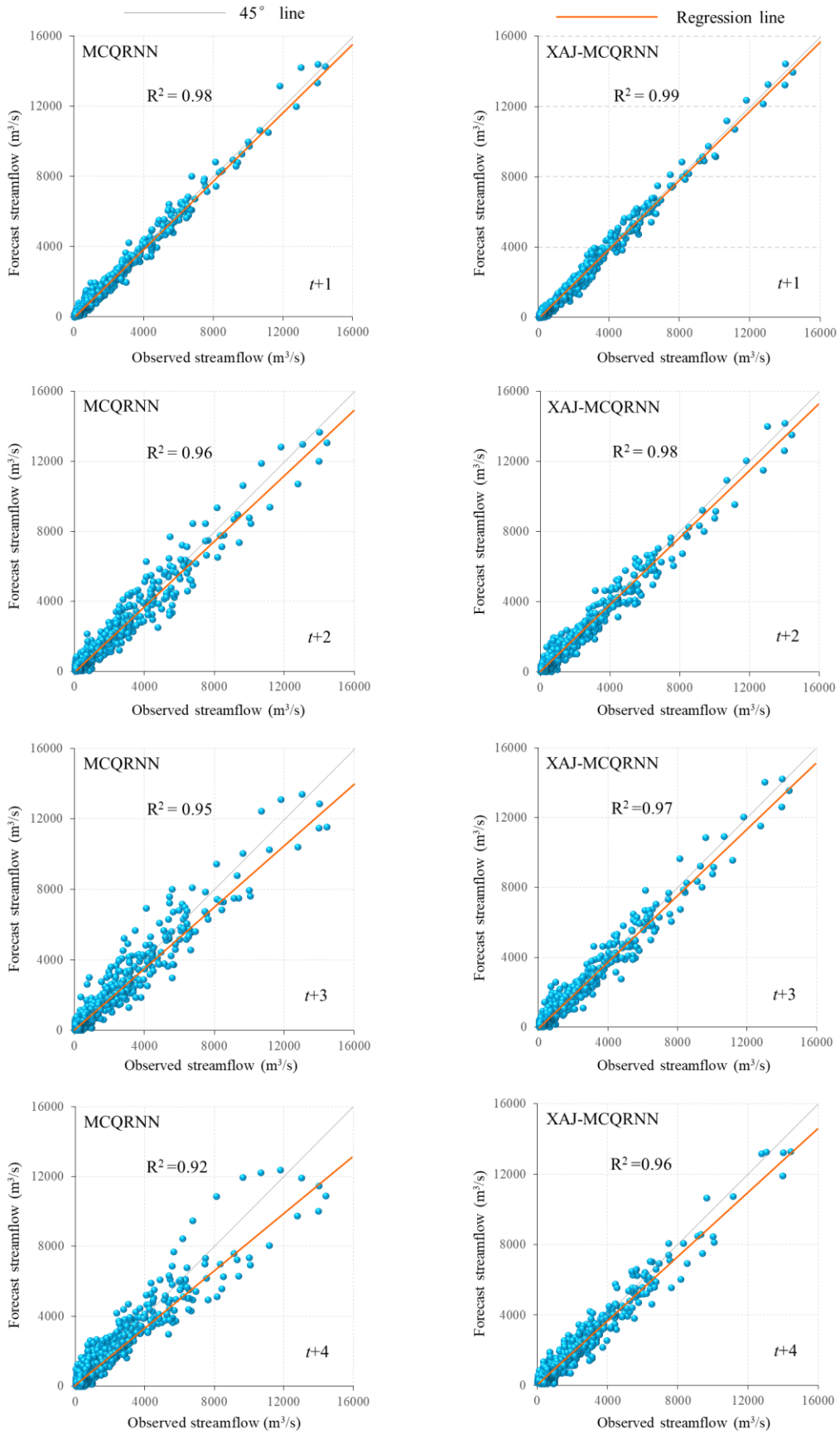
432

433 To further evaluate the forecast accuracy of MCQRNN models for making median  
434 forecasts of floods, the regression analysis of the observed and forecast streamflow data  
435 is presented in Fig. 4. It is too hard to judge the difference in model quality when the  
436 correlation between observations and forecasts is high. However, this is different for  
437 the case of low correlation, where the gap between the regression and 45-degree lines  
438 is large. A large gap denotes a significant biased-prediction. From the standpoint of  
439 correlation (Fig. 4), the XAJ-MCQRNN model can more adequately alleviate the  
440 biased-prediction phenomenon (under-prediction in our case) because of the larger  
441 values of the coefficient of determination  $R^2$  as well as the smaller gaps between the  
442 regression and 45-degree lines, compared to the MCQRNN model. As expected, there  
443 are higher correlations between observations and forecasts at horizons  $t+1$  and  $t+2$ ,  
444 whereas larger improvements of the correlation between observations and forecasts  
445 occur at horizons  $t+3$  and  $t+4$ .

446 The hybrid model still consistently underestimates most flood processes (Fig. 4).

447 The back-fitting algorithm with the autoregressive strategy (Zhang et al., 2018) was  
448 performed to correct the systematic bias of point forecasts of the hybrid model. After  
449 implementing bias-correction, Table 3 summarizes the Kolmogorov-Smirnov (KS) test  
450 results from the standpoint of density distribution. Due to the high variation of flood  
451 datasets (streamflow value  $\geq 1000 \text{ m}^3/\text{s}$ ), the observations at each horizon are divided  
452 into three parts (Part I:  $1000 \text{ m}^3/\text{s} \leq \text{value} < 3000 \text{ m}^3/\text{s}$ ; Part II:  $3000 \text{ m}^3/\text{s} \leq \text{value} <$   
453  $9000 \text{ m}^3/\text{s}$ ; and Part III:  $\text{value} \geq 9000 \text{ m}^3/\text{s}$ ) to effectively examine the predictability of  
454 the proposed model at various flood magnitudes. The larger KS test indicator values  
