Abstract. Design flood estimation is a fundamental task in hydrology. In this research, we propose a machine-learning-based approach to estimate design floods globally. This approach involves three stages: (i) estimating at-site flood frequency curves for global gauging stations using the Anderson–Darling test and a Bayesian Markov chain Monte Carlo (MCMC) method; (ii) clustering these stations into subgroups using a $K$-means model based on 12 globally available catchment descriptors; and (iii) developing a regression model in each subgroup for regional design flood estimation using the same descriptors. A total of 11 793 stations globally were selected for model development, and three widely used regression models were compared for design flood estimation. The results showed that (1) the proposed approach achieved the highest accuracy for design flood estimation when using all 12 descriptors for clustering; and the performance of the regression was improved by considering more descriptors during training and validation; (2) a support vector machine regression provided the highest prediction performance amongst all regression models tested, with a root mean square normalised error of 0.708 for 100-year return period flood estimation; (3) 100-year design floods in tropical, arid, temperate, cold and polar climate zones could be reliably estimated (i.e. $<\pm 25\%$ error), with relative mean bias (RBIAS) values of $-0.199$, $-0.233$, $-0.169$, $0.179$ and $-0.091$ respectively; (4) the machine-learning-based approach developed in this paper showed considerable improvement over the index-flood-based method introduced by Smith et al. (2015, https://doi.org/10.1002/2014WR015814) for design flood estimation at global scales; and (5) the average RBIAS in estimation is less than 18% for 10-, 20-, 50- and 100-year design floods. We conclude that the proposed approach is a valid method to estimate design floods anywhere on the global river network, improving our prediction of the flood hazard, especially in ungauged areas.

1 Introduction

Flood hazard is the primary weather-related disaster worldwide, affecting 2.3 billion people and causing USD 662 billion in economic damage between 1995 and 2015 (CRED and UNISDR, 2015). The frequency and severity of flood events are expected to increase in the future because of climate change and socio-economic growth in flood-prone areas (Sharma et al., 2018; Wing et al., 2018; Winsemius et al., 2016). Flood hazard models are mature tools to identify flood-prone areas and have been widely used in flood risk management at catchment or regional scales (Hammond et al., 2015; Teng et al., 2017). With the development of new remote sensing techniques and an increase in computing power, global flood hazard models (GFHMs) are now a practical reality and have been successfully applied for large-scale flood mapping and validated in several countries (Bates et al., 2020; Schumann et al., 2018). GFHMs can identify flood-prone areas in ungauged basins and provide a consistent and comprehensive understanding of the flood hazard at national, continental and global scales.

The “cascade” model type and “gauged flow data” model type are the two most frequently used approaches in global flood hazard modelling, and both map the flood hazard based on return period flows (Trigg et al., 2016). The cas-
The aim of this research is therefore to provide an improved method for reliable design flood estimation, ad-

1. The global RFFA approach of Smith et al. (2015) was developed based on 945 stations in the Global Runoff Data Base (GRDB) and the United States Geological Survey (USGS) database. This limited number of stations means that it cannot provide a reliable estimation in some regions at global scale. To improve the coverage and density of discharge stations, nearly 12,000 stations from the newly published Global Streamflow Indices and Metadata (GSIM) archive were selected for model development in this research.

2. The flood frequency curve in the Smith et al. (2015) approach was assumed to obey a generalised extreme value (GEV) distribution for the global coverage. Studies have suggested alternate distributions, such as GEV, generalised logistic (GENLOGIS) and Pearson type III (P3), whilst log-normal (LN3) distributions are mandated for use in the United States (Water Resources Council (US), 1975). In this research, the at-site flood frequency curve was selected from eight widely used distributions based on the Anderson–Darling goodness-of-fit tests.

3. The global RFFA approach of Smith et al. (2015) adopted only three catchment descriptors (rainfall, slope and catchment area) for clustering and flood estimation. These three factors can only provide a basic description of global catchment characteristics. In this research, 12 catchment descriptors covering meteorological, physiographical, hydrological and anthropological aspects were considered for clustering and design flood estimation.

4. The global RFFA approach of Smith et al. (2015) was proposed based on the index-flood method, and the index flood in ungauged areas was computed with a power-form function. As the coefficient of variation of flood flows generally varies from site to site, the index-flood method is not recommended if available samples are sufficient or highly cross-correlated (Stedinger, 1983). Moreover, the simple power-form function may fail to capture complicated relationships within the data, since the relationship between flood and each descriptor is assumed to obey an explicit power-form function, which may not always be appropriate. In this research, the design flood in ungauged areas is estimated based on a direct regression method, and machine learning models were adopted to describe the unknown relationship between catchment descriptors and at-site design floods. These machine-learning-based methods have shown advantages over ordinary regression approaches in RFFA at regional scales (Gizaw and Gan, 2016; Shu and Ouarda, 2008; Zhang et al., 2018) and are tested here for the first time in a global study.
dressing the deficiencies identified with the previous global-scale study of Smith et al. (2015). A three-phase model framework is applied, where Bayesian Markov chain Monte Carlo (MCMC), K-means and support vector machine (SVM) models were applied for at-site flood estimation, subgroup delineation and regional flood estimation, respectively. Specifically, 11,793 stations selected from the GSIM archive are used for model development, and the stations were divided into 16 subgroups using a K-means model and 12 catchment descriptors. For each subgroup, 70% and 30% stations were randomly selected for model training and validation respectively. Three types of regressions including power-form function (PF), SVM and random forest (RF) were compared for regional flood estimation. Finally, the proposed direct regression approach is compared with the previous results of Smith et al. (2015) in each climate zone.

