Global-scale massive feature extraction from monthly hydroclimatic time series: Statistical characterizations, spatial patterns and hydrological similarity

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Abstract: Hydroclimatic time series analysis focuses on a few feature types (e.g., autocorrelations, trends, extremes), which describe a small portion of the entire information content of the observations. Aiming to exploit a larger part of the available information and, thus, to deliver more reliable results (e.g., in hydroclimatic time series clustering contexts), here we approach hydroclimatic time series analysis differently, i.e., by performing massive feature extraction. In this respect, we develop a big data framework for hydroclimatic variable behaviour characterization. This framework relies on approximately 60 diverse features and is completely automatic (in the sense that it does not depend on the hydroclimatic process at hand). We apply the new framework to characterize mean monthly temperature, total monthly precipitation and mean monthly river flow. The applications are conducted at the global scale by exploiting 40-year-long time series originating from over 13 000 stations. We extract interpretable knowledge on seasonality, trends, autocorrelation, long-range dependence and entropy, and on feature types that are met less frequently in the literature. We further compare the examined hydroclimatic variable types in terms of this knowledge and, identify patterns related to the spatial variability of the features. For this latter purpose, we also propose and exploit a hydroclimatic time series clustering methodology. This new methodology is based on Breiman’s random forests. The descriptive and exploratory insights gained by the global-scale applications prove the usefulness of the adopted feature compilation in hydroclimatic contexts. Moreover, the spatially coherent patterns characterizing the clusters delivered by the new methodology build confidence in its future exploitation. Given this spatial coherence and the scale-independent nature of the features (which makes them particularly useful in forecasting and simulation contexts), we believe that this methodology could also be beneficial within regionalization frameworks, in which knowledge on hydrological similarity is exploited in technical and operative terms.

Keywords: autocorrelation; entropy; hydroclimatic signatures; seasonality; statistical hydrology; trends
1. Introduction

1.1 Representations and characterizations of hydroclimatic variables

The study of hydroclimatic variables and related topics and themes—such as precipitation, temperature and river flow dynamics—across spatio-temporal scales is a strategic research priority in a changing world. In line with this priority, pathways of hydroclimatic research are largely focused on the underlying mechanisms of hydroclimatic variables, their role in the sustenance of Earth systems, their changes, interrelationships, and relationships with climatic regimes and catchment characteristics (see e.g., Montanari et al. 2013; Blöschl et al. 2019a; Fan et al. 2019). In this context, representations and characterizations can be exploited to advance our understanding and scientific models of this important family of real-world variables.

Representations and characterizations can take various formulations not only as the core of diagnostic and exploratory frameworks, but also being hidden behind predictions of all possible types (see e.g., Pechlivanidis et al. 2014; Tyralis and Koutsoyiannis 2017; Papacharalampous et al. 2019a; Tyralis et al. 2020), and as the basis for hydrological and hydroclimatic (stochastic) simulation frameworks (see e.g., Perrin et al. 2003; Kumar et al. 2006; Langousis and Koutsoyiannis 2006; Lee and Salas 2011; Grimaldi et al. 2012; Papalexiou 2018). The candidate formulations may include (but are not limited to) statistical characterizations and representations in terms of marginal probability (or cumulative) distribution functions (see e.g., Kroll et al. 2002; Papalexiou and Koutsoyiannis 2013; Papalexiou et al. 2013; Nerantzaki and Papalexiou 2019), joint probability distribution functions and copulas (see e.g., Serinaldi et al. 2009; Kuchment and Demidov 2013; Wong et al. 2013), time series or regression models (see e.g., Carlson et al. 1970; Koutsoyiannis 2011; Khatami 2013; Khazaei et al. 2019; Papalexiou and Montanari 2019; Kagawa-Viviani and Giambelluca 2020), process-based (including conceptual) representations (see e.g., the reviews in Langousis and Koutsoyiannis 2006; Langousis and Veneziano, 2007, 2009; Langousis et al., 2009; Veneziano and Langousis 2010; Koutsoyiannis and Langousis 2011; Langousis and Kaleris 2014; Langousis et al. 2016a; Davtalab et al. 2017; Széles et al. 2018; Khatami et al. 2019; Tyralis and Langousis 2019; Emmanouil et al. 2020; Khatami et al. 2020; Perdios and Langousis 2020), and characterizations through feature extraction; see Section 1.2 below.
1.2 Features of hydroclimatic variables: Definition, extensions and examples

In their typical form, features (also known as “signatures”, “statistical characteristics”, or simply “statistics”) are sample statistics or model parameter estimates that can summarize or measure specific properties of real-world processes. They can also be exploited in a straightforward way (i.e., through regression analyses) for identifying important relationships between such properties. For instance, the Hurst parameter of the fractional Gaussian noise (fGn) process—initially introduced by Kolmogorov (1940), extensively studied by Mandelbrot, Wallis, and Van Ness in the 1960s (see e.g., Mandelbrot and Wallis 1968), and popularized in recent works (e.g., in Beran 1994; Koutsoyiannis 2002; Montanari 2003; O’Connell et al. 2016)—is a feature indicating the magnitude of long-range temporal dependence (when computed for non-seasonal processes). Global-scale investigations on this dependence and its relationships with other statistical properties of annual precipitation and annual runoff can be found in Tyralis et al. (2018; see also the references therein) and Markonis et al (2018b), respectively. Similarly, the shape parameter of the generalized extreme value distribution, when the latter is fitted to daily annual block maxima of streamflow, can serve as an indicator for flood extremity (see e.g., the investigations for North America by Tyralis et al. 2019c and the references therein).

By extension, less interpretable descriptive features (i.e., any statistic or model parameter estimate, independently of its interpretability) may also be relevant for various purposes and tasks (see e.g., Fulcher and Jones 2014; Christ et al. 2018; Fulcher 2018; Lubba et al. 2019), including feature-based time series clustering (distinguished from other time series clustering approaches e.g., in Aghabozorgi et al. 2015). Moreover, process predictability features can be extracted by characterizing the out-of-sample predictive performance (of statistical or process-based models) in terms of selected scores (see e.g., the global-scale predictability characterizations of monthly temperature and precipitation in terms of Nash-Sutcliffe efficiency by Papacharalampous et al. 2018). In this view, feature extraction facilitates the study of hydroclimatic (and other geophysical) processes from both the descriptive and predictive perspectives. These two perspectives, distinguished on a theoretical basis in Shmueli (2010), have important technical and operative implications, and may be linked (to a larger or smaller extent) to each other (see e.g., the investigations for North America and Europe on the relationships between selected predictability and descriptive annual river flow features in
Papacharalampous and Tyralis 2020, and the detailed study on the key hydroclimatic and physiographic drivers controlling seasonal river flow predictability across Europe by Pechlivanidis et al. 2020). In what follows, and unless specified differently, we will refer to descriptive features of hydroclimatic variables, obtained through statistical analyses in geoscience, since the present work is devoted to such features.

1.3 Features of hydroclimatic variables: Brief overview and investigated concepts

Features are regularly computed and studied in many diverse branches of geoscience, including statistical-stochastic geoscience (see e.g., Montanari et al. 1997; Grimaldi 2004; Koutsoyiannis 2011; Volpi and Fiori 2012; Markonis and Koutsoyiannis 2013; Papalexiou et al. 2013; Volpi et al. 2015; Villarini 2016; Markonis et al. 2018b; Tyralis et al. 2018; Volpi 2019; Marra et al. 2020; Serinaldi et al. 2020a) and catchment hydrology (see e.g., Pallard et al. 2009; Baratti et al. 2012; Euser et al. 2013; Toth 2013; Zhang et al. 2014; Shafii and Tolson 2015; Westerberg and McMillan 2015; Boscarello et al. 2016; Donnelly et al. 2016; Su et al. 2016; Westerberg et al. 2016; Fang et al. 2017; McMillan et al. 2017; Addor et al. 2018; Zhang et al. 2018). This latter field (in which features are referred to as “hydrological signatures”) shows the wide applicability of feature extraction with emphasis on feature-based catchment classification (see e.g., Burn and Boorman 1992; Wagener et al. 2007; Sivakumar 2008; Castellarin et al. 2011; He et al. 2011a; Ley et al. 2011; Di Prinzio et al. 2011; Sawicz et al. 2011; Ali et al. 2012; Coopersmith et al. 2012; Thomas et al. 2012; Toth 2013; Sawicz et al. 2014; Sikorska et al. 2015; Sivakumar et al. 2015; Auerbach et al. 2016; Ley et al. 2016; Tongal and Sivakumar 2017; Jehn et al. 2020), being viewed as (1) an effective approach to advance process perception and understanding, and (2) a necessary step for the regionalization of hydrologic models (e.g., Merz and Blöschl 2004) under a more general interpretation of hydrological similarity (i.e., similarity in specific hydrological features).

Other important concepts traditionally studied through feature extraction are those of variability and change (e.g., Montanari et al. 2013), with various trend, seasonality and temporal dependence features being among the most popular ones (e.g., Montanari et al. 1997; Grimaldi 2004; Koutsoyiannis 2011; Markonis and Koutsoyiannis 2013; Mallakpour and Villarini 2015; Archfield et al. 2016; Villarini 2016; Blöschl et al. 2017; Hall and Blöschl 2018; Markonis et al. 2018b; Tyralis et al. 2018; Blöschl et al. 2019b; Bertola et al. 2020; Kagawa-Viviani and Giambelluca 2020; Kelder et al. 2020; Serinaldi et
al. 2020b). Both variability and change, similar to feature extraction itself, are relevant to all temporal scales (i.e., daily, monthly, seasonal, annual and inter-annual), while feature selection is usually regarded as problem-dependent (as each study or research aim may require its own set of features). For a specific problem, a representative feature set could be determined either experimentally (see e.g., the extensive investigations by Tyralis et al. 2019c) or according to available past experience and experts' knowledge (see e.g., the guidelines by McMillan et al. 2017).