455 suggest smaller difference between observed and forecast distributions and better  
456 model performance. Interestingly, the XAJ-MCQRNN model creates a pretty good  
457 similarity between observed and forecast distributions of the three parts at all horizons  
458 whereas the MCQRNN model only performs well when flood magnitudes are small  
459 (Part I). From the table, we can see that the probability density distribution of the  
460 forecasts acquired from the XAJ-MCQRNN model is more similar in shape to that of  
461 observations at each horizon. In other words, the values of the forecasts obtained from  
462 the XAJ-MCQRNN model in three parts are closer to those of observations, in  
463 comparison to the forecasts obtained from the MCQRNN model. The results  
464 demonstrate that the XAJ-MCQRNN model can not only sufficiently forecast the  
465 probability density distribution of flood data but also accurately forecast different flood  
466 magnitudes at four horizons.





467

468

469

**Fig. 4** Regression analysis between the observed streamflow data and the median forecasts of streamflow data in the testing stage at four horizons.

470

471 **Table 3** Kolmogorov Smirnov (KS) test results of the two distributions of observations  
 472 and forecasts in three parts for each given horizon at the testing stage

Model	Horizon	KS test indicator*		
		Part I: 1000 m <sup>3</sup> /s ≤ value < 3000 m <sup>3</sup> /s	Part II: 3000 m <sup>3</sup> /s ≤ value < 9000 m <sup>3</sup> /s	Part III: value ≥ 9000 m <sup>3</sup> /s
MCQRNN	t+1	0.03	0.06	0.08
	t+2	0.03	0.07	0.10
	t+3	0.04	0.10	0.13
	t+4	0.05	0.13	0.15
XAJ- MCQRNN	t+1	0.01	0.03	0.06
	t+2	0.01	0.04	0.06
	t+3	0.02	0.06	0.08
	t+4	0.03	0.07	0.09

473 \*The KS test is performed at a significance level of 0.05. The null hypothesis states that the  
 474 probability density distribution of forecasts is similar in shape to that of observations. If the value  
 475 of the KS test indicator is smaller than the value of D(n, 0.05) (=0.05, 0.09 and 0.11 for the Part I,  
 476 II and III, respectively), the null hypothesis would not be rejected.