2 Study areas and data

2.1 Flood data

Observed annual maximum streamflow data in the GSIM archive were used to estimate at-site design floods (DFs) at different return periods. This archive is a collection of streamflow indices that includes more than 35,000 stations from seven national and five international streamflow databases (Gudmundsson et al., 2018; Do et al., 2018a). Compared with a widely used database in large-scale hydrological studies, the Global River Discharge Database (GRDB), which contains data from 9500 stations, the GSIM archive can help to improve the understanding of large-scale hydrological processes by improving the coverage and density of streamflow observations. After quality control of the daily streamflow data, 15 types of time-series indices are provided at yearly, seasonal and monthly resolutions in the GSIM archive (Do et al., 2018a; Gudmundsson et al., 2018). In this research, time series of annual maximal floods in the GSIM archive were adopted for at-site design flood estimation. To date, this archive has been successfully used in flood classification (Stein et al., 2019), streamflow trend analysis (Do et al., 2019) and hydrological model evaluation (Yang et al., 2019a) at the global scale.

To make reliable estimates for at-site DFs, a station selection is needed based on some quality control criteria. Firstly, the hydrological signatures of streamflow are reported to become stable during estimation with at least 20 years of record (Richter et al., 1997). Therefore, only stations with a historical streamflow record of 20 years or longer were selected for the analysis. Second, the traditional RFFA approach requires the assumption of flood stationarity. Stations experiencing obvious trends or sudden changes were detected by a Mann–Kendall test (MKT) (Hamed, 2008) and the standard normal homogeneity test (SNHT) (Alexandersson, 1986). Any stations exhibiting obvious non-stationarity or which do not obey the given hypothetical distributions identified by Anderson–Darling goodness-of-fit tests were not considered further in model development. Lastly, to better estimate DFs at the global scale, the selected stations were first divided into several subgroups based on a K-means clustering model, and separate regression models were developed for the different subgroups. The streamflow stations in each subgroup were also required to pass discordancy and heterogeneity tests. The adopted stationarity, discordancy and heterogeneity measures are described in Sect. 3, and the distribution of training and validation stations after selection is shown in Fig. 1.

Table 1 compares the number of stations used for model training and validation in each climate class between Smith et al. (2015) and this study. Compared with the research of Smith et al. (2015), the number of stations in this research is significantly improved in all climate classes.

2.2 Catchment descriptors

The main idea of an RFFA is to characterise a relationship between at-site DFs and catchment descriptors and then apply this relationship to estimate flood magnitudes along the river network in similar ungauged catchments. In this research, the river network of the global coverage is extracted from the 1 km resolution catchment area map for catchments exceeding a threshold area of 50 km². Twelve explanatory factors collected from open-access databases were selected as potential descriptors and applied for clustering and regression model development. A correlation analysis of all explanatory factors was done before model development to ensure none of them have strong correlation (Pearson’s correlation coefficient > 0.6) with each other. The statistics and data sources of these factors are summarised in Table 2.

These explanatory factors can be grouped into four categories as follows:

1. **Meteorological factors** included annual precipitation (AP), precipitation seasonality (PS), annual mean temperature (AT) and annual temperature range (TR). AP and AT represent the average annual precipitation and mean temperature of the upstream catchment respec-

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Table 1. The number of discharge stations for model development in each climate class. NA stands for “not available”.

| Climate class | Smith et al. (2015) | This research |
|---------------|---------------------|--------------|
|               | Training | Validation | Training | Validation |
| Tropical      | 163      | 8          | 716      | 298        |
| Arid          | 121      | 55         | 595      | 231        |
| Temperate     | 296      | 99         | 4231     | 1816       |
| Cold          | 109      | 80         | 2666     | 1099       |
| Polar         | 14       | NA         | 100      | 41         |
| Total         | 703      | 242        | 8308     | 3485       |
Figure 1. The distribution of discharge stations used for training and validation in this research.

Table 2. Statistics and data source of the explanatory descriptors.

| No. | Factor name (abbreviation) | Unit | Min  | Max  | Data source        |
|-----|---------------------------|------|------|------|-------------------|
| 1   | Annual precipitation (AP) | mm   | 0    | 7743 | WorldClim         |
| 2   | Precipitation seasonality (PS) | –    | 0    | 219.35 | WorldClim         |
| 3   | Annual mean temperature (AT) | °C  | −27.57 | 33.44 | WorldClim         |
| 4   | Temperature annual range (TR) | °C  | 0    | 74.79 | WorldClim         |
| 5   | Mean slope (SL)            | °    | 0    | 32.78 | MERIT DEM         |
| 6   | Lake fraction (LF)         | %    | 0    | 1    | GLWD              |
| 7   | Longitude (LO)             | °    | −180 | 180  | WGS 84            |
| 8   | Latitude (LA)              | °    | −60  | 85   | WGS 84            |
| 9   | Curve number (CN)          |      | 0    | 95   | NRCS CN dataset   |
| 10  | Catchment area (CA)        | km²  | 50   | 1 6 198 686 | MERIT DEM |
| 11  | Dam capacity (DC)          | 10⁶ m³ | 0  | 2648 | GRanD             |
| 12  | Population density (PD)    | number/km² | 0 | 5317 | GPW               |

Psy. PS is the coefficient of variation of the monthly rainfall series, and TR is the range between the maximal and minimal temperatures of the time series average over the upstream catchment. These four factors were collected from the WorldClim dataset (V2) at 30 arcsec (~ 1 km) resolution (Fick and Hijmans, 2017) and are used to represent the extreme value and seasonal distribution of precipitation and temperature.

2. Physiographical factors comprised discharge station location, slope (SL) and lake fraction (LF) of the upstream catchment. Station location is defined by the longitude (LO) and latitude (LA) of the discharge station in degree units of the World Geodetic System 1984 (WGS84) spatial reference frame. SL reflects the average slope of the upstream catchment, which is calculated based on the MERIT DEM (Yamazaki et al., 2017). LF represents the fraction of the catchment area upstream of the station covered with lakes. The location and area of global lakes are taken from the Global Lakes and Wetlands Database (GLWD) (Lehner and Döll, 2004).

