Highlights

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- We present a Matlab toolbox to calculate hydrologic signatures, which are metrics that quantify streamflow dynamics.
- The toolbox provides accessible, standardised signature calculations, with clear information on methodological decisions and recommended parameter values.
- We demonstrate the accuracy and robustness of the signature calculations by applying reproducible workflows to large streamflow datasets from the U.S. and Great Britain.

TOSSH: A Toolbox for Streamflow Signatures in Hydrology

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ARTICLE INFO

Keywords:
hydrology
hydrologic signatures
streamflow
reproducibility
Matlab

ABSTRACT

We present a Matlab toolbox to calculate hydrologic signatures, which are metrics that quantify streamflow dynamics. Signatures are widely used for catchment characterisation, hydrologic model evaluation, and assessment of instream habitat, but standardisation across applications and advice on signature selection is lacking. The toolbox provides accessible, standardised signature calculations, with clear information on methodological decisions and recommended parameter values. The toolbox implements three categories of signatures: basic signatures that describe the five components of a natural streamflow regime, signatures from benchmark papers, and an extended set of process-based signatures. The toolbox is designed for ease of use, including documentation, workflow scripts and example data to demonstrate implementation procedures, and visualisation options. We demonstrate the accuracy and robustness of the signature calculations by applying reproducible workflows to large streamflow datasets. The modular design of the toolbox allows for flexibility and easy future expansion. The toolbox is available from https://github.com/TOSSHtoolbox/TOSSH (https://doi.org/10.5281/zenodo.4451846).

1. Introduction

Information about streamflow dynamics is important for water resources management, hydrologic model building and evaluation, and assessment of instream habitat. Metrics that quantify streamflow dynamics are known as hydrologic signatures, and are widely used in hydrology and ecohydrology (Olden and Poff, 2003; Hrachowitz et al., 2014; McMillan, 2020b). Hydrologic signatures typically target one component of the catchment response, such as flashiness or recession shape. Signatures can be used to identify runoff generation processes (McMillan, 2020a), for catchment classification (Boscarello et al., 2016), and to detect hydrologic alteration such as urbanisation (McDaniel and O'Donnell, 2019). Signatures can quantify the dynamics of hydrologic variables including snow (Schaefli, 2016; Horner et al., 2020), soil moisture (Branger and McMillan, 2020) and groundwater (Heudorfer et al., 2019), but are most commonly used with rainfall and streamflow data.

Hydrologists must choose suitable sets of signatures to use. For example, Coxon et al. (2014) propose a collection of signatures for model evaluation, and Pfannerstill et al. (2014) describe a multi-signature evaluation framework for low flow modelling. These selections may rely on signatures used in previous studies (Coxon et al., 2014; Kuentz et al., 2017), or may be designed to encompass hydrologic behaviour across flow magnitudes and timescales (Sawicz et al., 2014; Westerberg et al., 2016). Clear selection criteria enable hydrologists to choose between competing signatures, enable more straightforward comparisons between studies, and promote robust, predictable signatures (McMillan et al., 2016; Addor et al., 2018). Methodological clarity in how signatures are defined and calculated is also essential as this has significant impact on signature values and spatial patterns (Westerberg and McMillan, 2015; Santos et al., 2019).

This paper addresses the need for accessible, standardised signature calculations, by presenting TOSSH: A Toolbox for Streamflow Signatures in Hydrology. The toolbox provides Matlab functions to calculate hydrologic signatures. There is a drive towards hydrological science that is reusable and reproducible through the use of common code (Hutton et al., 2016). Increasing availability of open source code has made hydrology-relevant toolboxes more common, e.g. for modelling (Coron et al., 2017; Knoben et al., 2019; Sadegh et al.,

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2019) and sensitivity analysis (Sarrazin et al., 2017). Previous toolboxes that analyse streamflow series include statistical metrics of forecast quality (Dawson et al., 2007), and specific aspects of runoff analysis, e.g. HydroRecession for recession analysis (Arciniega-Esparza et al., 2017), FDCfit for Flow Duration Curve analysis (Vrugt and Sadegh, 2015), HydRun for baseflow separation and event-based analysis (Tang and Carey, 2017) and lfstat for low flow analysis (Koffler and Laaha, 2012). Olden and Poff (2003) describe 171 streamflow statistics in the categories of magnitude, frequency, duration, timing and rate of change, and these can be calculated using a USGS GUI-based tool (Henriksen et al., 2006), via the EflowStats R package, and via the MATLAB Hydrological Index Tool (Abouali et al., 2016). The functional flow metrics proposed by Yarnell et al. (2020) quantify ecohydrology-relevant features of a Mediterranean flow regime, and are available via a website with data preloaded for California.