477 In brief, the point (i.e., median) forecasts of floods made by the XAJ-MCQRNN  
 478 model offered solid evidence of good model performance and favorable stability in  
 479 multi-step-ahead flood forecasting. The next subsection is concerned with the  
 480 comparison of the MCQRNN and XAJ-MCQRNN models for making interval  
 481 forecasts of floods.

482 **4.2 Reliability of MCQRNN models on interval forecasts of flood processes**

483 The interval forecasts of floods for the case of the quantiles ( $0.01 \leq \tau_k \leq 0.99$ , with  
 484 an increment of 0.01) were employed to test the reliability of the two models  
 485 (MCQRNN and XAJ-MCQRNN). The back-fitting algorithm with the autoregressive  
 486 strategy (Zhang et al., 2018) was also executed to correct the systematic bias of interval  
 487 forecasts of the hybrid model. Table 4 provides the RB and CR values of the MCQRNN  
 488 and XAJ-MCQRNN models in three stages at four horizons. The results indicate that

489 the XAJ-MCQRNN model acquires pretty good forecast accuracy at all the horizons  
490 whereas the MCQRNN model only performs well at shorter horizons of  $t+1$  and  $t+2$   
491 (CR is higher than 92%, but RB is lower than 12%). For 12-hour forecasts, the XAJ-  
492 MCQRNN model can enhance the CR value by 1.5% up to 5.9% and decrease the RB  
493 values by 8.8% up to 25.7% in the testing stages, as compared with the MCQRNN  
494 model. This means the XAJ-MCQRNN model can not only significantly improve  
495 probabilistic forecast accuracy in terms of a narrow prediction interval (as represented  
496 by CR values) but also adequately eliminate the impacts of flood magnitudes on the  
497 bandwidth of the prediction intervals (as represented by RB values). The 12-hour  
498 forecast accuracy of the XAJ-MCQRNN model is superior to that of the MCQRNN  
499 model since the XAJ-MCQRNN model utilizes the streamflow forecasts made by the  
500 XAJ model to reduce the uncertainties of the rainfall forecasts from the ECMWF,  
501 whereas the MCQRNN model adopts the rainfall forecasts of the ECMWF to make  
502 multi-step-ahead flood forecasts in testing stages.

503

504 **Table 4** Results of Coverage Ratio (CR) and Relative Bandwidth (RB) values acquired  
505 from the MCQRNN and XAJ-MCQRNN models in training, validation and testing  
506 stages at four horizons