3. Hydrological factors of catchment area (CA) and curve number (CN) reflect the area and runoff capacity of the upstream catchment respectively. CA is defined as the upstream flow accumulation area based on the D8 algorithm and the MERIT DEM. CN is an empirical parameter for runoff prediction in ungauged areas, which is calculated from the tables in the National Engineering Handbook of the United States, Section-4 (NEH-4) (United States Soil Conservation Service, 1985). The CN in this research is collected from a global CN dataset that utilises the latest Moderate Resolution Imaging Spectroradiometer (MODIS) land cover information and the Harmonized World Soil Database (HWSD) soil data (Zeng et al., 2017).

4. Anthropological factors included total dam capacity (DC) and population density (PD). DC is the total dam capacity of the upstream catchment. The location and capacity of each dam are provided by the Global Reservoir and Dam (GRanD) dataset, which includes about 7000 dams globally (Lehner et al., 2011). PD is a widely
3 Methodology

The flowchart for this research has three parts, which are shown in Fig. 2. Panel (a) includes the procedures of station selection and at-site design flood estimation that are described in Sect. 3.1 and 3.2 respectively. Panel (b) displays the procedure for subgroup delineation by using a K-means clustering model (in Sect. 3.3). Panel (c) describes the procedure of regression model development and regional flood estimation in ungauged areas. Three regression models, described in Sect. 3.4, were adopted for model comparison.

3.1 Station selection methods

3.1.1 Stationarity measures

Two widely used stationarity measures in hydrology, the Mann–Kendall test (MKT) (Hamed, 2008) and the standard normal homogeneity test (SNHT) (Alexandersson, 1986), were adopted for trend and change-point detection respectively in the research. One advantage of these two tests is that they provide an index reflecting the degree of trend or change. The details of the MKT and SNHT methods are described in Appendix A and B respectively.

The Z index in the MKT test was used to evaluate the trend that is descending (negative values) and ascending (positive values) in the time series. The change points occurred at the largest value of T index among the time series Tki, and a larger T represents a higher change. After stationarity measures were evaluated, each station has corresponding Zk and Tk indices. The stations experiencing obvious trends and/or sudden changes were removed based on the 95 % quantile value of the |Zk| and Tk indices.

3.1.2 Discardancy measures

The aim of using the discardancy measures was to detect potential outliers in each subgroup. Two discardancy measures are applied in this research to the time series of observed discharge. The first is the Z score method (Shiffler, 1988), which is based on the value of mean annual runoff (R). The global gauging stations are divided into several subgroups, and the R in each subgroup is normalised using Eq. (C1) in Appendix C. A station is regarded as an outlier with the Z score is larger than 3 (Garcia, 2012).

Another discardancy measure was proposed by Hosking and Wallis based on L-moment ratios (Hosking and Wallis, 2005). The discardancy of each station can be evaluated by Di as defined in Eqs. (C2) to (C4) in Appendix C. As suggested by Hosking and Wallis (2005), a station is considered as discordant if Di ≥ 3 when Nk is larger than 15.

3.2 At-site flood estimation

Table D1 (in Appendix D) describes the tested hypothetical distributions which have been widely recommended in flood frequency analysis in different countries. For example, a generalised Pareto distribution performs better in populated regions of Australia, whilst P3 is recommended as the national standard distribution for flood frequency analysis in China (Gao et al., 2019; Vogel et al., 1993; Wang et al., 2015).

The at-site flood estimation involves two steps. Firstly, the flood frequency curve for each station was selected from eight widely used hypothetical distributions based on the Anderson–Darling goodness-of-fit test. After the preferred distribution was selected, the parameters and design floods for this station were derived by a Bayesian MCMC method. The adopted Anderson–Darling test and Bayesian MCMC method are briefly described as follows.

3.2.1 Distribution selection

The Anderson–Darling (AD) test can detect whether a given sample of data follows a hypothetical distribution. It has been widely used in flood frequency analysis as it shows good skill for small sample sizes and heavy-tailed distributions (Haddad and Rahman, 2011). For each station, the A2 statistic was calculated for all hypothetical distributions, and the distribution with the minimum A2 was selected as the flood frequency curve for that station. The calculation process for the A2 statistic is described in Appendix E. After selection of a flood frequency curve for all stations, a threshold A25 % was determined by the 95 % quantile value of A2. The stations at which A2 exceeded the threshold were regarded as not obeying all hypothetical distributions, and these stations were not considered further for model development.

3.2.2 Parameter estimation

The adopted Bayesian inference consisted of three steps as follows:

a. Prior distribution and likelihood function calculation.

The first step is to determine the prior distribution for Bayesian analysis. As non-prior knowledge (i.e. population distribution function) was considered, a non-informative normal distribution was selected as a prior distribution. The likelihood function f(q|θ) can be computed as in Eq. (1).

\[
f(q|θ) = \prod_{i=1}^{n} f(q_i; θ),
\]

where \( q = (q_1, q_2, q_3, \ldots, q_n) \) are the given samples, and \( θ \) is a parameter vector.

b. Posterior distribution calculation. The posterior distribution \( f(θ|q) \) is computed using Bayesian inference as
in Eq. (16). As the integral in Eq. (2) cannot be solved analytically, the Metropolis–Hastings MCMC method (Chib and Greenberg, 1995) was used to generate samples from the posterior distribution.

\[
f(\theta | q) = \frac{f(q | \theta) \pi(\theta)}{\int f(q | \theta) \pi(\theta) \, d\theta},
\]

where \( \pi(\theta) \) is the density function of the prior distribution.

c. Parameter and design flood estimations. The final parameters \( \hat{\theta} \) can be calculated by the expected value of the posterior distribution. The probability density function of design flood \( Q \) can be described as in Eq. (3).

\[
f(Q | q) = \int_{\theta} f(Q | \theta) f(\theta | q) \, d\theta
\]

The three common methods for estimating the parameters of at-site flood frequency curves are based on moments (MOM), maximum likelihood (MLE) and Bayesian inference. Compared with MOM and MLE, the Bayesian approach can provide credibility intervals for the estimated design flood. The details of the adopted approach are comprehensively described in the research of Reis and Stedinger (2005), and the calculation is implemented based on a BayesianMCMC function (nsRFA package) in R software.