The aim of the TOSSH toolbox is to build on these previous works, and create a centralised Github repository of Matlab code to calculate hydrological signatures. TOSSH provides a wider range of signatures than previous toolboxes, with a stronger emphasis on signatures related to hydrological processes over statistical description of the time series. These signatures are particularly useful for model evaluation where the model should faithfully reproduce runoff generation processes. We provide standardised, default options and clear information on decisions in signature application, while also allowing the user to specify alternative methodological choices. TOSSH provides easy implementation of signatures from benchmark papers, as well as basic signatures that describe the streamflow regime.

2. Toolbox Design

2.1. Selection of signatures

The toolbox implements three categories of signatures: basic signatures, signatures from benchmark papers, and an extended set of process-based signatures. Motivation for the signature choice is described here.

The **basic set of signatures** covers the five components of a natural streamflow regime (Richter et al., 1996; Poff et al., 1997): magnitude, frequency, duration, timing and rate of change. As Poff et al. (1997) state, these components "can be used to characterise the entire range of flows and specific hydrologic phenomena, such as floods or low flows, that are critical to the integrity of river ecosystems". Many papers organise signatures around these components (Olden and Poff, 2003; Yarnell et al., 2020), or focus on one of these components, such as magnitude (Clausen and Biggs, 2000) or rate of change (Shamir et al., 2005).

We therefore include signatures in these five categories to provide an overview of the streamflow regime (Table 1). The signatures are drawn from papers that provide lists of signatures broadly structured around the five categories (Westerberg and McMillan, 2015; Yadav et al., 2007). Note that our implementation might have methodological differences to the original: we might use a signature called recession coefficient based on a signature in Yadav et al. (2007), but this will be our version based on the most up-to-date and robust algorithm (i.e. applicable to streamflow with a wide range of dynamics) that we found in the literature.

The second category enables users to reproduce **sets of signatures from three benchmark papers**. These papers are highly cited by later authors describing sets of signatures, and are therefore included to provide easy access, standardised forms of these signatures. Note that there is overlap in signatures between the benchmark papers and the basic set. The three sets are as follows, with all signatures listed in Table 1:

1. Addor et al. (2018): 15 commonly-used signatures that "characterize different parts of the hydrograph, and [...] are sensitive to processes occurring over different time scales". The paper explores the strength of relationships between signatures and catchment attributes.

Table 1
Signatures included in the toolbox from the basic set and three benchmark papers. BFI denotes the baseflow index, FDC denotes the flow duration curve. [a]These signatures are applied to different parts of the time series, e.g. the low flow period (May to September) or the high flow period (November to April).

	Magnitude	Frequency	Duration	Timing	Rate of Change
Basic Set	Mean flow, 5th and 95th flow percentiles, mean monthly flow, 7-day minimum flow, BFI, coefficient of variation at flow timestep	High, low, and zero flow frequency	High, low, and zero flow duration	Mean half flow date, mean half flow interval	Lag-1 autocorrelation, slope of FDC, exponential recession constant
Addor	Mean flow, 5th and 95th flow percentiles, runoff ratio, streamflow-precipitation elasticity, BFI	High, low, and zero flow frequency	High and low flow duration	Mean half flow date	Slope of FDC
Sawicz	Runoff ratio, BFI, streamflow-precipitation elasticity	Snow day ratio			Slope of FDC, rising limb density
Euser	Slope of distribution of peaks, low-flow[a] slope of distribution of peaks				FDC, low-flow[a] FDC, high-flow[a] FDC, lag-1 autocorrelation, low-flow[a] lag-1 autocorrelation, rising limb density

2. Sawicz et al. (2011): 6 signatures drawn largely from Yadav et al. (2007), that are uncorrelated and linked to catchment function. The paper analyses signature similarity between catchments, linking the resulting clusters to climate and landscape attributes.
3. Euser et al. (2013): 8 signatures that represent different aspects of hydrologic behaviour. The paper uses signatures to test the consistency of model performance.