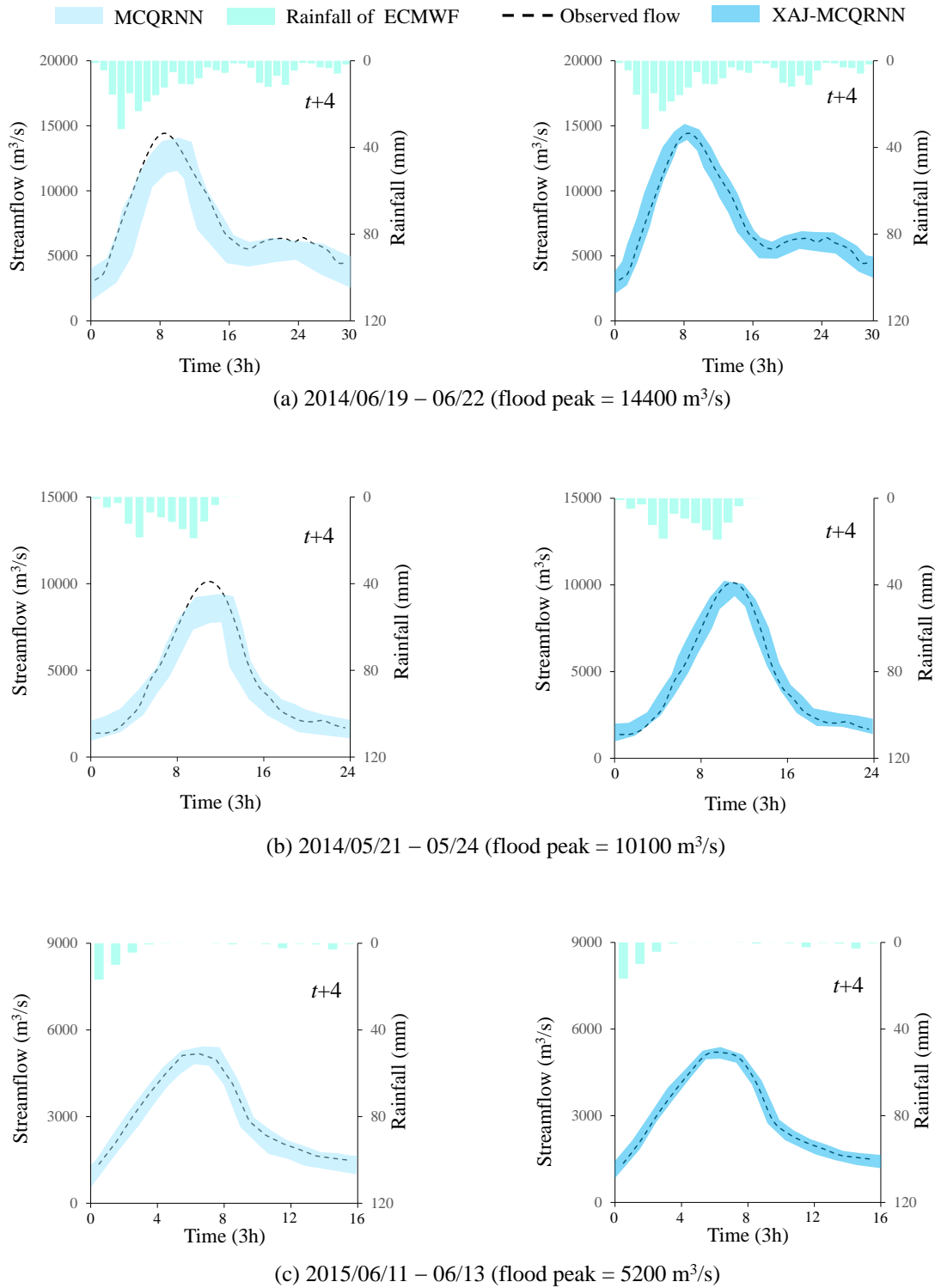
Stage	Horizon	RB (%)		CR (%)	
		MCQRNN	XAJ-MCQRNN	MCQRNN	XAJ-MCQRNN
Training	$t+1$	4.91	4.49 (8.5)*	95.17	96.98 (1.9)
	$t+2$	8.62	7.77 (9.9)	93.83	95.99 (2.3)
	$t+3$	12.56	11.20 (10.8)	90.60	94.04 (3.8)
	$t+4$	17.24	15.05 (12.7)	87.72	91.67 (4.5)
Validation	$t+1$	6.55	6.02 (8.1)	94.93	96.45 (1.6)
	$t+2$	10.10	9.15 (9.4)	93.26	95.31 (2.2)
	$t+3$	14.81	13.34 (9.9)	90.09	93.33 (3.6)
	$t+4$	19.37	16.62 (14.2)	86.36	90.07 (4.3)
Testing	$t+1$	8.16	7.44 (8.8)	94.32	95.73 (1.5)
	$t+2$	11.65	10.01 (14.1)	92.79	94.74 (2.1)

$t+3$	16.00	13.07 (18.3)	89.56	92.87 (3.7)
$t+4$	23.33	17.33 (25.7)	84.43	89.41 (5.9)

507 \* The number in the bracket is the improvement rate of the XAJ-MCQRNN model over the  
508 MCQRNN model.