### 3.3 Clustering method

#### 3.3.1 K-means model

The standard K-means model was adopted for clustering in this research. This model has been widely used in the area of hydrology, including in RFFA studies (Smith et al., 2015; Lin and Chen, 2006). The K-means model consists of two steps:

a. An input dataset \( D = \{x_j | j = 1, 2, 3, \ldots, N\} \), where \( N \) is the number of samples. The \( K \) centroids \( C = \{C_k | k = 1, 2, 3, \ldots, K\} \) are first randomly selected from the input dataset \( D \). Each sample \( x_j \) is assigned to its nearest \( C_k \) based on the squared Euclidean distance as in Eq. (4).

\[
\arg \min_{c_k \in C} \left[ \text{dis}(C_k, x_j) \right]^2,
\]

where \( \text{dis}(\cdot) \) is the function for Euclidean distance calculation.

b. The centroid \( C_k \) in step (a) is updated as in Eq. (5). Then, the algorithm iterates between centre assignment (a) and centre update (b) until the maximum number of iterations is reached or cluster assignments do not change.

\[
C_k = \frac{1}{N_j} \sum_{j=1}^{N_j} x_j, x_k \in A_k,
\]

where \( A_k \) is the subset of \( D \), and \( N_j \) is the number of samples in \( A_k \).
The $K$-means model was implemented based on the MATLAB kmeans function, and the maximum number of iterations was set to 1000 (https://www.mathworks.com/help/stats/kmeans.html, last access: 26 October 2021). Two sensitive parameters, the number of clusters and the clustering factors, were selected to maximise model performance during the validation procedure.

### 3.3.2 Heterogeneity measure

The heterogeneity of subgroup delineation is measured by a Davies–Bouldin index (Davies and Bouldin, 1979). This index considers both intra-subgroup diversity and inter-subgroup distances. The intra-subgroup diversity of a subgroup $i$ is computed as in Eq. (6)

$$ S_i = \left\{ \frac{1}{T_i} \sum_{j=1}^{T_i} \| x_j - C_i \|^2 \right\}^{1/2}, $$

where $C_j$ is the centroid of subgroup $i$; $x_j$ is the clustering factors of subgroup $j$; and $T_i$ is the number of samples in subgroup $i$.

The inter-subgroup distance between subgroup $j$ and subgroup $k$ is measured as in Eq. (7):

$$ R_{i,j} = \frac{s_j + s_j}{\text{dist}(C_i, C_j)}, $$

where $\text{dist}(C_i, C_j)$ is the Euclidean distance between $C_i$ and $C_j$.

The Davies–Bouldin index is computed as in Eq. (8) and (9):

$$ R_i = \max_{i \neq j} \{ R_{i,j} \}, $$

$$ \text{DBI} = \frac{1}{K} \sum_{i=1}^{K} R_i, $$

where $K$ is the number of subgroups, and DBI is the Davies–Bouldin index; a lower value means that the subgroups are better clustered.

### 3.4 Regression method

The direct regression method estimates design floods directly with catchment descriptors using a regression model as described in Eq. (10). Three types of regression models were compared in this research and are described below. The optimal regression model for the direct regression method was selected according to the highest prediction accuracy during the validation period. To the best of our knowledge, this research is the first in which three different regression models have been tested in an RFFA at the global scale.

$$ \text{DF} = f_{FQ}(d_1, d_2, \ldots, d_N), $$

where DF is the design flood for specific return periods, and $f_{FQ}$ is the regression model for design flood estimation in each subgroup.

#### 3.4.1 Power-form function (PF)

The power-form (PF) function is a simple non-linear regression model that has been successfully used in RFFA studies at a global scale (Smith et al., 2015). The basic formula of PF regression is described in Eq. (11).

$$ \text{DF} = \beta_0 d_1^{\beta_1} d_2^{\beta_2} d_3^{\beta_3} \ldots d_N^{\beta_N} \pm \epsilon, $$

where $\beta_n$ are the model parameters, $d$ is the explanatory descriptor used for model development, $N$ is the total number of descriptors and $\epsilon$ is the error term.

#### 3.4.2 Support vector machine (SVM)

SVM has shown advantages in solving complicated non-linear problems in the field of hydrology. The adopted SVM regression model was proposed by Drucker et al. (1997) and successfully used in forecasting of flood, drought and groundwater, etc. For a given training dataset $\{(x_1, y_1), (x_2, y_2), \ldots, (x_N, y_N)\}$, where $N$ is the number of training samples, the overall goal of SVM regression is to find a function $f(x)$ that has at most $\epsilon$ deviation from the observed $y_i$.

Thus, the SVM regression model can be described as a convex optimisation problem as in Eq. (12).

$$ \begin{align*}
\min_{w, b, \xi} & \frac{1}{2} \| w \|^2, \\
\text{s.t.} & \begin{cases}
    y_i - w^T x_i - b \leq \epsilon \\
    w^T x_i + b - y_i \leq \epsilon
\end{cases}, \\
\end{align*} $$

where $w$ and $b$ are hyperplane parameters, and $\epsilon$ is the insensitive loss.