The third category is a **larger set of process-based signatures**. We envisage that the toolbox provides a hub for signature calculations for different applications, requiring a variety of different signatures. We included signatures from the catalogue described by McMillan (2020a) that identify processes related to baseflow (including groundwater and catchment storage signatures) and processes related to overland flow (saturation and infiltration excess). We added seasonal signatures from Gnann et al. (2020), a catchment response time signature from Giani et al. (2020), and signatures from Horner (2020). Some of the signatures in the McMillan (2020a) catalogue are described only in visual or qualitative terms in their original papers. Where possible, we translated those signatures into a quantitative value, and we provide plotting functionality to enable the user to visualise the data. We note differences or interpretations from the original paper in the code for each signature.

The scope of the toolbox that guided our decisions on which signatures to include was that signatures should quantify an aspect of flow dynamics of interest to hydrologists, and have been described in a published paper. We did not add standalone signatures that were minor variations on existing signatures, as our aim is to provide a standardisation of signature methods. Instead, where signatures could be calculated in different ways, we added these as alternative options that the user could specify if desired. A list of all the signatures is available in our online documentation (`https://TOSSHtoolbox.github.io/TOSSH/`).

2.2. Toolbox structure and interface

2.2.1. User interaction with the toolbox

The user can interact with the toolbox in several ways (Figure 1). Signature code can be called directly (functions in the folder *TOSSH/TOSSH_code/signature_functions* with names beginning with *sig_*) or by requesting one of the signature sets of signatures (functions in the folder *TOSSH/TOSSH_code/calculation_functions* with names beginning with *calc_*). Example workflows that guide the user through these options are provided in the folder *TOSSH/example*; see Section 3 for a demonstration on their use.

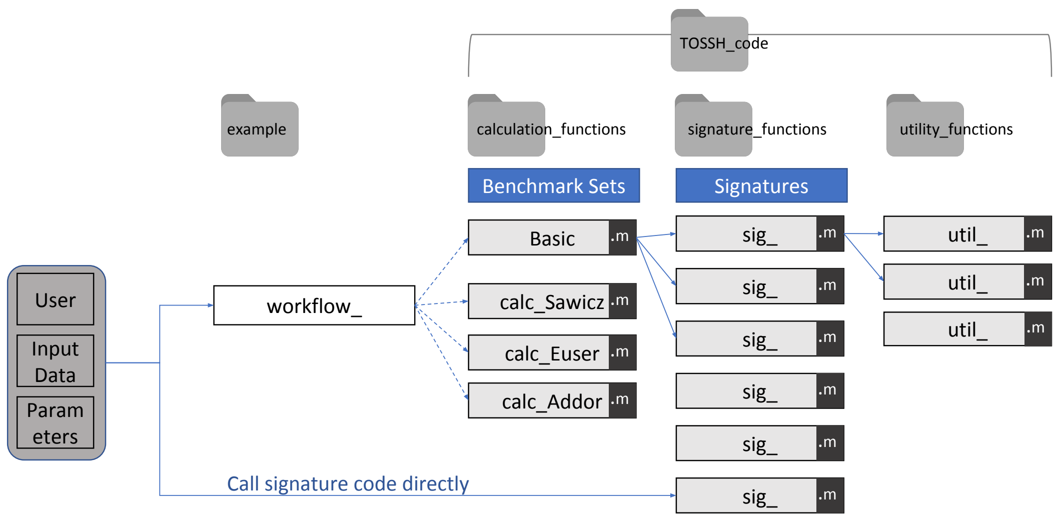

Figure 1: Overview of TOSSH toolbox structure.

When calling a signature or signature set, the user must provide input data. TOSSH includes signatures that require streamflow series with timestamps, and (for some signatures) concurrent precipitation, potential evapotranspiration or temperature series. Streamflow series must be given in units of mm/timestep. Some signatures are sensitive to the timestep of the data, and where possible we allowed for data of daily, hourly or 15 minute resolution. Example input data at these three timesteps are provided in the folder *TOSSH/TOSSH/example/example_data*.