Unarguably, during the last decade the study of hydroclimatic variable features has rapidly progressed following the increasing release of big hydroclimatic datasets, with many diverse and important topics being advanced through large-scale feature extraction, conducted at continental-scale regions (mostly in North America and Europe) and even at the global scale. Among the most characteristic topics are those related to:

- **Temperature means** (see e.g., Papacharalampous et al. 2018; Kagawa-Viviani and Giambelluca 2020).
- **Temperature extremes** (see e.g., Papalexiou et al. 2018b; Kagawa-Viviani and Giambelluca 2020).
- **Precipitation means** (Peel et al. 2002; Small et al. 2006; Papacharalampous et al. 2018; Tyralis et al. 2018).
- **Precipitation extremes** (see e.g., Papalexiou and Koutsoyiannis 2012, 2013; Langousis et al. 2016; Papalexiou et al. 2018a; Nerantzaki and Papalexiou 2019; Papalexiou and Montanari 2019; Kelder et al. 2020).
- **Streamflow means** (see e.g., Small et al. 2006; Markonis et al. 2018b; Papacharalampous et al. 2019a; Papacharalampous and Tyralis 2020).
- **Floods and streamflow maxima** (see e.g., Villarini et al. 2011; Mallakpour and Villarini 2015; Archfield et al. 2016; Berghuijs et al. 2016; Slater and Villarini 2016; Villarini 2016; Berghuijs et al. 2017; Blöschl et al. 2017; Do et al. 2017; Slater and Villarini 2017; Steirou et al. 2017; Hall and Blöschl 2018; Berghuijs et al. 2019a,b; Bertola et al. 2020; Blöschl et al. 2019b; Iliopoulou et al. 2019; Steirou et al. 2019; Tyralis et al. 2019c; Brunner et al. 2020; Do et al. 2020; Kemter et al. 2020; Perdios and Langousis 2020; Stein et al. 2020; see also the overviews by Hall et al. 2014; Blöschl et al. 2015; Zaghloul et al. 2020).
- **Droughts and low flows** (see e.g., Tongal et al. 2013; Van Loon et al. 2014; Hanel et al.
1.4 Aims and novelties of the present work

Here we: (1) develop a detailed framework for complete hydroclimatic variable characterization through massive feature extraction (with this massive character being the major theme of our work); (2) develop a new hydroclimatic time series clustering methodology that can also be perceived as a geographical location clustering methodology (since hydroclimatic time series correspond to geographical locations), thereby formalizing the identification of spatial patterns related to the spatial variability of the features; and (3) demonstrate the new framework and the new methodology within three global-scale applications to (a) characterize three hydroclimatic variable types (i.e., mean monthly temperature, total monthly precipitation and mean monthly river flow) and their spatial patterns, (b) inspect the statistical (dis)similarities of these variable types, (c) investigate the relationships between features, and (d) characterize the importance of the features in terms of variance explanation and in hydroclimatic time series clustering.

Our work complements the existing literature on the topic, while advancing the state-of-the-art knowledge, as summarized here below:

- Massive extraction of a variety of features is performed for three global hydroclimatic datasets. More precisely, 59 features are computed and extracted, without particular focus on a specific category (e.g., on trend or autocorrelation features).

- Based on these features, a new hydroclimatic time series clustering methodology is proposed. With this methodology, we aspire to exploit a larger part of the available information encompassed in monthly hydroclimatic time series than we could with existing methodologies.

- Feature compilation is supported by past experience and experts’ knowledge. The latter is largely sourced from scientific fields beyond geosciences (e.g., neuroscience, biology, biomedicine, forecasting), and has not been exploited so far in hydroclimatic and environmental contexts. Therefore, it should be encountered as a new concept for such contexts, whose usefulness is demonstrated through the present work.

- Focus spreads to three hydroclimatic variable types (examined at the same timescale), rather than being limited to a single one, thus allowing for direct comparisons within and across hydroclimatic variables under the concept of
hydrological similarity.

2. Data and methods

In this Section, we present our data and methods. Statistical software information is independently summarized in Appendix A.

2.1 Global hydroclimatic datasets

We compile a global dataset based on three large freely available temperature (Menne et al. 2018), precipitation (Peterson and Vose 1997), and river flow (Do et al. 2018) datasets. Basic data retrieval information is provided in Appendix B. We extract complete 40-year mean monthly time series from 2 432 temperature stations and complete 40-year total monthly time series 5 071 precipitation stations. From the entire river flow dataset, we first retrieve all the 40-year mean monthly river flow time series that have resulted from the aggregation of daily time series with missing up to 1% of their values (i.e., 5 849 time series). From these initially retrieved time series, we retain those that pass a visual inspection quality control (i.e., 5 601 time series that are not characterized by abrupt changes or irregularities). The geographical locations of the 13 104 exploited stations are presented in Figure 1.

Figure 1. Geographical locations of the temperature (Menne et al. 2018), precipitation (Peterson and Vose 1997), and river flow (Do et al. 2018) stations exploited in the study.
2.2 Feature description and extraction

Our methodological framework extends hydroclimatic signatures to a comprehensive set of 59 features. This feature set characterizes a wide range of the entire information content encompassed in hydroclimatic (and other geophysical) time series. A brief description of these features, adapted from Kang et al. (2017), Hyndman et al. (2020b) and Kang et al. (2020), is provided in Table 1. For their computation, we use various statistical-stochastic models, such as the sample autocorrelation function, the sample partial autocorrelation function, time series decomposition models, and the autoregressive fractionally integrated moving average (ARFIMA) model, to name a few (see Table 1 for details). Stochastic models (see e.g., Box and Jenkins 1970; Wei 2006) are certainly of interest to hydrologists and geoscientists (see e.g., Hurst 1951; Carlson et al. 1970; Yevjevich 1987; Hipel and McLeod 1994; Montanari et al. 1997; Koutsoyiannis 2002; Grimaldi 2004; Sivakumar and Berndtsson 2010; Veneziano and Langousis 2010; Grimaldi et al. 2011; O’Connell et al. 2016); however, in most hydrological and geoscientific studies this interest is limited to a small number of models (which is not the case herein). Another important remark to be made, at this point, is that the computed features do not depend on the scale (i.e., the magnitude) of the time series (to not be confused with the temporal resolution of the time series). Therefore, our methodological framework allows direct comparisons within and across geophysical and environmental variables (including hydroclimatic variables).

Table 1. Features computed in the study. Their brief description is adapted mostly from Hyndman et al. (2020b) but also from Kang et al. (2017, 2020) and the related vignette (https://github.com/robjhyndman/tsfeatures/blob/master/vignettes/tsfeatures.Rmd), while further information can be found in Fulcher et al. (2013), Hyndman et al. (2015), and Fulcher and Jones (2017). A loose categorization of the features is provided in the Supplement (see Table S1 herein).

| S/n | Abbreviation | Brief description |
|-----|--------------|-------------------|
| 1   | x_acf1       | Lag-1 sample autocorrelation of the original time series. |
| 2   | ac_9         | Lag-9 sample autocorrelation of the original time series, an autocorrelation feature from software package hctsa (Fulcher and Jones 2017; see also Fulcher et al. 2013) that is included for competency purposes (along with other autocorrelation features from the same package; see Table S1) in software package tsfeatures (Hyndman et al. 2020b) and herein. |
| 3   | x_acf10      | Sum of the squared sample autocorrelation values for the first ten lags of the original time series. |
| 4   | diff1_acf1   | Lag-1 sample autocorrelation of the first-order differenced time series. |
| 5   | diff1_acf10  | Sum of the squared sample autocorrelation values for the first ten lags of the first-order differenced time series. |
| 6   | diff2_acf1   | Lag-1 sample autocorrelation of the second-order differenced time series. |
| 7   | diff2_acf10  | Sum of the squared sample autocorrelation values of the first ten lags of the second-order differenced time series. |
| 8   | seas_acf1    | Sample autocorrelation for lag equal to one season. |
### Abbreviation