The SVM regression is formulated as follows by adding two slack variables in Eq. (13).

$$ \begin{align*}
\min_{w, b, \xi, \xi^*} & \frac{1}{2} \| w \|^2 + C \sum_{i=1}^{N} (\xi_i + \xi_i^*), \\
\text{s.t.} & \begin{cases}
    f(x_i) - y_i \leq \epsilon + \xi_i \\
    y_i - f(x_i) \leq \epsilon + \xi_i^* \\
    \xi_i, \xi_i^* \geq 0, \quad i = 1, 2, \ldots, N
\end{cases}
\end{align*} $$

where $\xi_i$ and $\xi_i^*$ are the two slack variables, and $C$ is a parameter that controls the trade-off between the support line and training samples. The solution of Eq. (13) is described in Garndareh et al. (2018) and Gizaw and Gan (2016).

#### 3.4.3 Random forest (RF)

RF regression is a representative type of ensemble machine learning model. Unlike SVM, which makes decisions based on a single trained model, RF is based on the average result of numerous independent regression tree models (RTMs). In RF, $n$ subsets were selected using a bootstrap aggregating method from the whole training samples, where $n$ is the number of subsets. For each subset
$T = \{(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)\}$, an RTM is developed by minimising the loss as in Eq. (14).

$$\min_{\theta} \sum_{m=1}^{M} \sum_{x_i \in R_m} (p_m - y_i). \quad (14)$$

where $x$ is the input, $y$ is the observed training target, $M$ is the amount of leaf of an RTM, $R$ is the subset of whole model inputs and $p_m$ is the predicted value of leaf $m$.

In each RTM, the factors were randomly selected for model development, and the final prediction of the RF model is calculated as the average of the results of different RTMs. This strategy means RF usually has good performance in terms of reducing overfitting, outliers and noise (Zhao et al., 2020, 2018).

The out-of-bag (OOB) samples (samples not selected by the bootstrap method) are applied to test its accuracy. Once an RF is developed, the error of OOB samples can be computed as in Eq. (15).

$$E_{\text{OOB}} = \frac{1}{n} \sum_{i=1}^{n} (y_i - \hat{y}_i). \quad (15)$$

where $n$ is the total number of OOB samples, and $\hat{y}_i$ is the predicted value of RF.

Each factor in the OOB samples is permuted one at a time, and the permuted $E_{\text{OOB}}$ can be computed with the permuted OOB samples and the trained RF model. The RF estimates the factor importance by comparing the difference between the original and permuted $E_{\text{OOB}}$, while all others are unchanged. RF has been successfully applied for tasks such as flood assessment, discharge prediction and ranking of hydrological signatures (Zhao et al., 2018; Hutengs and Vohland, 2016; Li et al., 2016), including RFFA at regional scales (Dessai and Ouarda, 2021).

### 3.5 Validation indices

Two widely used indices, the root mean square normalised error (RMSNE) and the relative mean bias (RBIAS), were applied for model evaluation (Salinas et al., 2013; Shu and Ouarda, 2008; Smith et al., 2015). The RMSNE and RBIAS are computed as in Eqs. (16) and (17) respectively. RMSNE is a negatively oriented index, where lower value means better model performance. Since the errors in RMSNE are squared before they are averaged, it should be more useful than RBIAS when large errors are particularly undesirable. However, as well as its use in error evaluation, RBIAS can describe if the model has positive bias (underestimation) or negative bias (overestimation).

$$\text{RMSNE} = \sqrt{\frac{1}{N} \sum_{i=1}^{N} \left( \frac{q_i - \hat{q}_i}{q_i} \right)^2}, \quad (16)$$

$$\text{RBIAS} = \frac{1}{N} \sum_{i=1}^{N} \left( \frac{q_i - \hat{q}_i}{q_i} \right), \quad (17)$$

where $q_i$ is the specific flood quantile derived by observed data, $\hat{q}_i$ is the specific flood quantile estimated by the RFFA method and $N$ is the total number of stations.

### 4 Results and discussion

#### 4.1 At-site flood estimation

Firstly, 16854 stations with a historical streamflow record of 20 years or longer were selected from all stations in the GSIM archive. Then, the MK, SNHT and AD tests were applied to these stations. As shown in Fig. 3, the thresholds of the MK, SNHT and AD tests were derived based on the 95 % quantile value of the $|Z|$, $T$ and $A^2$ indices, respectively. A total number of 1951 stations which experience obvious trends (or sudden changes), or at which the discharge data did not obey the given hypothetical distributions, were not considered further. The selected stations were then clustered into several subgroups based on a $K$-means clustering model, and the discordancy measures described in Sect. 3.1.2 were further applied to these stations in each subgroup. Finally, 11 793 stations were selected for model development in this research.

Taking one selected station (no. AT0000032) as an example, as shown in Fig. 4a, the P3 distribution was selected as the optimal flood frequency curve for this station as this gives the minimal $A^2$ of 0.43 among all hypothetical distributions. After the flood frequency curve was defined, the parameters and uncertainties of the P3 curve were estimated based on the Bayesian MCMC method described in Sect. 3.2.2. As shown in Fig. 4b, the uncertainties (band between 0.05–0.95 confidence interval) improved with the increase of return periods, and the 100-year return period could be estimated within 25 % RBIAS for this station. The results of flood frequency curve selection and 100-year return period flood estimation for all stations are shown in Fig. 4c. We found that P3 and GENLOGIS are the two most favoured distributions and that only a small percentage of stations obey a NORM distribution.

#### 4.2 Subgroup delineation

For subgroup delineation, the number of clusters ($K$) and the clustering factors are two sensitive parameters. The value of $K$ is selected by considering both the heterogeneity (reflected by the DB index) and the number of stations in the subgroup. Figure 5 describes the selection process of $K$ when using all factors for clustering. As shown in Fig. 5a, the DB index
reached an optimal value at $K = 16$ and then fluctuated with the increase of $K$. From Fig. 5b, we found that the number of stations in subgroups reduced with a larger $K$. To ensure a sufficient number of stations for model development for each subgroup, $K$ greater than 40 is not considered in this research.