Many signatures have parameters that control signature behaviour, e.g. degree of smoothing. Most parameters are optional as we have specified a default based on common usage in the literature. Other parameters have no default, (e.g. the flow percentile for which to calculate event frequency) and therefore the parameter is required. All optional inputs are parsed using a name-value convention so that parameters can be specified in any order.

Documentation is provided via Github at `https://TOSSHtoolbox.github.io/TOSSH/`. An overview of the toolbox aims and structure is provided, with examples of deployment and troubleshooting information. Lists of signatures in each signature set (e.g. basic set) are provided, with a brief description and link to the Matlab code.

2.2.2. Visualisation

Many signatures have a plotting parameter – when set, the function produces a visualisation of the signature value (see Figure 3). Visualisations are useful in several cases: to determine the suitability of input parameters (such as criteria for recession event selection), to determine the suitability of signature assumptions (e.g. near-exponential recessions), and to allow for judgement of visual evidence for a particular flow pattern (e.g. little flow after intense summer storms).

2.2.3. Software details

Signature code was written in Matlab R2020a, using Github for version control and distribution. We assume access to two Matlab toolboxes – Statistics and Machine Learning and Optimization – and a few signatures will fail if these are not installed. All signatures use a common template for consistency of layout, and provide information on function inputs, outputs, and options on typing *help <function_name>*.

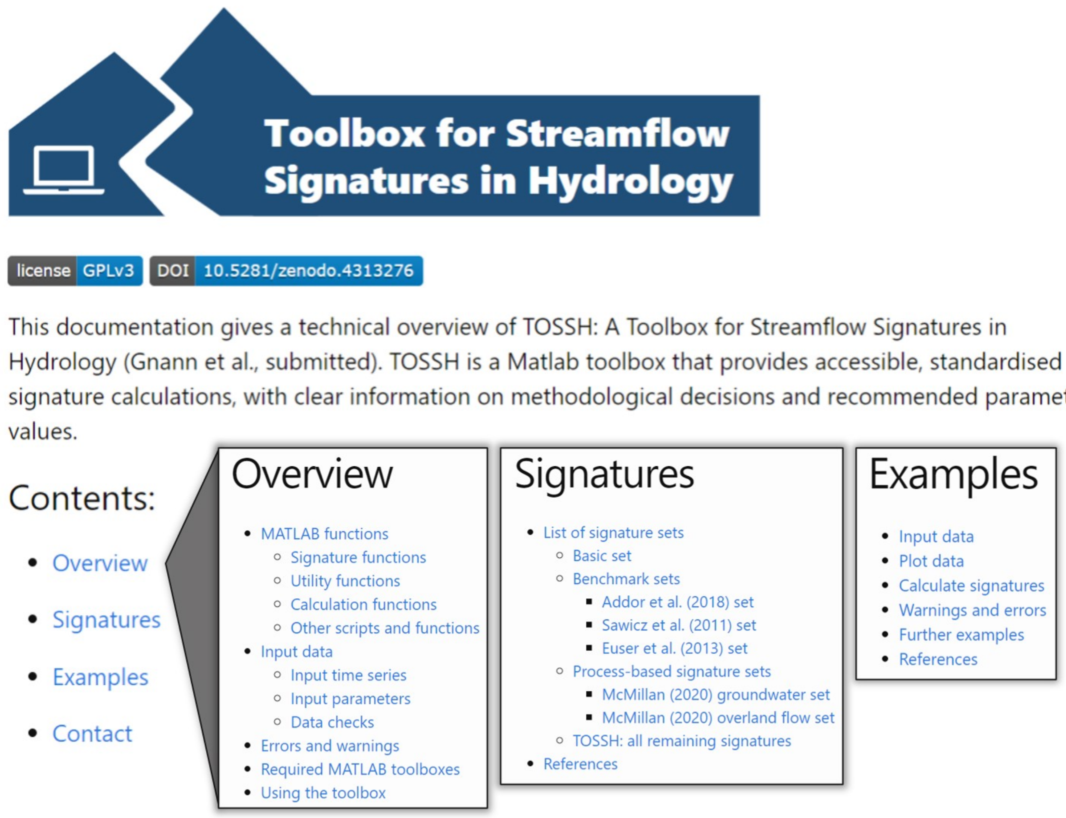

Figure 2: Front page and contents of the documentation available at `https://TOSSHtoolbox.github.io/TOSSH/`.