| S/n | Abbreviation                | Brief description                                                                                                                                 |
|-----|-----------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------|
| 9   | firstzero_ac               | Lag where the first zero crossing of the autocorrelation function is attained.                                                                  |
| 10  | firstmin_ac                | Lag where the first minimum of the autocorrelation function is attained.                                                                        |
| 11  | embed2_incircle_1          | Proportion of points inside a given circular boundary in a 2-dimensional embedding space. The circular boundary is obtained by setting the respective argument to 1 in CompEngine (e.g., through the software package hctsa). |
| 12  | embed2_incircle_2          | Proportion of points inside a given circular boundary in a 2-dimensional embedding space. The circular boundary is obtained by setting the respective argument to 2 in CompEngine (e.g., through the software package hctsa). |
| 13  | trev_num                   | The numerator of trev function, a normalized nonlinear autocorrelation function from software package hctsa. The feature is computed for the first lag of the original time series. |
| 14  | motiftwo_entro3            | A feature for identifying local motifs in a binary symbolization of the time series. For its computation, coarse-graining is performed; time series values above the mean are set to 1, and those below the mean are set to 0. |
| 15  | walker_propcross           | A hypothesis of a time series characterizing the time series through the time domain, is simulated. The walker moves in response to values of the time series at each point, narrowing the gap between its value and that of the time series by 10%. Then, walker_propcross is the fraction of time series length that the walker crosses time series. |
| 16  | x_pacf5                    | Sum of the squared sample partial autocorrelation values for the first five lags of the original time series.                                      |
| 17  | diff1x_pacf5               | Sum of the squared sample partial autocorrelation values for the first five lags of the first-order differenced time series.                       |
| 18  | diff2x_pacf5               | Sum of the squared sample partial autocorrelation values for the first five lags of the second-order differenced time series.                    |
| 19  | seas_pacf                  | Sample partial autocorrelation for lag equal to one season.                                                                                       |
| 20  | localsimple_mean1          | Lag τ where the first zero crossing of the autocorrelation function of the residuals from the prediction of the local mean is attained. The prediction is obtained by applying a linear model, with predictor the immediate preceding value in the time series. |
| 21  | localsimple_lfitac         | Lag τ where the first zero crossing of the autocorrelation function of the residuals from the prediction of the local mean is attained. The prediction is obtained by applying a linear model, with predictors the last three values in the time series. |
| 22  | sampen_first               | The second sample entropy of a time series, modified from Fulcher’s EN_SampEn (Fulcher and Jones 2017, Supplementary information), which uses a code from PhysioNet (Richman and Moorman 2000). |
| 23  | std1st_der                 | Standard deviation of the first-order differenced time series (with a standardization procedure additionally applied).                               |
| 24  | spreadrandomlocal_mantaul_50 | Bootstrap-based stationarity measure from software package hctsa. First, 100 time series segments, each containing 50 consecutive points, are selected at random from the time series. Then, the feature is computed as the ensemble mean of the lags where the first zero-crossing of the autocorrelation function is attained in all segment. |
| 25  | spreadrandomlocal_mantaul_ac2 | Bootstrap-based stationarity measure from software package hctsa. First, 100 time series segments, each containing / consecutive entries, where / equals twice the first zero-crossing of the autocorrelation function, are selected at random from the time series. Then, the feature is computed as the ensemble mean of the first zero-crossings of the autocorrelation function in all segments. |
| 26  | histogram_mode_10          | Mode of a data vector using a 10-bin histogram. The data is z-scored before computing the feature.                                                |
| 27  | outlierinclude_mdrmd       | Feature measuring the evolution of the median of a sample, as more and more outliers, located further from the mean, are included in the calculation according to a specified rule. The threshold for including data points in the analysis increases from zero to the maximum deviation, in increments of 0.01×σ, where σ is the standard deviation of the time series. At each threshold, proportion of time series points included and mean are calculated, and outputs from the algorithm measure how these statistical quantities change as more extreme points are included in the calculation. The data is z-scored before computing the feature. Outliers are defined as furthest from the mean. Fluctuation analysis is performed. A polynomial of order 1 is fitted and the range is returned. The order of fluctuations is 2, corresponding to root mean square fluctuations. |
| 28  | fluctanal_prop_r1          | The number of times a time series crosses the median.                                                                                           |
| 29  | crossing_points            | The number of times a time series crosses the median.                                                                                           |
| S/n | Abbreviation | Description |
|-----|--------------|-------------|
| 30  | entropy      | The spectral entropy of a time series computed from a univariate normalized spectral density, estimated using an autoregressive (AR) model ([Jung and Gibson 2006](#)). This feature can be used as a measure of time series "forecastability", with smaller values indicating larger forecastability ([Goerg 2012](#)). |
| 31  | flat_spots   | The number of flat spots in the time series, computed by dividing the sample space of a time series into ten equal-sized intervals, and computing the maximum run length within any single interval. |
| 32  | arch_acf     | First, the original time series is pre-whitened using an AR model resulting in a new time series ($\phi$). Then, $\text{arch}_\text{acf}$ is calculated as the sum of the squares of the first 12 autocorrelation values of ($\phi$). |
| 33  | garch_acf    | First, the original time series is pre-whitened using an AR model resulting in a new time series ($\phi$). Then, a GARCH(1,1) model is fitted to ($\phi$) and the residuals ($e$) are obtained. Lastly, $\text{garch}_\text{acf}$ is calculated as the sum of the squares of the first 12 autocorrelation values of ($e$). |
| 34  | arch_r2      | First, the original time series is pre-whitened using an AR model resulting in a new time series ($\phi$). Then, $\text{arch}_\text{r2}$ is calculated as the R$^2$ value of an AR model fitted to ($\phi$). |
| 35  | garch_r2     | First, the original time series is pre-whitened using an AR model resulting in a new time series ($\phi$). Then, a GARCH(1,1) model is fitted to ($\phi$) and the residuals ($e$) are obtained. Lastly, $\text{garch}_\text{r2}$ is calculated as the R$^2$ value of an AR model fitted to ($e$). |
| 36  | alpha        | First smoothing parameter $\alpha$ of Holt-Winters’ seasonal method ([Hyndman and Athanasopoulos 2018](#), Chapter 7.3), an extension of the Holt’s linear trend method ([Hyndman and Athanasopoulos 2018](#), Chapter 7.2). Holt-Winters’ seasonal method considers additive seasonal trend. |
| 37  | beta         | Second smoothing parameter $\beta$ of Holt-Winters’ seasonal method. |
| 38  | gamma        | Third smoothing parameter $\gamma$ of Holt-Winters’ seasonal method. |
| 39  | lumpiness    | First, the variances of all tiled windows are calculated. Then, lumpiness is the variance of the variances. |
| 40  | stability    | First the means of all tiled windows are calculated. Then, stability is the variance of the means. |
| 41  | max_level_shift | The largest shift (mean shift) between two consecutive windows. |
| 42  | time_level_shift | The time index of max_level_shift. |
| 43  | max_var_shift  | The largest variance shift between two consecutive windows. |
| 44  | time_var_shift  | The time index of max_var_shift. |
| 45  | max_kl_shift  | The largest shift in Kulback-Leibler divergence between two consecutive windows. |
| 46  | time_kl_shift  | The time index of max_kl_shift. |
| 47  | ARCH.LM    | Feature based on the Lagrange Multiplier (LM) test of [Engle 1982](#) for autoregressive conditional heteroscedasticity (ARCH), specifically the R$^2$ value of an autoregressive model of order 12 applied to the squared de-meaned data. |
| 48  | nonlinearity | Nonlinearity feature based on Teräsvirta’s nonlinearity test. The feature is $10X^2/T$, where $X^2$ is the Chi-squared statistic from Teräsvirta’s test, and $T$ is the length of the time series. Large values indicate nonlinearity, and values around 0 indicate linearity. |
| 49  | unitroot_kpss  | The statistic of the unit root test by [Kwistowski et al. (1992)](#), for linear trend and lag 1. |
| 50  | hurst        | First, classical time series decomposition is performed using the additive model ([Hyndman and Athanasopoulos 2018](#), Chapter 6.3) according to the following equation: $x_t = S_t + T_t + R_t$. In this equation, $x_t$ denotes the data at time $t$, while $S_t$ and $R_t$ denote the seasonal and remainder components, respectively, at time $t$. A measure of long-range dependence is measured through the following equation ([Wang et al. 2006](#)): $\text{hurt} = 1 - \text{var}(R_t)/\text{var}(x_t - S_t)$. |
| 51  | trend       | First, STL decomposition ([seasonal and trend decomposition using Loess; see e.g., Hyndman and Athanasopoulos 2018](#), Chapter 6.6) is applied to the original series ([Hyndman and Khandakar 2008](#); [Hyndman et al. 2020](#)), according to the following equation: $x_t = S_t + T_t + R_t$. In this equation, $x_t$ denotes the data at time $t$, while $S_t$ and $R_t$ denote the seasonal, smoothed trend and remainder components, respectively, at time $t$. The trend strength is then measured through the following equation ([Wang et al. 2006](#)): $\text{trend} = 1 - \text{var}(R_t)/\text{var}(x_t - S_t)$. |
| 52  | spike       | STL decomposition (see above) is applied to the original series. The computed measure of "spikiness" is the variance of the leave-one-out variances of the remainder component ($R_t$); see above. |
### 2.3 Statistical learning algorithms

In addition to the large variety of classical statistical-stochastic models utilized herein (see Section 2.2), we also apply four statistical learning (else referred to as “machine learning”) algorithms (see e.g., Hastie et al. 2009; James et al. 2013; Alpaydin 2014). These algorithms are principal component analysis (see Section 2.3.1), linear regression (see Section 2.3.2), hierarchical clustering (see Section 2.3.3) and random forests (see Section 2.3.4). As documented in Mukhopadhyay and Wang (2020), statistical learning algorithms have their roots in nonparametric statistics. These algorithms are known to offer benefits (e.g., they can become fully automated and provide improved solutions as the dataset size increases; see also the relevant discussions in Breiman 2001b), which are insightful for geoscientific and environmental studies (Quilty et al. 2019; Sahoo et al. 2019; Tyralis et al. 2019a; Papacharalampous et al. 2020; Quilty and Adamowski 2020; Rahman et al. 2020).