509

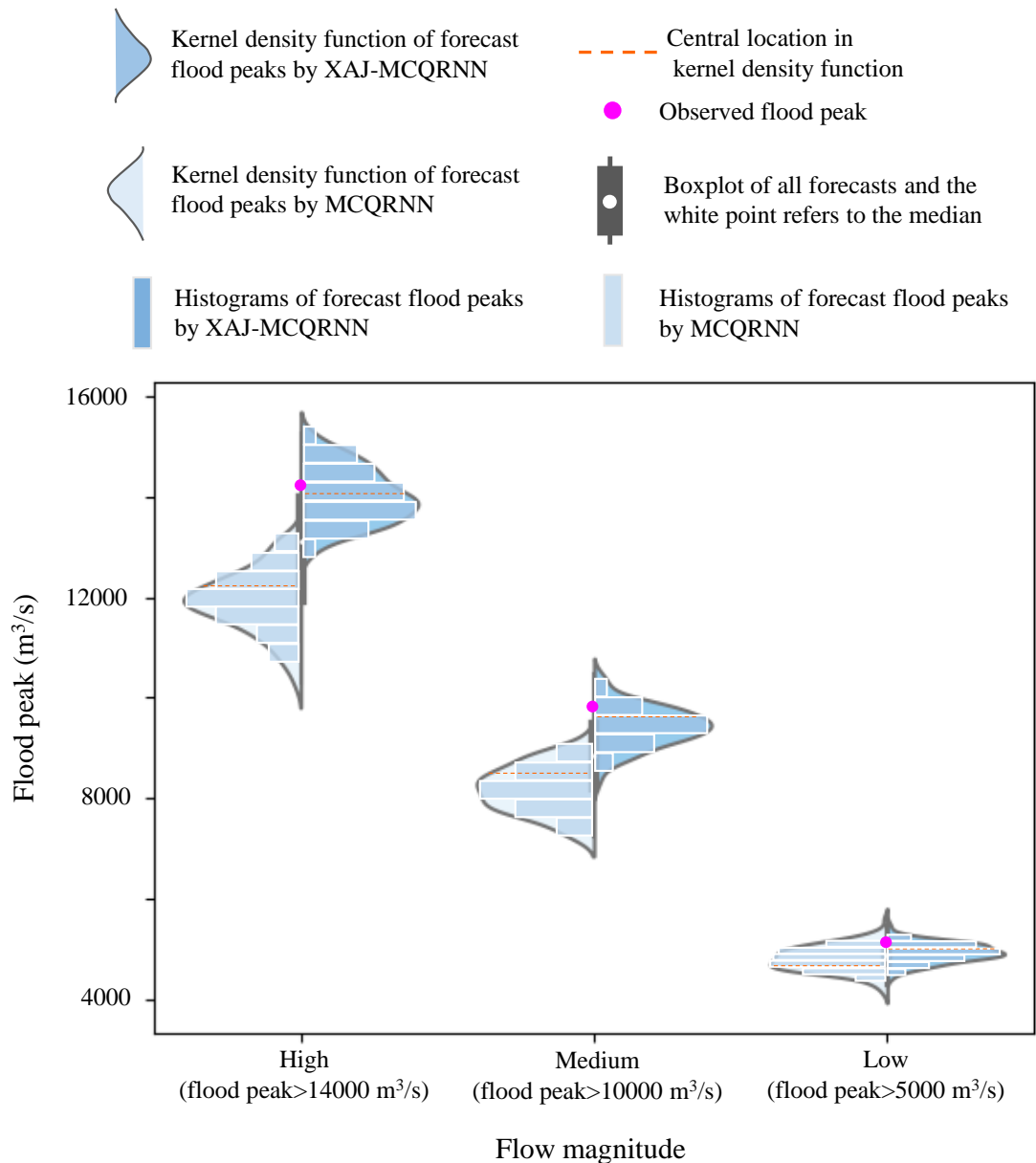
510 Moreover, to clearly determine the predictabilities of the MCQRNN and XAJ-  
511 MCQRNN models, the three flood events: (a) high flood magnitude with total  
512 precipitation of 134 mm and maximal streamflow of 14400 m<sup>3</sup>/s (maximum streamflow  
513 with a return period of 45a); (b) medium flood magnitude with total rainfall of 60 mm  
514 and maximal streamflow of 10100 m<sup>3</sup>/s (the return period of this peak is 20a); and (c)  
515 low flood magnitude with total rainfall of 26 mm and maximal streamflow of 5200 m<sup>3</sup>/s  
516 (the return period of this peak is 10a), were selected to examine both models by  
517 assessing whether the observed streamflow data fall within the 90% prediction interval,  
518 i.e. [5% quantile, 95% quantile], at horizon  $t+4$  in testing stages, as illustrated in Fig. 5.  
519 Three interesting results are acquired. First, the 90% prediction intervals made by the  
520 XAJ-MCQRNN model can cover the majority of the observed streamflow data, in  
521 comparison to those of the MCQRNN model. Second, the XAJ-MCQRNN model can  
522 create a predictive distribution narrower than that of the MCQRNN model in each flood  
523 event. Third, the XAJ-MCQRNN model can largely mitigate the biased-prediction  
524 phenomenon (under-prediction in our case). The prediction interval aims to promote  
525 the sharpness of the predictive distributions as much as possible, where sharpness is  
526 used to represent the concentration of the predictive distributions. Concerning short-  
527 term forecasts, the XAJ-MCQRNN model can raise the concentration of the predictive  
528 distributions while obtaining high coverage of the observed streamflow data in all cases.