Input time series are automatically tested for common issues. Where data contains missing values or NaN values, a warning is returned, but the signature is calculated if possible. Signature values will become less reliable as the proportion of missing values increases, but we leave it up to the user to specify how to treat missing values. More serious errors such as negative flow values and mismatched time series lengths prevent calculation of the signature. Less clear cases occur because the interpretation of some signatures is not suitable for some types of flow patterns (see Section 4 for a short discussion of this), a warning is returned when these cases are identified.

2.2.4. Errors and warnings

Every signature function optionally returns an error flag (a number describing the error type) and an error string (e.g. *Error: Negative values in flow series.*). These contain warnings and errors that might occur during the data check or during signature calculation. If such an error occurs, NaN is returned as signature value without stopping code execution. This enables signature calculations for large samples of catchments without breaking. The error strings indicate why a certain signature could not be calculated for a certain catchment. There are still normal Matlab warnings and errors, for example if input parameters are specified incorrectly. Such errors stop code execution but can be avoided if the functions are called with input data that are in the correct format.

3. Testing and Evaluation

3.1. Workflows

The toolbox includes workflow scripts that facilitate easy user uptake by guiding the user through common usages of the toolbox. The scripts include setting Matlab directories, loading data, creating data structures to hold the output, calculating signatures, and plotting the results. To test the toolbox, we use 5 workflows that test different aspects of the functionality of the toolbox. This method allows full reproducibility of our evaluation results by re-running the workflows. Workflows 1 and 2 are basic workflows intended to guide the users and not used in the evaluation section; workflows 3, 4 and 5 are described further in the next section.