#### 2.3.1 Principal component analysis

Principal component analysis is an unsupervised learning algorithm (i.e., an algorithm that “learns” using unlabelled data, without human “supervision”) for interpretable dimensionality reduction and variance explanation characterizations, used in geosciences (Burn and Boorman 1992; Euser et al. 2013; Jehn et al. 2020) and beyond (Abdi and Williams 2010; Jolliffe and Cadima 2016). For detailed literature and tutorial information on principal component analysis, the reader is referred to Abdi and Williams (2010), Bro
and Smilde (2014), Shlens (2014), and Jolliffe and Cadima (2016). In summary, principal component analysis uses an input variable set to compute new variables that are linear combinations of the original ones and are obtained under the following rules: (1) The first of the new variables (also referred to as “principal components”) should explain the largest possible portion of the total variance of the original (i.e., the input) data; (2) the second principal component should be orthogonal to the first principal component and explain the largest possible portion of the total variance of the original data; and (3) the remaining principal components should be computed likewise. According to Jolliffe and Cadima (2016), the roots of principal component analysis trace back to Pearson (1901) and Hotelling (1933). Herein, principal component analysis is used for extracting variance explanation information.

2.3.2 Linear regression

Linear regression supports supervised learning (i.e., learning based on input-output examples, which can be interpreted as some short of human “supervision”), specifically regression tasks, and is widely exploited for both statistical inference and prediction. In this work, it is used for inference and correlation analysis. Its theoretical properties are well-discussed in the literature (see e.g., James et al. 2013; Hastie et al. 2009).

2.3.3 Hierarchical clustering

Hierarchical clustering is a form of unsupervised learning. Once a measure of dissimilarity between (disjoint) groups of observations has been selected, the algorithm begins by assigning each data point to its own cluster and progresses by gradually joining the two most similar clusters, until a single cluster is obtained (containing all the data). At each stage, it also re-computes the distances between the clusters. Hierarchical clustering is explained in detail in Hastie et al. (2009, pp. 520–528).

2.3.4 Random forests

Breiman’s random forests (Breiman 2001a) belong to the family of ensemble learning algorithms (extensively reviewed e.g., by Sagi and Rokach 2018). They are used across a range of geoscientific and geoengineering applications (e.g., Tyralis and Papacharalampous 2017; Addor et al. 2018; Althoff et al. 2020; Rahman et al. 2020), and big data comparisons with stochastic and/or other machine learning algorithms (see e.g., Papacharalampous et al. 2019a, 2019b; Tyralis et al. 2020). Tyralis et al. (2019b) provide
long list of water resource engineering applications of random forests (published in 30 representative journals until 31 December 2018) together with the algorithm’s theoretical summary. In short, random forests are bagging (acronym for “bootstrap aggregation”; Breiman 1996) of classification and regression trees (CARTs; Breiman et al. 1984) with some additional degree of randomization, which aims at reducing the correlation between the trees and, consequently, the variance of the predictions (Tyralis et al. 2019b, Section 2.1.4). Their main parameter is the number of trees. They can be exploited either in supervised mode (for regression and classification) or in unsupervised mode (for clustering; see e.g., Yan et al. 2013). In this work, they are used in both these modes, specifically for classification and clustering.

2.4 Feature-based time series clustering methodology

We propose a new feature-based methodology for hydroclimatic time series clustering. This methodology relies on unsupervised random forests (see Section 2.3.4) and the feature set adopted in this study (see Section 2.2), with all the computed features simply being the random forests’ inputs. Together with the scale-independent nature of these features and their large variety (which also constitute the novelty of the methodology), the following properties of random forests contribute to making this methodology properly designed and useful for hydroclimatic time series clustering (Tyralis et al. 2019b, Section 2.8.1):

- They demonstrate increased predictive performance.
- They can handle highly correlated predictor variables.
- They can operate successfully when interactions are present.
- They are invariant to monotone transformations of the predictor variables.

Importantly, the proposed hydroclimatic time series methodology is applicable to different types of hydroclimatic (and environmental) data, with no need for input pre-processing via dimensionality reduction. Spatial information (i.e., the proximity of locations and spatial dependencies) and information on the time series magnitude are not considered by this methodology.

2.5 Global-scale application and pattern searching workflow

2.5.1 Monthly hydroclimatic time series characterizations and analyses

Hydroclimatic time series feature extraction and feature-based hydroclimatic time series
analyses are conducted at monthly time scale, as outlined here below:

- Under our feature-based approach to analysing hydroclimatic time series data (see Section 2.2), each monthly hydroclimatic time series (see Section 2.1) is converted into a vector of 59 features, representing its corresponding time series for any further analyses. In total, 13 104 feature vectors are computed and grouped under three feature datasets, each dataset corresponding to one of the hydroclimatic variable types examined in the study. The dimensions of the resulted mean monthly temperature, total monthly precipitation and mean monthly river flow feature data matrices are 2 432 × 59, 5 071 × 59 and 5 601 × 59, respectively.

- We summarize the information contained in the three feature datasets (see the above point) by conducting histograms. On this ground, we characterize and compare the three different hydroclimatic variable types.

- We characterize each of the three feature datasets in terms of variance explanation by conducting principal component analyses (see Section 2.3.1). As suggested in the literature (see e.g., Bro and Smilde 2014), pre-processing of the inputs via auto-scaling precedes the principal component analyses (because features are not dependent on the scale-magnitude of the time series, but range within different scales-magnitudes with regard to each other). On this ground, we search for patterns within and across the three different hydroclimatic variable types.

- We also perform linear regression (see Section 2.3.2) and compute the linear correlations between the features for each of the feature datasets. We present the corresponding correlograms for the entire feature datasets and for those 15 features contributing the most to the first and second principal components, as these components have been previously derived through our principal component analyses (see above point). For conducting the correlograms, we additionally apply hierarchical clustering (see Section 2.3.3) to the computed correlations and test their significance.

2.5.2 Spatial hydroclimatic patterns and hydroclimatic time series clustering

Identification of patterns related to the spatial variability of the features, as well as feature-based hydroclimatic time series clustering and hydroclimatic time series cluster characterizations, are conducted at monthly timescale, as outlined here below:

- We search for coherent spatial patterns characterizing the computed features by
conducting maps for continental-scale regions around the globe.

- We use the computed features to apply the new time series clustering methodology (see Section 2.4), separately for each hydroclimatic variable type. In this context, random forests (see Section 2.3.4) are applied with 5,000 trees, while the number of clusters is set to five.

- We also compute variable importance (i.e., the relative significance of the variables used by the algorithm for completing a statistical learning task) and use it for ranking the features.

- Once we have obtained the clustering outcomes, we perform spatial interpolation of the clusters by applying random forests (see Section 2.3.4) in classification mode. The application is again made with 5,000 trees. Separately for each hydroclimatic variable type, we use the location-cluster information for all stations (i.e., all the available location-cluster examples) as input-output examples for training the algorithm. Once the algorithm has been trained, it can be applied to predict the cluster of an arbitrary location of the globe (including locations other than those of the stations). To allow spatial pattern extraction, we present the spatial interpolation outcomes for continental-scale regions with a large number of stations.

3. Results and discussion

In this Section, we present the results of our global-scale analyses and investigations, and provide their interpretation in light of the study’s background. A portion of the conducted Figures is given the Supplement (for reasons of brevity).

3.1 Monthly hydroclimatic time series characterizations and analyses

3.1.1 Features of monthly hydroclimatic time series

Here, we summarize the results obtained through feature extraction. For this summary, we present and discuss a small sample of the histograms of the computed features (see Figures 2 and 3). This sample refers to ten selected features (i.e., \texttt{x\_acf1}, \texttt{x\_acf10}, \texttt{diff1\_acf1}, \texttt{seas\_acf1}, \texttt{x\_pacf5}, \texttt{stdlst\_der}, \texttt{entropy}, \texttt{nonlinearity}, \texttt{trend} and \texttt{seasonal\_strength}), for which at least one of the following conditions holds: (1) They are loosely identified (based on our intuition) as highly interpretable and/or highly relevant to the main interests spotted in the hydroclimatic literature (see the brief overview presented in Section 1.3); (2) They are objectively identified as among...
the top-10 important ones in explaining the variance of our three feature datasets (see Section 3.1.2), and in clustering the hydroclimatic time series (see Section 3.2.2). We choose to focus on 30 histograms for reasons of brevity only, with no intention to imply that the remaining histograms are not important, as such an implication would have been in opposition to our main premise (that by adopting a multi-faced and massive approach to hydroclimatic time series representation via feature extraction we can capture and explore the largest part of the information encoded in hydroclimatic time series). For this reason, the remaining histograms (i.e., 147 histograms) are provided in the Supplement (see Figures S1–S10 therein).

To better understand what the here-provided quantitative information implies in practical terms, and to facilitate further discussions on it, it might be useful to first recall the definitions of the ten selected features (see also Table 1), as well as to discuss their utilities and relevance to hydroclimatic concepts:

- Feature $x_{acf1}$ (i.e., the lag-1 sample autocorrelation of the original time series) is considered as a good autocorrelation measure in the hydrological literature and, thus, widely computed for interpretable characterizations of hydroclimatic variables (see e.g., Markonis et al. 2018; Papacharalampous et al. 2019a; Papacharalampous and Tyralis 2020). It takes values from $-1$ to $1$, and the larger its absolute value the larger the magnitude of the correlation (positive or negative, depending on the sign) between two subsequent data points in the original time series.

- On the contrary, $x_{acf10}$ is a new feature in hydroclimatic contexts. It is the sum of the squared sample autocorrelation values for the first ten lags of the original time series. This feature summarizes more information than $x_{acf1}$ and is quite interpretable (yet less interpretable than $x_{acf1}$). It takes positive (or zero) values, and the larger its values the stronger the temporal dependence structure of the hydroclimatic variables.