Taking the 100-year flood estimation as an example, different combinations of clustering factors were tested using the optimal $K$. As shown in Table 3, the best combination is to use all factors for clustering, and this result reaches the best RMSNE of 0.708 and RBIAS of $-0.174$ among all combinations for the validation periods. The design flood still could be satisfactorily estimated (RBIAS < 25%) when using meteorological, physiographical or hydrological factors for clustering, respectively. Anthropological factors alone are not recommended for clustering as this results in the worst RMSNE of 1.788 and RBIAS of $-0.909$ among all combinations.

### 4.3 Regression model comparison

Three regression models, PF, SVM and RF, were compared for 100-year flood estimation. Figure 6 describes the accuracy of the three models during training and validation periods. We found that PF showed the worse accuracy, with an RMSNE of 1.175 and 1.089 in training and validation periods, respectively, whereas SVM and RF showed better results with lower RMSNE values.
Table 3. The impact of clustering factors on regional 100-year flood estimation.

| Clustering factors             | Optimal | Training | Validation |
|-------------------------------|---------|----------|------------|
|                               | K       | RBIAS    | RMSNE      | RBIAS    | RMSNE    |
| All factors                   | 16      | -0.179   | 0.703      | -0.174   | 0.708    |
| Meteorological factors (AP, PS, AT, TR) | 11      | -0.202   | 0.768      | -0.185   | 0.746    |
| Physiographical factors (SL, LF, LO, LA) | 5       | -0.214   | 0.829      | -0.244   | 0.824    |
| Hydrological factors (CA, CN) | 30      | -0.207   | 0.781      | -0.243   | 0.876    |
| Anthropological factors (DC, PD) | 7       | -0.379   | 1.235      | -0.909   | 1.788    |

Figure 5. Optimal $K$ selection by (a) DB index and (b) the number of stations in subgroups during delineation.

Table 4 compares the training and validation results of 10-, 20-, 50- and 100-year return period floods derived by the proposed direct regression method. By using the proposed direct regression method, all design floods could be estimated within the RBIAS of $0.18$ (18%). We found, unsurprisingly, that the prediction accuracy decreases with a larger flood magnitude. This is mainly because the at-site design flood
Figure 6. Comparison of three regression models (PF, SVM and RF) during training and validation periods.

(a) PF training  
(b) SVM training  
(c) RF training

(d) PF validation  
(e) SVM validation  
(f) RF validation

Table 4. Result for different return period flood estimation.

| Return periods | Training | Testing | Training | Testing |
|----------------|----------|---------|----------|---------|
|                | RBIAS    | RMSNE   | Mean RBIAS | RMSNE   |
| 10             | -0.160   | 0.655   | -0.165   | 0.664   |
| 20             | -0.165   | 0.663   | -0.168   | 0.672   |
| 50             | -0.175   | 0.695   | -0.166   | 0.684   |
| 100            | -0.179   | 0.703   | -0.174   | 0.708   |

is derived by observed data based on several assumptions, not the truth, and large return period floods are more difficult to be reliably estimated with limited observed data (Gaume, 2018). Regarding the natural and epistemic uncertainties in flood frequency analysis, the RBIAS of at-site design flood estimation was reported to be as large as 30% in some studies (Di Baldassarre et al., 2012; Di Baldassarre and Montanari, 2009; Halbert et al., 2016; Merz and Thieken, 2005). As the at-site design flood is regarded as a training target, this error will be introduced in the regression and will directly affect the approach accuracy. Therefore, an RBIAS of 20% or less
is very impressive considering the uncertainties of at-site design flood estimation.

4.5 Discussion

In this research, we adopted a simple hold-out validation strategy such that 70 % and 30 % of stations were randomly selected for training and validation, respectively. To test the influence of hold-out samples on the model results, a 10-fold cross-validation strategy (Garmdareh et al., 2018; Lee et al., 2020) was applied. All stations in one subgroup were randomly divided into 10 folds. For every fold $i$ ($i = 1, 2, \ldots, 10$), the model$_i$ was trained by the remaining 9 folds (except the $i$th fold) and validated by the $i$th fold. Using this strategy, 10 models were developed for each subgroup, and each sample in the original dataset was used for validation once. Table 5 describes the best, worse and median model performances validated by the different folds. We found that the selection of hold-out samples had a moderate impact on the PF model, and the RMSNE performance ranged from 0.97 to 1.49. Both SVM and RF showed more stable performances than PF, and SVM provided the narrowest range. We suggest using ensemble results from SVM models trained by different split samples to reduce the errors in sample selection.

We compared the flood estimation accuracy in different catchment sizes (Fig. 9a). Both over- and underestimations were found from small to large catchments. The range of RBAIS in small catchments is wider than that in large catchments. This reveals that design floods in small catchments are more difficult to estimate than large catchments. This is mainly because the catchment descriptors derived from global satellite images can have large uncertainties (McCabe et al., 2017) when describing small catchments and can lead to more substantial errors at low discharge. The negative value of RBAIS reflected some overestimation. Some studies suggested that the trends in observed discharge can lead to overestimation (or underestimation) of flood quantiles if such non-stationarity is not taken into consideration in RFFA (Kalai et al., 2020; O’Brien and Burn, 2014). Before model development, some non-stationary or discordant stations were eliminated from the whole dataset using a threshold of 5 %. This threshold is an empirical value and may remove some reliable stations if the sample is homogeneous. Figure 9b presents the model performances of training, testing and eliminated stations. We found that the proposed approach showed stable performance in the training and testing stations. However, the wide range of RBAIS in eliminated stations reveals that there may be some downsides in applying the proposed approach to a station where flows are changing rapidly. To address this limitation, the non-stationary RFFA approach should be explored in further research.

Table 5. Results of 100-year design flood estimation using 10-fold cross-validation.

| Models | RBAIS | | | RMSNE | | |
|---|---|---|---|---|---|---|
| | Worse | Best | Median | | | |
| PF | $-0.37$ | $-0.21$ | $-0.29$ | 1.49 | 0.97 | 1.12 |
| SVM | $-0.20$ | $-0.16$ | $-0.19$ | 0.74 | 0.69 | 0.71 |
| RF | $-0.21$ | $-0.14$ | $-0.18$ | 0.78 | 0.69 | 0.74 |
All the proposed methods have not been implemented in a totally optimised way, the SVM model being slightly favoured in terms of the selected stations, not the whole initial GSIM dataset. Although only one-third of GSIM stations were selected, this research significantly improved the station density and model accuracy in all climate zones compared with the global RFFA of Smith (2015). The proposed approach achieved similar performances to some regional studies by adopting a global coverage of stations (Shu and Ouarda, 2008; Salinas et al., 2013). However, there can still be large errors in design flood estimation, especially in arid zones. This is consistent with previous research and is likely to be a result of drier regions being more heterogeneous (Salinas et al., 2013; Smith et al., 2015). In this study, the subgroups are delineated based on a widely used K-means model using squared Euclidean distance. Some studies showed that this model is not recommended for solving highly non-linear problems (Bárdossy et al., 2005; Samaniego et al., 2008; Raykov et al., 2016), and this may make it difficult to properly reflect the heterogeneous characteristics of the study area. Other clustering models and distance metrics that can better describe the non-linear relationship between descriptors should be compared in future studies.

5 Conclusions

A three-phase machine-learning-model-based approach was proposed to estimate design floods along river networks at the global scale. The at-site floods for global gauging station data were estimated based on a Bayesian MCMC method. The global stations were then clustered into several subgroups using a K-means clustering model, and a SVM regression was developed in each subarea for design flood estimation. Three widely used regression techniques, power-form function (PF), support vector machine (SVM) and random forests (RF), were compared for regression in each subgroup. The regional floods were final estimated using the same descriptors and the optimal SVM regression model.

The main conclusions of this study are summarised below:

1. To make reliable estimates, 11793 stations from the GSIM archive were selected for model implementation using stationarity, discordancy and homogeneity measures. For clustering, the impact of clustering number and clustering factors on estimation accuracy was tested. The best clustering number (K) was 16, which gave the lowest RMSNE of 0.708 for 100-year flood estimation when using all factors for clustering in a K-means model.

2. Three regression models were compared for 100-year flood estimation, and the SVM method showed the highest accuracy during the validation period, with an RMSNE of 0.708 and RBIAS of −0.174. Factor importance was identified using the RF model, and different combinations of factors were tested for the optimal SVM regression implementation. When only using the top two factors (annual precipitation and catchment area) for regression and a large number of stations (3485 stations) for validation, the design flood cannot be accurately estimated (RMSNE > 1.0) for some subgroups. After considering the top 10 factors for regression, the RMSNE for subgroups became stable and did not significantly improve by further adding factors.

3. The proposed approach showed good performance (i.e. the bias < ±20%) in tropical, temperate, cold and polar climate zones, with an RBIAS of −0.199, −0.169, −0.179 and −0.091 respectively. A satisfying performance was found in arid areas with an RBIAS of −0.233. The negative value of RBIAS reflected some overestimation in RFFA.

This approach shows considerable promise for the estimation of extreme flood magnitudes at global scales, and the
average RBIAS in estimation is less than 18% for all design floods. This is likely to yield a significant improvement in the skill of global flood inundation models.

Appendix A: Mann–Kendall test (MKT)

For a discharge series \( \{ Y_i \}_{i=1}^n \), the process of MKT is described in Eqs. (A1) to (A4):

\[
S = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \text{sgn} (Y_j - Y_i), \quad (A1)
\]

\[
\text{sgn} (y) = \begin{cases} 
1, & y > 0 \\
0, & y = 0 \\
-1, & y < 0 
\end{cases}, \quad (A2)
\]

The variance of \( S \) is computed as follows:

\[
\text{Var}(s) = \frac{1}{18} (n(n-1)(2n+5) - \sum_{i=1}^{n} t_i (i-1)(2i+5)), \quad (A3)
\]

where \( n \) is the total number of time series \( Y_i \); \( \text{Var}(s) \) is the variance of \( S \); and \( t_i \) is the number of data points contained in the \( i \)th tie group.

The MKT statistic \( Z \) is given by

\[
Z = \begin{cases} 
\frac{S-1}{\sqrt{\text{Var}(s)}}, & S > 0 \\
0, & S = 0 \\
\frac{S+1}{\sqrt{\text{Var}(s)}}, & S < 0 
\end{cases}. \quad (A4)
\]

Appendix B: Standard normal homogeneity test (SNHT)

For a discharge series \( \{ Y_i \}_{i=1}^n \), the SNHT is described in Eqs. (B1) to (B4).

\[
T_d = d \frac{\overline{z}_1^2 + (n-d) \frac{\overline{z}_2^2}{d}}, \quad d = 1, 2, \ldots n, \quad (B1)
\]

\[
Z_1 = \frac{1}{d} \sum_{i=1}^{d} \frac{(Y_i - \overline{Y})}{\delta}, \quad (B2)
\]

\[
Z_2 = \frac{1}{n-d} \sum_{i=d+1}^{n} \frac{(Y_i - \overline{Y})}{\delta}. \quad (B3)
\]

The SNHT statistic \( T \) is given by

\[
T = \max (T_d), \quad (B4)
\]

where \( n \) is the total number of time series \( Y_i \); and \( \overline{Y} \) and \( \delta \) are the mean and standard deviation of time series \( Y_i \).

Appendix C: Discordancy measure methods

The \( Z \) score (ZS) method is described in Eq. (C1).

\[
zs_i = \frac{R_i - \overline{R}}{sd(R)}, \quad (C1)
\]

where \( R_i \) is the mean annual runoff of station \( i \) in one subgroup; \( \overline{R} \) is the mean value of \( R_i \) in one subgroup; and \( sd(R) \) is the standard deviation of \( R_i \) in one subgroup.

The \( L \)-moment-based method is presented in Eqs. (C2) to (C4).

\[
D_i = \frac{1}{3} N_k (U_i - \overline{U}) \frac{T}{S^{-1}} (U_i - \overline{U}), \quad (C2)
\]

\[
\overline{U} = \frac{1}{N_k} \sum_{i=1}^{N_k} U_i, \quad (C3)
\]

\[
S = \sum_{i=1}^{N_k} (U_i - \overline{U}) \frac{T}{S^{-1}} (U_i - \overline{U}), \quad (C4)
\]

where \( N_k \) is the number of stations in cluster \( k \), and \( U_i = [t_1^i, t_2^i] \) is the vector of the coefficient of \( L \) variation (\( L \) CV), \( L \) skewness and \( L \) kurtosis of the station \( i \) as defined by Hosking and Wallis (2005).
Table D1. Hypothetical distributions adopted in this research.

| No. | Hypothetical distributions | Probability density function $f(x)$ or cumulative distribution function $F(X)$ |
|-----|----------------------------|--------------------------------------------------------------------------------|
| 1   | Normal distribution (NORM) | $f(x) = \frac{1}{\sqrt{2\pi b^2}} \exp\left(-\frac{(x-a)^2}{2b^2}\right)$ |
| 2   | Exponential distribution (EXP) | $F(x) = 1 - \exp\left(-\frac{x-a}{b}\right)$ |
| 3   | Gumbel distribution (GUMBEL) | $F(x) = \exp\left[-\exp\left(-\frac{x-a}{b}\right)\right]$ |
| 4   | Generalised extreme value distribution (GEV) | $F(x) = \exp\left[-\left(1 - \frac{b}{a} (x-c)\right)^{\frac{1}{b}}\right]$ |
| 5   | Generalised logistic distribution (GENLOGIS) | $F(x) = \frac{1}{1+\exp\left(\frac{x-c}{a}\right)}$ |
| 6   | Generalised Pareto distribution (GENPAR) | $F(x) = 1 - \left(1 + c \left(\frac{x-a}{b}\right)^{\frac{1}{c}}\right)^{-1}$ |
| 7   | Log-normal distribution (LN3) | $f(x) = \frac{1}{\sqrt{2\pi b(x-c)}} \exp\left(-\frac{1}{2} \left(\frac{\log(x-c) - h}{a}\right)^2\right)$ |
| 8   | Pearson type III distribution (P3) | $f(x) = \frac{1}{a^b \Gamma(b)} \left(\frac{x-c}{a}\right)^{b-1} \exp\left(-\frac{x-c}{a}\right)$ |

Note that $x$ is the random variable; $a$, $b$ and $c$ are parameters of distributions.

Appendix E: Anderson–Darling (AD) test

Given a sample of data $x_i (i = 1, 2, \ldots, m)$, the AD test will determine if a given dataset comes from a candidate cumulative distribution function $F(x, \theta)$ as in Eq. (E1), where $\theta$ is the parameter estimated by the sample $x_i$.

$$
\begin{align*}
F_m(x) &= 0, \quad x < x_{(1)} \\
F_m(x) &= i/m, \quad x_{(i)} \leq x < x_{(i+1)} \\
F_m(x) &= 1, \quad x_{(m)} \leq x
\end{align*}
$$

(E1)

where $F_m(x)$ is the empirical cumulative distribution function; $x_{(i)}$ is the $i$th element of the sample in increasing order; and the AD test statistic $A^2$ can be calculated as in Eq. (E2) (Ahmad et al., 1988; Laio, 2004).

$$
A^2 = -m - \frac{1}{m} \sum_{i=1}^{m} \left\{ (2i-1) \ln[F(x_{(i)}, \theta)] + (2m+1-2i) \ln[1 - F(x_{(i)}, \theta)] \right\}
$$

(E2)
Code availability. The MKT and SNHT were implemented using the “trend” package (https://cran.r-project.org/web/packages/trend/index.html, Pohlert, 2021). The discordancy and at-site design floods were estimated based on the nsRFA package (https://CRAN.R-project.org/package=nsRFA, Vigliione, 2021). The K-means, SVM and RF models are available from https://www.mathworks.com/help/stats/kmeans.html (MathWorks, 2021a), https://uk.mathworks.com/help/stats/support-vector-machine-regression.html (MathWorks, 2021b) and https://www.stat.berkeley.edu/~breiman/RandomForests/ (Breiman and Cutler, 2021) respectively.

Data availability. The Global Streamflow Indices and Metadata Archive (GSIM) is freely available at https://doi.org/10.1594/PANGAEA.887477 (Do et al., 2018b). To access WorldClim – Global Climate Data, visit http://www.worldclim.org/ (Fick and Hijmans, 2021). The adopted terrain data are the MERIT-DEM at http://hydro.iis.u-tokyo.ac.jp/~yamadai/MERIT_DEM/ (Yamazaki, 2021). The Gridded Population of the World (GPW) dataset is available from https://sedac.ciesin.columbia.edu/data/collection/gpw-v4 (CIESIN, 2021). The Global Lakes and Wetlands Database (GLWD) is available from https://www.worldwildlife.org/pages/global-lakes-and-wetlands-database (Lehner and Döll, 2021). The data sources of the NRCS curve number dataset are described at https://doi.org/10.1080/2150704X.2017.1297544 (Zeng et al., 2017). The Global Reservoir and Dam Database (GRanD) can be downloaded by visiting http://globaldamwatch.org/grand/ (Beames et al., 2021).

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