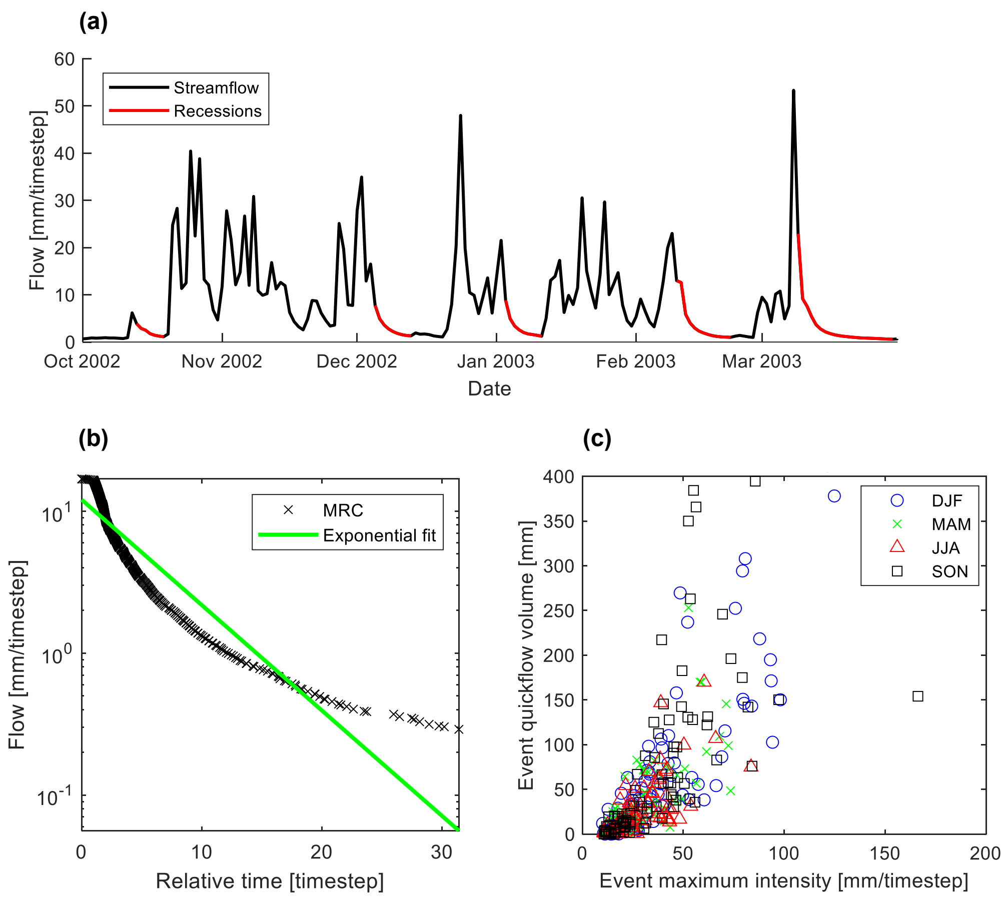

Figure 3: Examples of the plotting functionality. (a) Recession segments chosen using *util_RecessionSegments.m*. (b) Fitted exponential master recession curve (MRC) using *sig_BaseflowRecessionK.m*. (c) Event quickflow volume vs. maximum storm event intensity coloured according to season using *sig_EventGraphThresholds.m*.

Table 2
Overview of workflows provided with the toolbox.

Workflow	Description
workflow_1_basic.m	Shows basic functionalities of TOSSH with example data from one catchment.
workflow_2_advanced.m	Shows advanced functionalities of TOSSH with example data from multiple catchments.
workflow_3_time_resolution.m	Shows how to use TOSSH with example data from the same catchment but with different time resolution.
workflow_4_CAMELS_US.m	Shows how to use TOSSH to calculate the Addor et al. (2018) signatures using the CAMELS dataset (Newman et al., 2015; Addor et al., 2017).
workflow_5_CAMELS_GB.m	Shows how to use TOSSH to calculate various signatures using the CAMELS GB dataset (Coxon et al., 2020).

3.1.1. Comparison of signatures using different timesteps

Workflow *workflow_3_time_resolution.m* compares the toolbox results when using example time series from a UK catchment at daily, hourly and 15 min resolution, to demonstrate the impact of the time resolution of input flow data. Results for three signatures are shown in Table 3. The results demonstrate that some signatures are virtually unaffected by data time resolution (e.g. slope of FDC, BFI because the parameter is adjusted to the timestep) while some signatures are affected because the dynamics of the flow series are smoothed when longer timesteps are used (e.g. rising limb density).

3.1.2. Reproduction of CAMELS US signatures using daily flow data

Workflow *workflow_4_CAMELS_US.m* calculates the 13 signatures described by Addor et al. (2018) for daily flow data from the 671 mostly-natural U.S. catchments of the CAMELS dataset (Newman et al., 2015; Addor et al., 2017). We test whether our code gives the same signature values as those provided with the CAMELS dataset, providing a test across a wide range of flow dynamic characteristics (Figure 4). The results show that

Table 3
Comparison of three signatures applied to time series from the same catchment but with different timesteps. Default parameters were used; these may differ according to timestep.

	Daily	Hourly	15min
Slope of FDC [-]	-2.49	-2.50	-2.50
BFI [-]	0.84	0.82	0.82
Rising limb density [1/d]	0.43	0.55	0.56

for most signatures, our code matches the CAMELS data within the limits of small differences in signature definition, as shown by the Spearman rank correlation ρ_s given for each signature. In the case of the FDC slope, we verified with CAMELS authors that the large differences stem from an error with CAMELS signature values.