- Another feature that is scarcely computed in hydroclimatic contexts is $diff1_acf1$. This feature is defined as the lag-1 sample autocorrelation of the first-order differenced time series, and contributes—together with the remaining (partial) autocorrelation features of our framework—to better representing the temporal dependence structure of hydroclimatic variables. It takes values from $-1$ to $1$. 

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Figure 2. Histograms of the mean monthly temperature, total monthly precipitation and mean monthly river flow features (part 1). For comparison purposes, the limits of the horizontal axes have been set common for features of the same type. Outliers have been removed for $x_{\text{acf10}}$. The features are defined in Table 1.
Figure 3. Histograms of the mean monthly temperature, total monthly precipitation and mean monthly river flow features (part 2). For comparison purposes, the limits of the horizontal axes have been set common for features of the same type. Outliers have been removed for std1st_der, entropy, nonlinearity and trend. The features are defined in Table 1.
Similarly to \texttt{x\_acf1}, \texttt{seas\_acf1} is intuitively considered as an effective and interpretable autocorrelation measure for monthly (and more generally seasonal) hydroclimatic variables, as it is the sample autocorrelation for lag equal to one season. It takes values from \(-1\) to 1.

In opposition to other partial autocorrelation features (e.g., the lag-1 sample partial autocorrelation of the original time series), \texttt{x\_pacf5} has not been computed so far in hydroclimatic contexts to our knowledge. This feature is the sum of the squared sample partial autocorrelation values for the first five lags of the original time series; therefore, it summarizes more information than a sample partial autocorrelation value at a single lag. It takes positive (or zero) values.

Feature \texttt{std1st\_der} is the standard deviation of the first-order differenced time series (with a standardization procedure additionally applied) and, to our knowledge, has not been computed before in hydroclimatic contexts.

Feature \texttt{entropy} (i.e., the spectral entropy of the time series) can be used for characterizing hydroclimatic variables in terms of “forecastability” (Goerg 2013). This feature is computed from a univariate normalized spectral density, estimated using an autoregressive (AR) model, and takes values from 0 to 1. A variety of entropy-based analyses and calibration measures can be found in the hydrological literature (see e.g., Papalexiou and Koutsoyiannis 2012; Pechlivanidis et al. 2014; Tongal and Sivakumar 2017; Papacharalampous and Tyralis 2020); nonetheless, to our knowledge the estimator used in this study is new in hydroclimatic contexts.

Another feature that is relevant to the scientific interests identified in the hydroclimatic literature (see e.g., Khatami 2013; Xu et al. 2013; Fleming and Dahlke 2014; Zhou et al. 2016) is nonlinearity, a feature based on Teräsvirta’s nonlinearity test. This feature takes positive (or zero) values, with its large values indicating nonlinearity and its values around 0 indicating linearity.

Hydroclimatic trends are regularly analysed (see e.g., Khatami 2013; Do et al. 2017; Papalexiou et al. 2018b; Khazaei et al. 2019; Bertola et al. 2020). The trend strength of the time series (i.e., \texttt{trend}) is an interpretable and dimensionless measure for investigating trends that has only been computed so far for annual (i.e., non-seasonal) river flow time series (specifically, in Papacharalampous and Tyralis 2020) in the hydrological literature. Its usefulness arises from the fact that it allows comparisons
between (a) the magnitude of the variance of the remainder component (known as the “random” component of the time series) obtained by applying STL decomposition (i.e., the variation remaining in the data after the “removal” of its seasonal and trend components; Cleveland et al. 1990) and (b) the magnitude of the time series with only its seasonal component removed, thereby informing us in relative terms on the trend’s magnitude (compared to the “random” component’s magnitude). This feature takes values from 0 to 1, with smaller values indicating relatively weaker trends.

- Hydroclimatic seasonality is also of interest (see e.g., Villarini 2016; Hall and Blöschl 2018). The strength of seasonality (i.e., seasonal_strength) is an interpretable measure for relevant investigations. Similarly to trend, this feature provides information in relative terms on the strength of the seasonal component, obtained by applying STL decomposition, compared to the remainder component. This feature takes values from 0 to 1, with smaller values indicating relatively weaker seasonality.

As implied by our aim 3(b) (see Section 1.4), the presentation of all histograms is made in a way that allows a direct comparison between mean monthly temperature, total monthly precipitation and mean monthly river flow (see also the mean and median feature values presented in Table 2). For instance, we observe that larger values are computed for the mean monthly temperature autocorrelation and partial autocorrelation features summarized in Figure 2 (i.e., x_acf1, x_acf10, diff1_acf1, seas_acf1 and x_pacf5), than for the total monthly precipitation and mean monthly river flow autocorrelation and partial autocorrelation features (summarized in the same Figure), thereby revealing the temperature’s much stronger temporal dependence characteristics. Moreover, the temporal dependence structure of mean monthly river flow is found to be somewhat more intense on average than the temporal dependence structure of total monthly precipitation (see Table 2). Similar observations are made for seasonal_strength (see Figure 3m–o and Table 2), indicating somewhat stronger seasonality patterns in mean monthly river flow than those in total monthly precipitation (and the strongest seasonality patterns in mean monthly temperature). The histograms of the six above-discussed features are left-skewed for mean monthly temperature (see Figures 2 and 3m), and right-skewed or not skewed for total monthly precipitation (see Figures 2 and 3n) and mean monthly river flow (see Figures 2 and 3o).
Table 2. Medians and means of ten selected mean monthly temperature, total monthly precipitation and mean monthly river flow features. The features are defined in Table 1.

| Hydroclimatic time series feature | Corresponding histograms | Summary statistic | Mean monthly temperature | Total monthly precipitation | Mean monthly river flow |
|----------------------------------|--------------------------|-------------------|--------------------------|-----------------------------|------------------------|
| x_acf1                           | Figure 2a–c              | Median            | 0.825                    | 0.251                       | 0.492                  |
|                                  |                          | Mean              | 0.822                    | 0.278                       | 0.491                  |
| x_acf10                          | Figure 2d–f              | Median            | 3.666                    | 0.241                       | 0.484                  |
|                                  |                          | Mean              | 3.614                    | 0.405                       | 0.571                  |
| diff1_acf1                       | Figure 2g–i              | Median            | 0.538                    | -0.403                      | -0.226                 |
|                                  |                          | Mean              | 0.534                    | -0.357                      | -0.187                 |
| seas_acf1                        | Figure 2j–l              | Median            | 0.923                    | 0.281                       | 0.377                  |
|                                  |                          | Mean              | 0.919                    | 0.316                       | 0.385                  |
| x_pacf5                          | Figure 2m–o              | Median            | 1.698                    | 0.112                       | 0.297                  |
|                                  |                          | Mean              | 1.683                    | 0.172                       | 0.331                  |
| stdlst_der                       | Figure 3a–c              | Median            | 0.587                    | 1.224                       | 1.007                  |
|                                  |                          | Mean              | 0.591                    | 1.193                       | 0.998                  |
| entropy                          | Figure 3d–f              | Median            | 0.174                    | 0.924                       | 0.875                  |
|                                  |                          | Mean              | 0.191                    | 0.860                       | 0.848                  |
| nonlinearity                     | Figure 3g–l              | Median            | 0.190                    | 0.167                       | 0.514                  |
|                                  |                          | Mean              | 0.208                    | 0.349                       | 0.550                  |
| trend                            | Figure 3j–l              | Median            | 0.220                    | 0.145                       | 0.293                  |
|                                  |                          | Mean              | 0.227                    | 0.150                       | 0.311                  |
| seasonal_strength                | Figure 3g–l              | Median            | 0.964                    | 0.432                       | 0.517                  |
|                                  |                          | Mean              | 0.960                    | 0.453                       | 0.522                  |

On the other hand, the exact opposite holds for stdlst_der and entropy, with their computed values being smaller for mean monthly temperature (see Figure 3a,d) than for total monthly precipitation (see Figure 3b,e) and mean monthly river flow (see Figure 3c,f), and the corresponding histograms being right-skewed for the former hydroclimatic variable type and left-skewed or approximately non-skewed for the latter two hydroclimatic variable types. Furthermore, larger stdlst_der values are computed on average for total monthly precipitation than for mean monthly river flow, indicating somewhat stronger temporal variation in the former. Also notably, similar mean entropy values are computed for total monthly precipitation and for mean monthly river flow, indicating a similar degree of “forecastability” between them. Lastly, for all hydroclimatic variable types, the histograms of nonlinearity and trend are right-skewed (see Figure 3g–l), with the nonlinearity values on average smallest for mean monthly temperature and largest for mean monthly river flow (see Table 2), and the trend values on average smallest for total monthly precipitation and largest for mean monthly river flow (but in general indicating weak trend strength on average, although some large trend values are also computed, mostly for river flow).

3.1.2 Characterizations in terms of variance explanation

Here, we focus on the most representative characterizations in terms of variance explanation for the three feature datasets (to better understand these datasets, and the
similarities and differences across the three examined hydroclimatic variable types. These characterizations are summarized in Figure 4, while a more detailed presentation is given in the Supplement (see Figures S11–S17 therein). For the below provided and discussed information, it might be useful to recall that (1) each principal component is a linear combination of our features, and (2) the total variance is collectively explained by all principal components (with the contributions of these components in variance explanation being smaller as we move from the first one to the last one); see again Section 2.3.1 for a short summary of principal component analysis.

For our three feature datasets, the first three principal components explain ~50% of the total variance (see Figure S11). The 1st principal component explains 30.5% of the total variance of the mean monthly temperature feature dataset (see Figure S12), while the respective percentages for the total monthly precipitation and mean monthly river flow feature datasets are 34.1% (Figure S13) and 24.1% (Figure S14). For mean monthly temperature, 18 features contribute ~3–5% to the 1st principal component (maximum contribution computed for seas_acf1), with the remaining features contributing less to this component and more to the remaining ones (see Figure 4). The numbers of features contributing more than 3% to the 1st principal component are 15 and 17 for total monthly precipitation and mean monthly river flow, respectively. The maximum contributions are ~4.5% for total monthly precipitation and 6% for mean monthly river flow, and the features exhibiting these contributions are seasonal_strength and x_pacf5, respectively. Interestingly, several feature types are among the top contributors to the 1st principal component for all three (or at least for two) main hydroclimate variable types (e.g., x_acf1, x_acf10, diff1_acf1, seas_acf1, diff2x_pacf5, x_pacf5, std1st_der, entropy and seasonal_strength; see Figure 4a). To the contrary, the top contributing features to the 2nd principal component are distinct for each main type of hydroclimate variables (see Figure 4b). In the mean monthly temperature, total monthly precipitation and mean monthly river flow feature datasets, the 2nd principal component explains 10.9%, 9.4% and 14.4%, respectively, of the total variance.
Figure 4. Rankings of the features according to their contributions to the (a) first, (b) second, (c) third, and (d) fourth principal components. (Each principal component is a linear combination of the features). The features are defined in Table 1.
3.1.3 Feature relationship characterizations and analyses

To better understand the three feature datasets obtained through massive feature extraction, and to extract further empirical evidence on the statistical similarities (and differences) characterizing the three examined hydroclimatic variable types, we examine the relationships between the features. Hierarchically clustered correlograms, conducted for the entire mean monthly temperature, total monthly precipitation and mean monthly river flow feature datasets, are provided in the Supplement (Figures S18–S20). Here, we focus on the top-15 contributing features to the 1st and 2nd principal components for each hydroclimatic variable type (as identified in Figure 4) by presenting and discussing the hierarchically clustered correlograms of Figures 5–7. Half of these correlograms (see Figures 5a, 6a and 7a) depict medium to large (positive or negative) linear correlations, while the other half (see Figures 5b, 6b and 7b) depict linear correlations of various magnitudes (including statistically insignificant values).

As derived mainly from the former half, some features are highly correlated with each other (in terms of Pearson’s correlation) for all three hydroclimatic variable types, suggesting intense feature relationships and some sort of statistical similarity across the examined hydroclimatic variable types. Among the most characteristic examples of such features are the following autocorrelation and partial autocorrelation ones: $x_{acf1}$, $x_{acf10}$, $diff1_{acf1}$, $diff1_{acf10}$, $seas_{acf1}$, $x_{pacf5}$, $diff1x_{pacf5}$ and $seas_{pacf}$. These features are also found to be (mostly) highly correlated with $std1st_{der}$, $ARCH.LM$ and $seasonal_strength$, to name a few relevant examples. Other features whose relationships are found to be intense are entropy and $seasonal_strength$ with correlations $-0.91$ and $-0.87$ for total monthly precipitation and mean monthly river flow, respectively, and hurst and trend with correlations $0.88$ and $0.86$ for mean monthly temperature and mean monthly river flow, respectively. These two latter features are also found to be highly correlated with alpha. Statistical differences are also identified between the examined variable types. For instance, the relationships between entropy and several autocorrelation features are very intense for the total monthly precipitation dataset, and medium for the mean monthly temperature and mean monthly river flow datasets.
Figure 5. Linear correlations (a) between the fifteen mean monthly temperature features contributing the most to the first principal component, and (b) between the fifteen mean monthly temperature features contributing the most to the second principal component. The contributions of the mean monthly temperature features to the first and second principal components are presented in the Supplement (see Figure S15). The correlograms are hierarchically clustered. Statistically insignificant correlations are marked with crosses. The features are defined in Table 1.
Figure 6. Linear correlations (a) between the fifteen total monthly precipitation features contributing the most to the first principal component, and (b) between the fifteen total monthly precipitation features contributing the most to the second principal component. The contributions of the total monthly temperature features to the first and second principal components are presented in the Supplement (see Figure S16). The correlograms are hierarchically clustered. Statistically insignificant correlations are marked with crosses. The features are defined in Table 1.
Figure 7. Linear correlations (a) between the fifteen mean monthly river flow features contributing the most to the first principal component, and between (b) the fifteen mean monthly river flow features contributing the most to the second principal component. The contributions of the mean monthly temperature features to the first and second principal components are presented in the Supplement (see Figure S17). The correlograms are hierarchically clustered. Statistically insignificant correlations are marked with crosses. The features are defined in Table 1.
3.2 Spatial hydroclimatic patterns and hydroclimatic time series clustering

3.2.1 Spatial variability of hydroclimatic time series features

To facilitate the detection of spatial patterns, we produce continental-scale maps for several regions around the globe (see Figure S21 in the Supplement and Figures 8–12). These maps refer to selected mean monthly temperature, total monthly precipitation and mean monthly river flow features. We select only four features for reasons of brevity. Specifically, we select x_acf1, entropy, trend and seasonal_strength due to their high interpretability (see also Table 1 and Section 3.1.1) and relevance to the main themes identified in the hydroclimatic literature (see Sections 1.3 and 3.1.1). Notably, the selection of x_acf1, entropy and seasonal_strength is also supported by their importance in terms of variance explanation (see Section 3.1.2) and in hydroclimatic time series clustering (see Section 3.2.2). Their latter importance could be helpful in inspecting and interpreting the clustering outcomes presented in Section 3.2.2.

Interestingly, total monthly precipitation across the Indian subcontinent and Australia exhibits small trend (see Figures 8c and 9c), without any particular patterns being noticed, except for the fact that the trend values are slightly larger for Australia than for India. By recalling the definition of this dimensionless feature (see Table 1), we interpret this result as follows: The variance of the remainder component obtained by applying STL decomposition is comparably large to the variance of the deseasonalized total monthly precipitation time series (i.e., the total monthly precipitation time series with only its seasonal component removed). This suggests that the trend component is relatively weak (compared to the remainder component, which can be interpreted as the “random” component of the time series; see also Section 3.1.1).

Furthermore, the other three total monthly precipitation features under study (see Figures 8a,b,d and 9a,b,d) suggest some degree of spatial coherence in these two regions. Specifically, both x_acf1 and seasonal_strength are notably higher for the West Coast of India (region exhibiting tropical monsoon climate) than for the inner Indian subcontinent and the East Cost of India for the same latitudes (respectively suggesting stronger autocorrelation structure and stronger seasonality patterns for the West Coast compared to these latter regions). Moreover, entropy is remarkably lower for the same tropical monsoon region (suggesting larger degree of “forecastability” for total monthly precipitation variables across this region; Goerg 2013). Analogous spatial patterns can
also be extracted for other regions in the Indian subcontinent and Australia; nonetheless, perhaps the most notable findings are those related with the large differences (in terms of features’ magnitude) between the Indian subcontinent and Australia. For instance, it is found that _entropy_ (mostly) takes much larger values across Australia than it takes across India and its neighbouring regions (suggesting that the former continental-scale region is characterized by smaller “forecastability” than the latter). Total monthly precipitation in Australia is also characterized by a less pronounced autocorrelation structure and by less intense seasonal patterns than total monthly temperature in the Indian subcontinent (as suggested by the smaller \(x_{acf1}\) and \(seasonal\_strength\) values computed for Australia). Also notably, Figures 8 and 9 show high (positive or negative) correlation between \(x_{acf1}\), _entropy_ and _seasonal_strength_, thereby suggesting intense relationships between them (and serving as graphical illustrations of the findings already presented and discussed in Section 3.1.3).

Distinct spatial patterns are also observed for mean monthly river flow. Since most river flow stations are from North America and Europe, Figures 10–12 are devoted to these two continental-scale regions. The (medium or) high (positive or negative) correlation between \(x_{acf1}\), _entropy_ and _seasonal_strength_ is also evident for the mean monthly river flow processes of North America (see Figures 10 and 11). For the same continental-scale region, distinct sub-regions can be identified with similar feature values. For instance, central North America is characterized by smaller values of \(x_{acf1}\) and _seasonal_strength_ with respect to its neighbouring sub-regions and notably larger _entropy_ values. For Europe, patterns are less evident, but not ignorable. For instance, mean monthly river flow in Alps exhibit stronger seasonality and autocorrelation patterns compared to their adjacent regions (as indicated by larger _seasonal_strength_ and \(x_{acf1}\) values, respectively), and larger “forecastability” (as indicated by smaller _entropy_ values). Lastly, we observe several large values for _trend_, rather scattered across North America and Europe.

Since we do not identify any patterns for mean monthly temperature, its corresponding results are only presented in the Supplement (see Figure S21 therein). As shown, \(x_{acf1}\) and _seasonal_strength_ are high for all stations in and around Europe, while _entropy_ and _trend_ are quite low. The same applies for other regions; for a justification, see the ranges of the computed features in Figures 2 and 3.
Figure 8. Maps of selected total monthly precipitation features across the Indian subcontinent. The presented features are: (a) $x_{acf1}$, (b) entropy, (c) trend and (d) seasonal_strength. For their definitions, see Table 1.
Figure 9. Maps of selected total monthly precipitation features across Australia. The presented features are: (a) $x_{acf1}$, (b) entropy, (c) trend and (d) seasonal_strength. For their definitions, see Table 1.
Figure 10. Maps of selected mean monthly river flow features across North America (part 1). The presented features are: (a) $x_{acf1}$ and (b) entropy. For their definitions, see Table 1.
Figure 11. Maps of selected mean monthly river flow features across North America (part 2). The presented features are: (a) trend and (b) seasonal_strength. For their definitions, see Table 1.
Figure 12. Maps of selected mean monthly river flow features across Europe. The presented features are: (a) $x_{acf1}$, (b) entropy, (c) trend and (d) seasonal_strength. For their definitions, see Table 1.

3.2.2 Feature-based hydroclimatic time series clustering

Here, we present the clustering outcomes for the hydroclimatic time series examined in this work and, by extension, for the geographical locations in which these hydroclimatic time series have been observed. The presentation is made across the globe (Figure 13; see also Figure S22 in the Supplement for the percentages of the time series attributed to each cluster for each hydroclimatic variable type) and across selected continental-scale
regions (Figures 14–16), with T1, T2, T3, T4 and T5 simply signifying the five clusters obtained for mean monthly temperature and similar notations being used for the five clusters obtained for total monthly precipitation (i.e., P1, P2, P3, P4 and P5), as well as for the five clusters obtained for mean monthly river flow (i.e., R1, R2, R3, R4 and R5). For the selected continental-scale regions, we also present the categorical spatial interpolation outcomes to ease the identification of spatial patterns. Regarding these spatial interpolations, it might be relevant to note that the emerging shapes are somewhat different from the shapes that we would have obtained with linear spatial interpolation, as already expected (due to the internal of the random forest algorithm). Spatial interpolation outcomes are especially meaningful for regions with high density of stations, with North America being one of the most characteristic examples of such regions for its river flow stations (see Figure 16).

The spatial coherence of the clusters is evident in Figures 13–16. For instance, the largest part of the mean monthly temperature time series observed in Europe (mostly those observed in northern regions) is attributed to the same cluster, specifically to cluster T1 (see Figure 14a), while East Asian temperature is mostly attributed to clusters T4 and T5. Distinct spatial patterns are also identified for mean monthly precipitation. The Indian subcontinent is an interesting example on this hydroclimatic variable type, already examined in terms of x_acf1, entropy, trend and seasonal_strength (see Section 3.2.1, specifically Figure 8 therein). The spatially coherent patterns observed for this continental-scale region under our hydroclimatic time series clustering approach (see Figure 15b) are consistent with those previously identified (based on Figure 8), with the mean monthly precipitation time series observed in the West Coast of India being attributed to a different cluster (specifically, to cluster P5) from those observed in the inner and eastern Indian subcontinent for the same latitudes (i.e., clusters P3 and P4). Lastly, distinct spatial patterns are also found for mean monthly streamflow in North America with latitudes up to approximately 50° (see Figure 16), with those time series originating from its western and northern parts belonging to cluster R1 (except for some originating from adjutant stations that belong to cluster R2), while the time series originating from its middle and eastern parts (mostly) belong to clusters R3 and R5, respectively.
Figure 13. Clusters of the (a) mean monthly temperature, (b) total monthly precipitation and (c) mean monthly river flow time series.
Figure 14. Clusters of the mean monthly temperature and categorical spatial interpolations for (a) Europe and its neighbouring regions, (b) North America, and (c) East Asia.
Figure 15. Clustering outcome for the total monthly precipitation time series and outcome of the categorical spatial interpolation for (a) North America and (b) the Indian subcontinent.
Figure 16. Clustering outcome for the mean monthly river flow time series and outcome of the categorical spatial interpolation for North America.

It is also relevant to explore which are the most important hydroclimatic time series features in solving the three clustering problems, as well as to compare these features with the ones contributing the most to the first principal components obtained for the same datasets (see Figure 9). For these explorations and comparisons, we present Figure 17. Among the most important features for all three (or at least for two of) the examined main hydroclimatic variable types, as identified by random forests, are the following ones: $x_{acf1}$, $x_{acf10}$, $diff1_{acf1}$, $seas_{acf1}$, $x_{pacf5}$, $diff1x_{pacf5}$, $diff2x_{pacf5}$, $std1st_{der}$, $entropy$, $spike$ and $seasonal_strength$. Indeed, most of these features are also important from a variance explanation perspective. In general, it seems that the rankings presented in Figure 17 are mostly comparable (though not identical) with those corresponding to the contributions to the 1st principal components.
**Figure 17.** Rankings of the features according to their importance for time series clustering using random forests. The features are defined in Table 1.
3.2.3 Monthly hydroclimatic time series cluster characterizations and analyses

To characterize the hydroclimatic time series clusters obtained by applying the new feature-based methodology, in Figure 18 we present −conditional on the cluster− the violin plots of the top-12 important mean monthly river flow features in time series clustering, as identified by random forests (see Figure 17). Analogous visualizations are also provided for the top-12 important mean monthly temperature features (see Figure S23) and the top-12 important mean monthly precipitation features (see Figure S24). In general, we observe that there are overlaps in the ranges of the computed features across the different clusters, with these overlaps being larger or smaller depending on the feature.

An interesting feature for someone to examine in detail is seasonal_strength. This feature is, in fact, one of the most interpretable ones (see also the discussions in Section 3.1.1) and its magnitude can be (largely) evident through an optical inspection of the time series. For this inspection, we also present the side-by-side boxplots of the mean monthly river flow values for the twelve months of the year (see Figure 19), while in the Supplement we enclose similar visualizations for mean monthly temperature and precipitations (see Figures S25 and S26 therein). We first observe in Figure 18f that seasonal_strength is mostly larger for cluster R2 and smaller for R3 than for the remaining clusters. We also observe that clusters R4 and R5 are characterized by seasonal_strength values with very similar (almost identical) ranges (although they are quite different with respect to other features; see e.g., Figure 18a–e), and that cluster R1 is characterized by seasonal_strength values that cover the entire range of possible values. This information is easily cross-checked by using Figure 19. Specifically, in this latter Figure we observe that clusters R4 and R5 are characterized by very similar seasonality patterns, which are also quite intense (see Figure 19d,e), but less intense than seasonality in cluster R2 (see Figure 19b).
Figure 18. Violin plots of the top-12 important monthly river flow features in time series clustering using random forests conditional on the cluster. The features are presented from (a) the most important to (l) the least important. The corresponding rankings of the features are presented in Figure 17. Outliers have been removed for spike and x_acf10. The features are defined in Table 1.
Figure 19. Side-by-side boxplots of the mean monthly river flow values conditional on the cluster and the month. The vertical axes have been truncated at 75 m$^3$/s.

As the data availability time periods are not the same for all stations (since we needed the largest number of 40-year-long time series possible for our experiments), we should lastly check whether the formation of clusters depends on the time period of our time series. For this test, in Figure 20 we present the densities of the last year of the mean monthly river flow time series characterizing the five clusters obtained for mean monthly river flow. These densities show that the formation of clusters is independent of the time period of the time series. Mean monthly temperature and total monthly precipitation clustering exhibit a similar independence (see Figures S27 and S28).
4. **Further discussion, selected findings and key recommendations**

In this Section, we further discuss selected findings of the study by emphasizing the implications of the proposed methodological framework (including the new hydroclimatic time series clustering methodology), and by providing additional interpretations and recommendations in line with our research objectives.

4.1 **On seasonality, trends, temporal dependence, entropy and more**

Our premise that a multi-faced and massive approach to time series representation via feature extraction would be meaningful in hydroclimatic contexts has been empirically confirmed by the three global-scale applications of the introduced framework, specifically by the competitive contributions of (most of) the computed features in explaining the total variance of our three big data feature datasets (see Section 3.1.2). Moreover, it has led to the delivery of new descriptive insights into the nature of the examined hydroclimatic variables. These insights are particularly important under the concepts of hydrological variability, hydrological change and hydrological similarity, and include those related to the quantification of the similarities and differences observed between the three examined hydroclimatic variable types (see Section 3.1), as well as those related
to the identification of homogenous spatial patterns characterizing feature variability in space (see Section 3.2). For facilitating these specific quantifications and spatial investigations, we have exploited the entire amount of information resulted from massive feature extraction. This information is summarized in Section 3.1.1 and in the Supplement, and can be used by the interested reader to better understand the computed features and the nature of the three examined hydroclimatic variable types (also by comparing them).

We have also ranked the features according to their contributions in the various principal components (obtained through principal component analyses) and provided ex post knowledge on which of them have been the most informative in solving our three time series clustering problems. Features that have been both (a) identified among the top-10 contributing ones to the 1st principal components formed for (at least two of) the three feature datasets (see the results presented in Section 3.1.2), and (b) ranked in the first 10 places by the clustering algorithm for (at least two of) the three examined clustering problems (see the results presented in Section 3.2) are the following: \texttt{x_acf1}, \texttt{x_acf10}, \texttt{diff1_acf1}, \texttt{seas_acf1}, \texttt{x_pacf5}, \texttt{std1st_der}, \texttt{entropy} and \texttt{seasonal_strength}. Most of these features are also quite interpretable. Although the adoption of the entire feature compilation is highly recommended by this study (for its multi-faced and massive character, which resulted in complete hydroclimatic time series characterizations herein), the above-provided ex post knowledge-information may have some practical value for future investigations focusing on monthly temperature, monthly precipitation and monthly river flow. This practical value holds especially for cases in which we cannot afford massive feature extraction solutions, but we are still interested in capturing as much information as possible (given this scale limitation).

By considering this same above-provided information along with the main interests spotted in the hydroclimatic literature (see Section 1.3), in our discussions we have also emphasized (to some extent) on selected interpretable characterizations on seasonality, trends, temporal dependence, entropy, etc. (for reasons of brevity). A feature extensively discussed in this respect is spectral entropy (\texttt{entropy}). This feature has been found to vary significantly from region to region for both total monthly precipitation and mean monthly river flow, suggesting regions characterized by lower “forecastability” than others (according to Goerg 2013). Such regions are the greatest part of the examined Australia (identified as the one with the less “forecastable” total monthly precipitation in
our conducted maps), a region in the Indian subcontinent (again for total monthly precipitation), approximately half of North America (for its mean monthly river flow) and the largest part of Europe (again for its mean monthly river flow). As it is shown in Papacharalampous and Tyralis (2020) by using approximately 600 mean annual river flow time series and by computing Goerg’s (2003) spectral entropy, in situations characterized by larger “forecastability”, persistent schemes (e.g., the naïve forecasting scheme simply setting the forecasts equal to the last available observation for the case of non-seasonal processes) are more likely to perform better (compared to sophisticated methodologies) than they are in situations characterized by smaller “forecastability”.

Another feature found to be particularly relevant to characterizing hydroclimatic variables in interpretable terms (and in line with the main interests identified in the hydroclimatic literature) is trend strength (\textit{trend}), a practical appealing dimensionless feature that (to our knowledge) has not been exploited before for the investigation of monthly hydroclimatic variables. Although the investigation of trends is quite common in the hydrological and geoscientific literature (Serinaldi et al. 2020a), with many useful descriptive features being exploited in this respect, we believe that this new feature could offer additional descriptive insights and could, therefore, be computed in future works (alongside with other features facilitating the study of trends; see e.g., Papalexiou and Montanari 2019; Bertola et al. 2020).

Herein, we have found trend strength to be more intense for mean monthly river flow, while trends have been found to be rather weak (but not negligible) for mean monthly temperature and total monthly precipitation (when contrasted to the magnitude of the “random” variations in the time series). Perhaps, this latter finding is also related to the fact that BATS and Prophet (forecasting methods with trend components) have been found to perform equally well with other sophisticated methods (with no trend components) in the global-scale forecasting investigations on mean monthly temperature and total monthly precipitation by Papacharalampous et al. (2018). Moreover, we have found that the trend values of mean monthly river flow that are (roughly) larger than 0.5 are rather scattered across the world (mostly across North America and Europe, since river flow station concentration is larger for these two continental-scale regions). Such spatial patterns are not observed for the remaining features on which we have focused in Section 3.2.1. For instance, quite homogenous spatial patterns characterize the very characteristic feature of sample autocorrelation at lag 1 (\textit{x_acf1}), as well as the spectral
entropy and the seasonality strength \( \text{(seasonal\_strength)} \) features.

To our knowledge, investigations on seasonality strength are also new in hydrology and geoscience. We believe that such investigations could offer some additional interpretable insights into the nature of seasonal hydroclimatic variables, along with previously proposed approaches to analysing seasonality (see e.g., Villarini 2016; Hall and Blöschl 2018). Such approaches extensively analyse both the timing and magnitude of seasonal patterns within the year (herein assessed with the side-by-side boxplots of Figure 19), while \text{seasonal\_strength} summarizes in a compact way (i.e., into a single value) and in relative terms information about the magnitude of seasonal fluctuations compared to the magnitude of the “random” fluctuations in the time series (i.e., the component remaining after the removal of the trend and seasonal components).

### 4.2 On the spatial patterns revealed through hydroclimatic time series clustering

Distinct spatially coherent patterns have been identified based on our cluster characterizations (see Section 3.2.2). For instance, most of the mean monthly temperature time series observed in European regions with latitude larger than 45° (or 50°) are attributed to the same cluster. Interestingly, this specific cluster has been shown to mostly characterize these European regions at the global scale. Another continental-scale region identified as worth-discussed is East Asia, with the mean monthly temperature time series observed there being mostly attributed to two clusters with spatial homogeneity. Especially, the cluster characterization holding for the largest part of East Asia seems to be extremely rare in other regions across the globe.

Spatial coherence also applies to the cluster characterizations delivered for total monthly precipitation and river flow, with the latter hydroclimatic variable type being perhaps the most interesting to examine (because of the large concentration of river flow stations with long observation periods in North America). Notably, total monthly precipitation time series observed in the West Coast of India, a region with tropical monsoon climate, are attributed to a different cluster from those observed in the inner and eastern Indian subcontinent for the same latitudes, while mean monthly river flow time series originating from the western parts of North America and its parts with latitudes from approximately 45° to approximately 50° mostly belong to the same cluster. This cluster is different from the clusters characterizing the mean monthly river flow time series originating from the middle and eastern parts of North America.
The above-outlined information highlights the efficiency of our methods in delivering descriptive and exploratory insights in a completely automatic way (in the sense that the procedures do not depend on the hydroclimatic process at hand). Such insights are important in terms of progressing our understanding of hydroclimatic variable behaviours (primary consideration within our global-scale analyses). Moreover, they build some confidence in using the new time series clustering methodology (and its possible extensions) in the future. Given the spatial coherence characterizing the delivered clusters and the scale-independent nature of the computed features (exploited as inputs to the random forests algorithm), we believe that this methodology could be particularly relevant within regionalization frameworks, in which methodological advances and knowledge on hydrological similarity are exploited in technical and operative terms.

5. **Summary and conclusions**

We have developed a detailed framework to facilitate complete hydroclimatic variable characterizations. This new framework relies on massive feature extraction and four statistical learning (else referred to as “machine learning”) algorithms. The adopted feature compilation (composed by 59 diverse features) is supported by past experience and experts’ knowledge, which is mostly sourced from scientific fields beyond geoscience and environmental science (e.g., the fields of neuroscience, biology, biomedicine and forecasting), thereby constituting a new concept for our fields. We have empirically proven the high relevance of this new concept in hydrological and hydroclimatic contexts by applying our framework to three global hydroclimatic datasets. These datasets contain 40-year-long information on mean monthly temperature, total monthly precipitation and mean monthly river flow, which originates from over 13 000 stations in total.

Our big data analyses have provided a useful basis for extracting interpretable knowledge (e.g., on seasonality, trends, autocorrelation, long-range dependence, entropy and more, as well as on the relationships between all the computed features) at the global scale, for comparing the examined hydroclimatic variable types in terms of this knowledge, and for identifying distinct patterns related to the features’ spatial variability. For this latter purpose, we have also proposed a fully automatic feature-based methodology for hydroclimatic time series clustering, with which we have aspired to exploit a larger part of the information encompassed in the hydroclimatic observations.
than we could achieve with existing hydroclimatic time series clustering methodologies. Automation is needed in modelling (Chatfield 1988; Hyndman and Khandakar 2008; Taylor and Letham 2018), especially when we are interested in studying problems “at scale” and at a common base. The term “at scale” is used in the literature to imply a large number and variety of problems (see Taylor and Letham 2018), and is therefore relevant to the study of hydroclimatic variables (since these variables may differ with each other in many ways; see Papalexiou 2018). In addition to the benefits of our new time series clustering methodology stemming from its automatic nature, the spatially coherent patterns delivered with its use can build some further confidence in its future exploitation for the delivery of descriptive and exploratory insights into the nature of other geophysical variables. Although only such insights have been delivered in the present work, we deem that the technical exploitation of the new methodology within regionalization frameworks could also be beneficial (given the scale-independent nature of the computed features).

We conclude by emphasizing, once again, the massive and automatic character of our methodological framework. With this framework, we believe to have moved a step further from the traditional approach to feature extraction in hydroclimatic research, aiming both to (a) facilitate a better understanding of hydroclimatic variable behaviours, and to (b) deliver more reliable results in hydroclimatic time series clustering contexts.

Appendix A    Statistical software information

The analyses and visualizations have been performed in R Programming Language (R Core Team 2020). The following contributed R packages have been used: cluster (Maechler et al. 2019), devtools (Wickham et al. 2020c), dplyr (Wickham et al. 2020b), factoextra (Kassambara and Mundt 2020), forecast (Hyndman and Khandakar 2008; Hyndman et al. 2020a), fracdiff (Maechler 2020), gdata (Warnes et al. 2017), geoR (Ribeiro et al. 2020), ggbio (Vu 2011), ggcroplot (Kassambara 2019), ggnewscale (Campitelli 2020), ggplot2 (Wickham 2016a; Wickham et al. 2020a), gstat (Gräler et al. 2016; Pebesma and Gräler 2020), knitr (Xie 2014, 2015, 2020), lubridate (Grolemund and Wickham 2011; Spinu et al. 2020), maptools (Bivand and Lewin-Koh 2020), maps (Brownrigg et al. 2018), randomForest (Liaw and Wiener 2002; Liaw 2018), readr (Wickham et al. 2018),
Appendix B  Original data sources

Basic information on real-world data retrieval is provided in Table B.1.

| Data type      | Original data source link                                      | Retrieved     |
|----------------|----------------------------------------------------------------|--------------|
| Temperature    | https://www.ncdc.noaa.gov/ghcnm/v4.php                         | 2019-12-29   |
| Precipitation  | https://www.ncdc.noaa.gov/ghcnm/v2.php                         | 2019-12-28   |
| River flow     | https://doi.org/10.1594/PANGAEA.887477                         | 2019-05-20   |

Supplement: Table S1 and Figures S1–S28 are provided in the online version of the paper.

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