529

530 **Fig. 5** Interval forecast results of three flood events at horizon  $t+4$  in the testing stages,  
531 given a 90% prediction interval of [5% quantile, 95% quantile]. The rainfall forecasts  
532 during horizons  $t+1$  up to  $t+4$  were collected from the ERA-Interim datasets of the  
533 ECMWF. Left panel for MCQRRN, and right for XAJ-MCQRRN.

534 The density distribution (i.e., violin plot) is also adopted to evaluate the reliability  
535 of interval forecasts. Fig. 6 illustrates the predictive violin-plots of the flood peaks of  
536 the above-specified flood events at horizon  $t+4$  in testing stages. In each violin plot, the  
537 probability density distribution of the forecasts made by the MCQRNN (XAJ-  
538 MCQRNN) model is located at the left (right) part, while the statistical boxplot of all  
539 forecasts is located at the central part. The violin plots point out that the difference  
540 between the forecasts acquired from MCQRNN and XAJ-MCQRNN models displays  
541 a trend climbing from the low, the medium to the high values of flood peaks at horizon  
542  $t+4$ . The bandwidths of the prediction intervals are notably larger in the medium-high  
543 flood peaks than in the low flood peak due to the larger fluctuations of flood magnitudes  
544 in the former. Interestingly, the range of kernel density functions corresponding to the  
545 XAJ-MCQRNN model is significantly narrower than that of the MCQRNN model  
546 while the central locations (orange dashed lines) of kernel density functions related to  
547 the XAJ-MCQRNN model are closer to the observed flood peaks (purple points) in all  
548 cases. That means the XAJ-MCQRNN model produces higher sharpness and  
549 predictions with smaller bias than the MCQRNN model. Briefly, the XAJ-MCQRNN  
550 model not only can produce more accurate and reliable probability density forecasts but  
551 also can alleviate the biased-prediction phenomenon associated with the extreme flood  
552 events through integrating the data-driven and conceptual-based mechanisms for  
553 rainfall-runoff modelling.



554

555 **Fig. 6** Violin plots for evaluating the uncertainty of MCQRNN and XAJ-MCQRNN  
 556 model forecasts on flood peaks of high, medium and low flood magnitudes at horizon  
 557  $t+4$  in the testing stages.

558

## 559 **5 Conclusions and discussion**

560 The demand for the hybridization of machine learning and conceptual models is  
 561 motivated by real-world applications in the best interests of enhancing the accuracy and  
 562 reliability of short-term FPD forecasting. This study proposed a hybrid rainfall-runoff  
 563 model (i.e., XAJ-MCQRNN) that integrated the Xinanjiang (XAJ) conceptual model

564 and the MCQRNN to make short-term FPD forecasts. Its capability of efficient learning  
565 and accurate forecasting is tested and verified with the long-term (2009-2015) flood  
566 events at the Jianxi River catchment in China. The MCQRNN model is constructed and  
567 used for comparison purpose.