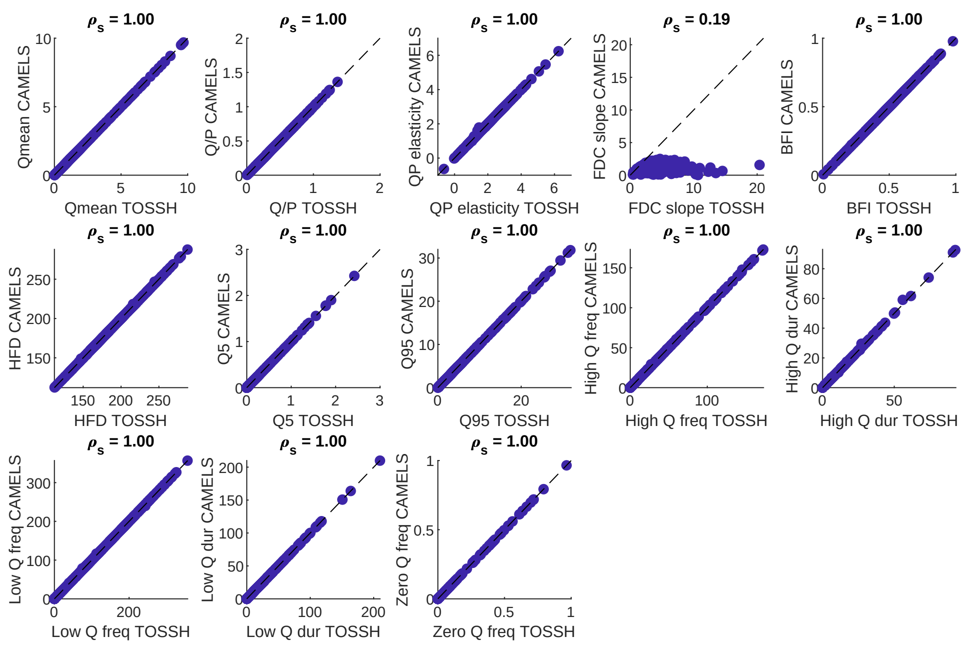

Figure 4: Addor et al. (2018) signatures calculated with TOSSH (*calc_Addor.m*) compared to signatures provided with CAMELS (Addor et al., 2017). See Table 1 for a list of all Addor et al. (2018) signatures.

3.1.3. Evaluation of signatures over CAMELS GB catchments

Workflow *workflow_5_CAMELS_GB.m* calculates the 13 signatures described by Addor et al. (2018) for daily flow data from the 671 UK catchments of the CAMELS GB dataset (Coxon et al., 2020). Again, we test whether our code gives the same signature values as those provided with the CAMELS GB dataset, providing a test across a wide range of flow dynamic characteristics. The results agree for complete time series, but disagree for time series with missing data which are treated differently in the two studies (not shown here). Additionally, the workflow calculates some of the process-base signatures that are not contained in the CAMELS datasets, shown in Figure 5. The patterns correspond well with the climate (more humid towards the north and the west) and the geology (e.g. Chalk in the south) of Great Britain.

4. Discussion

4.1. Transferability of signatures

Several of the signatures we implemented, particularly the process-based signatures, were originally designed for a specific catchment. Others were designed for a specific class of catchments, such as those where baseflow is low enough that events are clearly separated, or where recessions are approximately exponential. In catchments with different dynamics, those signatures may produce unreliable values; for example, event runoff coefficients

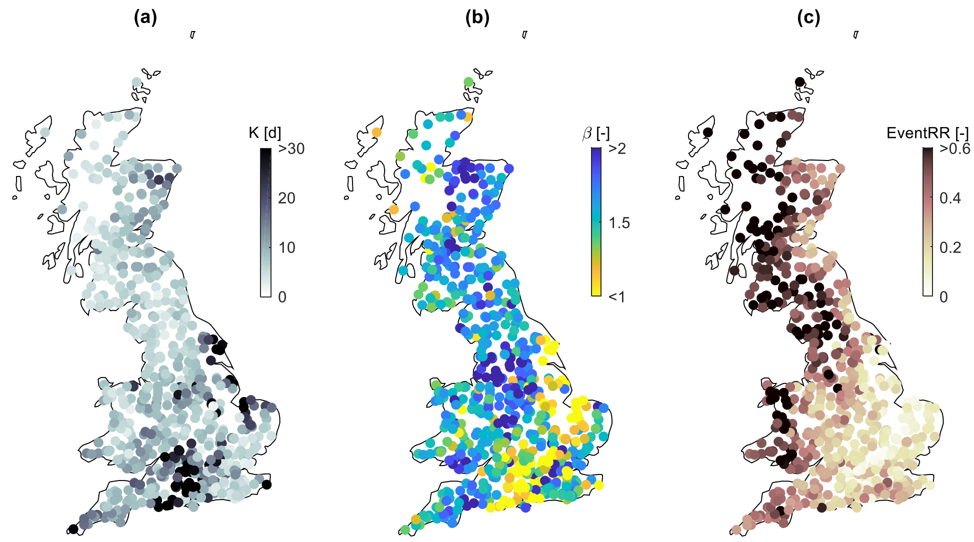

Figure 5: Maps of Great Britain showing (a) recession time constant (assuming exponential recession behaviour, *sig_BaseflowRecessionK.m*), (b) recession exponent obtained from fitting a power-law to the dQ/dt vs. Q point cloud (*sig_RecessionAnalysis.m*), and (c) event runoff ratio (*sig_EventRR.m*).

would be unreliable in karst or pumice landscapes where baseflow dominates. Many signatures rely on separating the rainfall and flow series into discrete events, which works better in drier climates. These signatures often failed to give meaningful values in the wetter British climate where many locations have more than 150 rain-days per year and events blend together. Streamflow series that are strongly affected by human impacts (e.g. flow regulation, abstractions) may also produce unreliable values due to unnatural flow dynamics. We therefore caution that the choice of signatures must consider local climate and streamflow dynamics.

The line between suitable/unsuitable catchments for a signature is not clear cut. Where possible, the toolbox functions screen the flow series and warn of inconsistencies with the signature. For example, a warning when is returned if less than ten recession periods are available to calculate recession-based signatures. However, the user is ultimately responsible for the choice of signatures. This issue is common to other signature tools, such as the eFlows web software (`https://eflows.ucdavis.edu/`) which calculates signatures designed for Mediterranean climates with a summer dry season (Patterson et al., 2020). The user may upload flow data for any catchment to the website, but in the case of a non-Mediterranean flow pattern the software may return either an unrealistic value or a null value.

4.2. Limitations

The toolbox does not provide estimates of the signature uncertainty. Signatures inherit the uncertainty of their underlying flow and precipitation data, which may be suppressed or amplified depending on signature design (Westerberg and McMillan, 2015). One way to estimate signature uncertainty is to draw samples of possible flow series based on the observed flow. This could use a site-specific uncertainty analysis, or a sensitivity analysis approach with synthetic flow data created by adding bias or random errors to the observed flow based on estimates of uncertainty magnitude (McMillan et al., 2012). Calculating the change in signature values using the sampled flow gives an estimate of signature uncertainty. This analysis is left to the user due to the site-specific nature of flow uncertainty (Coxon et al., 2015).

The toolbox implements the most common and robust version of each signature, based on our reading of the literature. However, there are often multiple other variations described by different authors. This was a conscious decision on our part, to promote the standardisation of signatures and to avoid overwhelming the toolbox user with methodological decisions. We aimed at easy to understand and robust code, which can sometimes compromise computational efficiency. Additionally, we made many decisions while implementing the signatures, such as how to handle missing values, which were not completely described in the host papers. For these reasons, minor differences in signature values may occur compared to previous implementations. The comments in the Matlab functions provide further information on specific implementations and relevant references.

4.3. Outlook

The modular design of the toolbox allows for easy use of signatures, and easy expansion. We anticipate future additions to the toolbox in the following categories: (1) individual signatures contributed by our team or toolbox users, (2) additional benchmark signature sets in the case of new papers that become widely used, (3) expansion to signatures based on different data types such as snow or soil moisture. In the case of readers wishing to contribute additional signatures that fit the scope of the toolbox, we ask you to code your signatures using one of the templates provided, and test the signatures using the example input data at daily, hourly and 15 minute time resolutions. A basic template is provided for a signature that only uses flow data (*sig_TemplateBasic.m*), and an advanced template (*sig_TemplateAdvanced.m*) that enables input of flow, precipitation, potential evapotranspiration and temperature data. Please use the Github issues forum (https://github.com/TOSSHtoolbox/TOSSH/issues) to report any bugs or suggestions or email the corresponding author.

5. Conclusions

This paper presented TOSSH: A Toolbox for Streamflow Signatures in Hydrology, which addresses the need for accessible, standardised signature calculations. The toolbox provides accessible, standardised signature calculations, with clear information on methodological decisions and recommended parameter values. The toolbox implements three categories of signatures: basic signatures that describe the five components of a natural streamflow regime, signatures from benchmark papers, and an extended set of process-based signatures. We presented workflow scripts and example data to demonstrate implementation procedures, and visualisation options. We demonstrated the accuracy and robustness of the signature calculations by applying reproducible workflows to large streamflow datasets from the U.S. and Great Britain using the CAMELS datasets. The modular design of the toolbox allows for flexibility and easy future expansion. We envisage the toolbox to provide a hub for signature calculations for various applications in hydrology and related fields.

Funding

This work is funded as part of the Water Informatics Science and Engineering Centre for Doctoral Training (WISE CDT) under a grant from the Engineering and Physical Sciences Research Council (EPSRC), grant number EP/L016214/1.

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