568 The results of median point forecasts on flood processes reveal that the proposed  
569 XAJ-MCQRNN model performs distinguishably better than the MCQRNN model in  
570 short-term (12 hours) flood forecasting with higher NSE and lower RMSE values as  
571 well as a better goodness-of-fit to observed flood processes. The results of interval  
572 forecasts of flood processes further demonstrate that the XAJ-MCQRNN model is  
573 superior to the MCQRNN model at four horizons. The XAJ-MCQRNN model has  
574 smaller RB, larger CR values, and higher sharpness of the predictive distribution. These  
575 achievements provide solid evidence that the XAJ-MCQRNN model can make  
576 considerably more reliable and accurate point and interval forecasts of flood processes  
577 at long forecast horizons and can more effectively overcome the phenomena of  
578 overfitting and time-shift than the MCQRNN model. Moreover, the reason that the  
579 XAJ-MCQRNN model is successful in obtaining superb probability density forecast  
580 results is attributed to the pivotal strategy that the XAJ conceptual model supplements  
581 the point forecasts of flood processes through training the MCQRNN model to alleviate  
582 predictive uncertainty.

583 Therefore, the XAJ-MCQRNN by virtue of data-driven and conceptual-based  
584 hydrological models can provide forecasting and early warning of flood processes, thus  
585 reducing flood risks associated with the extreme rainstorm phenomenon. This study is



586 a good demonstration of the hybrid approach which unites two different groups of  
587 scientists including data scientists and disciplinary scientists (e.g., hydrologists). To use  
588 the strength of various point forecasts meanwhile alleviating their weaknesses, model  
589 combinations in the form of hybridization (e.g., Zhang et al., 2018; Lin et al., 2020;  
590 Hosseiny et al. 2020; Konapala et al., 2020; Kao et al., 2021) have been applied to  
591 making short-term flood point forecasts for basins with humid subtropical climate. This  
592 is the first study to apply conceptual models with artificial neural networks for flood  
593 probability density (FDP) forecasting for such basins. Notwithstanding these promising  
594 achievements, further research can be conducted to investigate the far-reaching effects  
595 of short-term and even long-term flood probability forecasting and warning on flood  
596 prevention and water resources management in humid, semi-humid and arid areas by  
597 combining more hybrid modelling techniques with medium-long term weather forecast  
598 products.

599

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## Abstract

Making accurate and reliable probability density forecasts of flood processes is fundamentally challenging for machine learning techniques, especially when prediction targets are outside the range of training data. Conceptual hydrological models can reduce rainfall-runoff modelling errors with efficient quasi-physical mechanisms. The Monotone Composite Quantile Regression Neural Network (MCQRNN) is used for the first time to make probability density forecasts of flood processes and serves as a benchmark model, whereas it confronts the drawbacks of overfitting and biased-prediction. Here we propose an integrated model (i.e. XAJ-MCQRNN) that incorporates Xinanjiang conceptual model (XAJ) and MCQRNN to overcome the phenomena of error propagation and accumulation encountered in multi-step-ahead flood probability density forecasts. We consider flood forecasts as a function of rainfall factors and runoff data. The models are evaluated by long-term (2009-2015) 3-hour streamflow series of the Jianxi River catchment in China and rainfall products of the European Centre for Medium-Range Weather Forecasts. Results demonstrated that the proposed XAJ-MCQRNN model can not only outperform the MCQRNN model but also prominently enhance the accuracy and reliability of multi-step-ahead probability density forecasts of flood process. Regarding short-term forecasts in testing stages at four horizons, the XAJ-MCQRNN model achieved higher Nash-Sutcliffe Efficiency but lower Root Mean Square Error values, while improving Coverage Ratio and Relative Bandwidth values in comparison to the MCQRNN model. Consequently, the improvement can benefit the mitigation of the impacts associated with uncertainties of extreme flood and rainfall events as well as promote the accuracy and reliability of flood forecasting and early warning.

## **Highlights**

- Machine learning assists hybrid model to promote flood forecasting and early warning
- Hybridizing MCQRNN with XAJ model for flood probability density forecasting
- XAJ-MCQRNN conquers overfitting and biased-prediction bottlenecks
- XAJ-MCQRNN improves accuracy and reliability of flood probability density forecasts

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**Declaration of 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.

The authors declare the following financial interests/personal relationships which may be considered as potential competing interests: