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A review of hydrologic signatures and their applications

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Abstract

Hydrologic signatures are quantitative metrics or indices that describe statistical or dynamical properties of hydrologic data series, primarily streamflow. Hydrologic signatures were first used in eco-hydrology to assess alterations in flow regime, and have since seen wide uptake across a variety of hydrological fields. Their applications include extracting biologically relevant attributes of streamflow data, monitoring hydrologic change, analyzing runoff generation processes, defining similarity between watersheds, and calibrating and evaluating hydrologic models. Hydrologic signatures allow us to extract meaningful information about watershed processes from streamflow series, and are therefore seeing increasing use in emerging information-rich areas such as global-scale hydrologic modeling, machine learning, and large-sample hydrology. This overview paper describes the background and development of hydrologic signature theory, reviews hydrologic signature use across a variety of applications, and discusses ongoing hydrologic signature research including current challenges.

This article is categorized under:

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KEYWORDS

flow indices, flow metrics, hydrologic signatures

1 | INTRODUCTION

1.1 | Discovering the information in streamflow data

Streamflow timeseries show patterns: flood peaks and low flow periods, daily changes and seasonal cycles. These patterns are examples of information in streamflow data. The information might describe how the stream reacts to changes in weather, or what magnitudes and rates of change of flow are usual for the stream. Streamflow patterns depend on the physical characteristics of the watershed, telling a story about the path of water from precipitation to streamflow. Flow patterns in turn affect the stream's environment, informing us about riparian conditions and habitats. This paper describes how hydrologists use hydrologic signatures to extract this wealth of information from streamflow.

1.2 | What is a hydrologic signature?

Hydrologic signatures are quantitative metrics that describe statistical or dynamic properties of streamflow. They are also known as hydrologic metrics, hydrologic indices, or diagnostic signatures. Hydrologic signatures range from simple statistics such as the mean and quantiles of the timeseries, to complex metrics such as descriptors of recession shapes that are related to the storage-discharge behavior of the watershed (Figure 1). Hundreds of different hydrologic signatures have been proposed, for example a review of signature choice and redundancy considered 171 signatures (Olden & Poff, 2003). To organize and describe signatures, several categorizations have been proposed.

An early and well-known categorization groups signatures into five ecologically important features of flow regimes: magnitude, timing, frequency, duration, and rate of change (Richter, Baumgartner, Powell, & Braun, 1996) (Table 1). This work built on a previous suggestion to group signatures by flow variability, pattern of the flood regime, and extent of intermittent conditions (Poff & Ward, 1989). Many subsequent authors use the five categories. Notably, Poff et al. (1997) use the categories to quantify the natural flow regime of a river, proposing that these components completely describe the flow characteristics of importance to the aquatic ecosystem. Based on the categories, Richter et al. (1996) went on to propose five statistical signature types for describing hydrologic alteration caused by human influence. Those categories were: flow magnitude, magnitude and duration of annual maxima, timing of annual maxima, frequency and duration of high and low flow pulses, and rate and frequency of streamflow change.

Signatures may purely describe the streamflow timeseries (e.g., mean and quantiles of timeseries) or may describe a watershed process (e.g., recession shapes related to storage-discharge behavior). Some authors define these as different

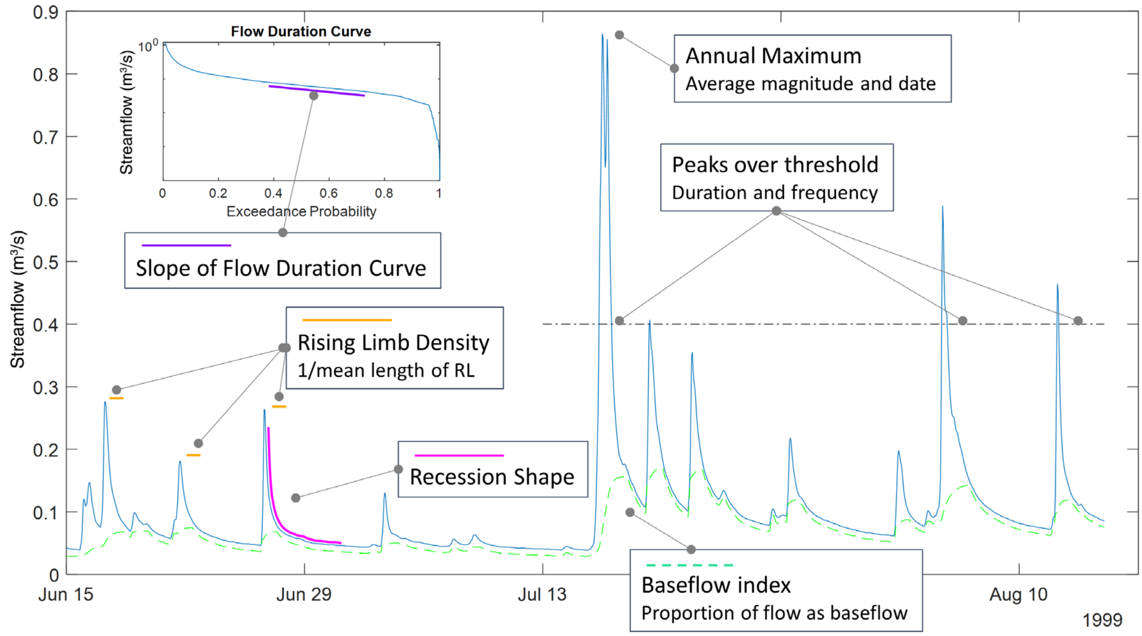

FIGURE 1 Examples of commonly used hydrologic signatures calculated as metrics of the streamflow timeseries

TABLE 1 Categorization of signatures described by Richter et al. (1996)

Type	Signature examples	Ecological relevance
1. Magnitude	Flow magnitude by year or month	Describes wetted area and availability of habitat
2. Timing	Seasonal timing of annual maxima and other annual flow events	Describes whether life-cycle requirements of instream species are met
3. Frequency	Frequency of events such as floods or droughts	Influences population dynamics by controlling reproduction or mortality events for instream species
4. Duration	Length of time for which a specific flow condition occurs	Controls life cycle phases; controls accumulated impact of floods or droughts
5. Rate of change	Rate of change of flow magnitude and stage height	Can strand organisms above the water's edge, and strand plant roots above the reach of groundwater

TABLE 2 Categories of signatures suggested by McMillan (2020)

Type	Description	Examples
1. Timeseries visuals	Visual interpretations of timeseries data	Double peaks in streamflow, diurnal cycles
2. Quantified event dynamics	Numerical descriptors of event-scale dynamics	Recession shapes, flow generation thresholds
3. Quantified seasonal dynamics	Numerical descriptors of dynamics, averaged over time	Rising limb density, baseflow index
4. Seasonal statistics	Statistical descriptors of the flow distribution	Runoff ratio, shape of the flow duration curve
5. Mini-model	Quantities derived from highly simplified models	Storage volumes, regression relationships

categories, with the former described as flow indices, metrics, or characteristics, and only the latter described as signatures (Wagener, Sivapalan, & McGlynn, 2008; Wagener, Sivapalan, Troch, & Woods, 2007). McMillan (2020) proposed a categorization that differentiates between statistics- and dynamics-based signatures, and between signatures at different timescales (Table 2). Statistics-based signatures are calculated at seasonal or longer timescales, require only the flow distribution and typically relate to storage volumes, while dynamics-based signatures describe shapes or patterns of the flow series and typically relate to partitioning of water between different flow pathways.

Hydrologic signatures, including the examples in Table 2, often build on earlier ideas. For example, early descriptions were published for the flow duration curve (the cumulative distribution function of flow that shows the percent of time that flow values are exceeded; Searcy, 1959), baseflow index (proportion of flow that is baseflow; Kunkle, 1962), and Pardé coefficients for flow variability (ratios of monthly mean discharges to the mean annual discharge; Pardé, 1933). However, the concept of combining these metrics into a more complete description of the flow regime did not occur until later.

1.3 | Hydrologic signatures in other fields

Hydrologic signatures originate in the idea that measurable hydrologic patterns can tell us about the underlying system. We can use accessible measurements to reveal inaccessible or complex processes: for example, using streamflow to learn about subsurface or overland flow. Other environmental fields use signatures similarly, such as using water level fluctuations in a wetland to learn about hidden inflows and outflows (Mitsch & Gosselink, 1986), or using ocean surface patterns to learn about deep currents (Millot, 1999). In tracer studies, isotope ratios in a water sample are called signatures, as they help identify the source of the water in time or space (Klaus & McDonnell, 2013; Sprenger et al., 2019; Xue et al., 2009). In remote sensing, reflectance ratios between wavelengths are called spectral signatures, as they can identify surface properties such as snow cover (Dozier, 1989) or water quality (Doxaran, Froidefond, Lavender, & Castaing, 2002). In geomorphology, signatures of drainage density are even used on Mars to interpret the ancient hydrological cycle (Hynek, Beach, & Hoke, 2010). In all these examples, signatures allow scientists to interpret measurements and extract information about the environment.

This review focuses on signatures describing streamflow data. However, signatures are applied to other hydrologic data types. Signatures combining flow and temperature data provide information on alpine snowfall and melt (Horner, Branger, McMillan, Vannier, & Braud, 2020; Schaefli, 2016). Signatures were used to categorize groundwater dynamics (Heudorfer, Haaf, Stahl, & Barthel, 2019), and to identify soil moisture dynamics that are less affected by soil heterogeneity (Branger & McMillan, 2019). Recent innovations include signatures created for karst hydrology (Hartmann, Wagener, et al., 2013), glacio-hydrology (He et al., 2018; Mackay et al., 2018), and for total water storage anomalies from GRACE data (Fang & Shen, 2017). These examples demonstrate the continuing and expanding use of signature methods in hydrology.

2 | APPLICATIONS OF HYDROLOGIC SIGNATURES

The following sections describe three main types of hydrologic signature applications: ecohydrology, watershed processes, and modeling (Figure 2).

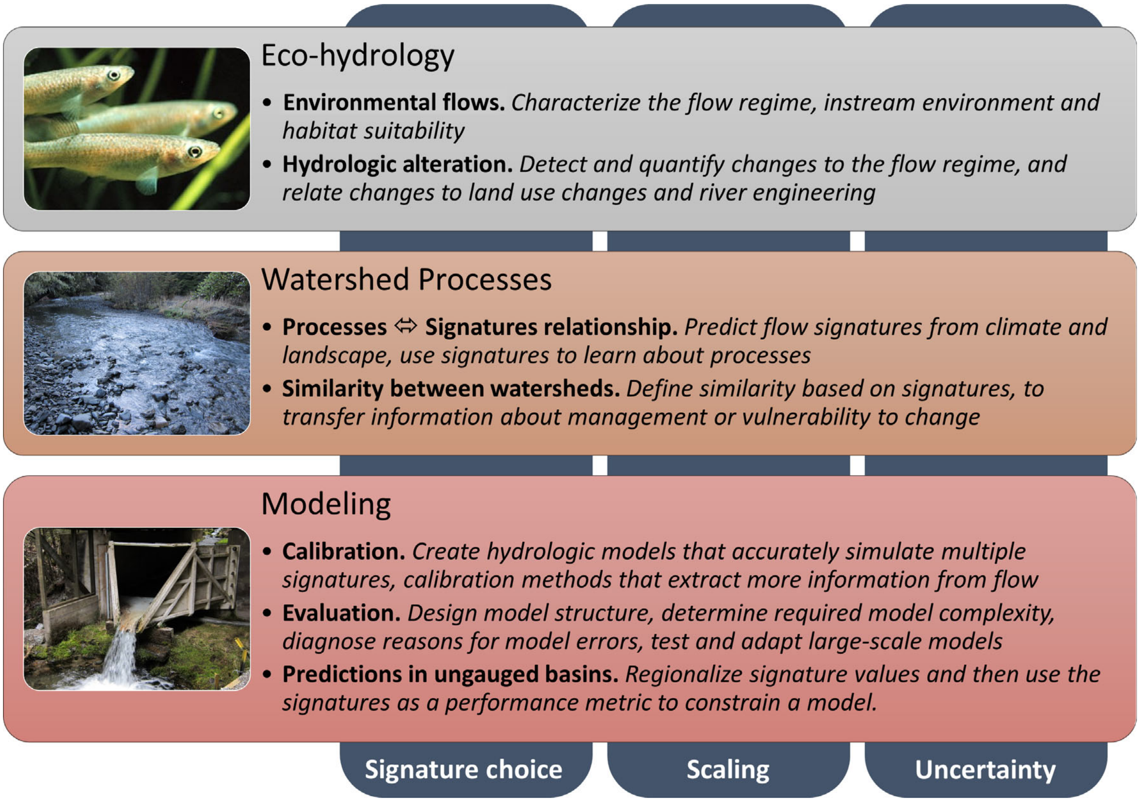

FIGURE 2 Summary of the three categories of hydrologic signature applications discussed in this paper (Eco-hydrology, Watershed Processes, and Modeling), with cross-cutting methodological considerations

2.1 | Ecohydrology, environmental flows, and hydrologic alteration

An important concept in ecohydrology is that the flow regime of a river controls channel and riparian habitat, and the suitability of the river to support freshwater species (Gordon, 2004). Flow velocity and its variability close to the streambed affect instream ecosystems via multiple mechanisms. Flows control bed sediments, nutrient levels, availability of refuges, and frequency of disturbance; and therefore control species dispersal, habitat use, resource acquisition, predator–prey interactions, and competition (Hart & Finelli, 1999).

Given the need to describe how flow characteristics impact stream ecology, ecohydrology was the first field to create catalogues of signatures that summarize the flow regime. Two foundational papers use signatures such as annual maximum flows and numbers of high and low flow events to characterize biologically relevant flow attributes (Poff et al., 1997; Richter et al., 1996). Their signatures emphasize the flow extremes—floods and low flows—that control channel shape and species survival.

2.1.1 | Environmental flows to preserve instream habitat

Stream habitat is influenced by multiple aspects of the flow regime. Flow variability, from milliseconds to decades, affects which species dominate the ecosystem (Biggs, Nikora, & Snelder, 2005). For example, invertebrates may tolerate variability only above or below certain limits (Konrad, Brasher, & May, 2008). Species may have very specific flow requirements, such as the endangered yellow-legged frog (*Rana boylii*) in California that relies on a consistent rate of river level fall in summer, allowing tadpoles to following the receding water's edge (Bondi, Yarnell, Lind, & Lind, 2013; Yarnell, Viers, & Mount, 2010). Species requirements can be encoded as signatures, for example by quantifying flow variability, or frequency and duration of unacceptable flow conditions. To encompass all the flow attributes required to sustain a healthy ecosystem, water managers use the term “environmental flows” (Acreman, 2016). Methods to assess whether a river meets environmental flow requirements are diverse, but typically rely on hydrologic or hydraulic signatures to rate habitat suitability (Tharme, 2003).

To rate habitat suitability, hydrologists search for signatures that explain species abundance, and where ecosystem theory explains why those flows are needed (Table 3). Other measures such as species presence/absence, diversity, or size and fitness of individuals may also be used. This method needs measurements of species abundance at large numbers of sites. Commonly measured species include periphyton (streambed organisms such as algae), invertebrates, and fish species. For example, Jowett and Duncan (1990) analyze 130 sites in New Zealand and find that high flow variability is negatively correlated with mean water velocity and relative bed stability, and positively correlated with trout habitat. In other species, flow variability reduces abundance, such as in stream salamanders where variability reduces survival through metamorphosis (Lowe, Swartz, Addis, & Likens, 2019). Clausen and Biggs (1997) find that the "Fre3" signature, that is, the frequency of floods higher than three times the median flow, predicts periphyton and invertebrate density because Fre3 flows have sufficient energy to disturb sand and gravel riverbed sediments. Once a relationship between signatures and species is established, it can be used to predict basin-wide species distribution (Ceola et al., 2014).

For general environmental flow assessments, not aimed at one particular species, the best choice of signatures is less clear. Yarnell et al. (2020) propose a method based on "functional flows," that is, flow features that affect species lifecycles, such as fall pulse flows, spring recessions, and summer low flows. For each feature, signatures are selected corresponding to flow magnitude, timing, frequency, duration, and/or rate of change. Online software is available to calculate these signatures in seasonal, Mediterranean climates (Patterson et al., 2020). Archfield, Kennen, Carlisle, and Wolock (2014) instead try to overcome subjectivity in signature choice by using their seven "fundamental daily streamflow statistics" for all rivers, including the moments of the flow series and descriptors of the seasonal cycle. Refer to Section 3.1 for a wider discussion of rationales behind signature choice.

2.1.2 | Detecting hydrological change

An important motivation for using signatures to quantify environmental flows is to understand how humans have altered river ecosystems by altering streamflow patterns. Modified flows encourage invasive species, to the detriment of native species that rely on natural water levels, seasonal flow changes, and floodplain connectivity (Bunn & Arthington, 2002). Signatures can be compared before and after a hydrologic change, to quantify how disturbances such as dams, levees, urbanization, afforestation, or drainage change the flow regime (Archer & Newson, 2002; Poff et al., 1997). The widely used ELOHA framework (Ecological Limits Of Hydrologic Alteration; Poff et al., 2010) uses signatures to classify rivers by flow and geomorphological regime, quantify flow changes from baseline conditions, and understand the ecological impacts of those changes.

The most disruptive changes for riverine ecosystems are depleted high flows, homogenization of flows, and erratic flows (for U.S. rivers; Carlisle, Grantham, Eng, & Wolock, 2017) as well as artificially reduced flow that reduces water velocity, depth, wetted width and therefore habitat and species diversity (Dewson, James, & Death, 2007). Larger changes in flow magnitude carry a greater risk of ecological change, but exact relationships between flow signatures and ecological change are place-specific (Poff & Zimmerman, 2010). Most studies analyze changes in flow magnitude (e.g., flow peaks, average flow, baseflow, and daily variation), whereas changes in flow timing, frequency, duration, and rate of change are less commonly studied. Evaluating signature changes on a large scale can help to identify the underlying causes. Mahe et al. (2013) used signatures to describe decadal changes in the baseflow and flow variability of African rivers, and investigated the influence of climate, land use, and other anthropogenic changes. As well as past changes, signatures can help summarize how flows may change in future. By calculating signatures from future flows predicted by coupled climate and hydrologic models, we can identify changes such as timing of the snowmelt peak or the duration of summer low flows (Hayhoe et al., 2007). Signatures are valuable to identify causes and impacts of flow regime changes, in the past and for the future.

2.2 | Watershed processes

While ecohydrology uses signatures to study how flow regime affects instream habitat, hydrologic process research uses signatures to study how the upstream watershed affects the flow regime. Using watershed attributes (e.g., soil, geology

TABLE 3 Four freshwater species highlighted in this article and the hydrologic signatures that help explain their abundance in instream environments

				
Species	Periphyton and invertebrates (*various species*)	Mayfly (*Baetis muticus*, *Baetis rhodani*, *Ecdyonurus venosus*)	Rainbow trout (*Oncorhynchus mykiss*)	Yellow-legged frog (*Rana boylii*)
Signature	Frequency of floods 3× the median flow	Quantiles of flow duration curve	Flow variability (coefficient of variation of flow)	Stage height recession rate
Explanation	Relates to frequency of disturbance events	Relates to shear stress distribution that controls grazing behavior	Low flow variability relates to cleaner water and larger food production area	Egg masses and tadpoles rely on steady fall of water level in summer
Reference	Clausen and Biggs (1997)	Ceola et al. (2014)	Jowett and Duncan (1990)	Bondi et al. (2013), Yarnell et al. (2010)

and topography) to predict flow signatures enables us to estimate flows and stream habitat in ungauged basins. To this end, many early signature papers describe relationships between watershed attributes and signature values (Jowett & Duncan, 1990; Poff & Ward, 1989). It is also useful to reverse the inference and use flow signatures to predict watershed processes. Examples of process predictions could include whether overland flow occurs, or how connected is water in the hillslopes and channel. By using intensively studied basins to establish relationships between signatures and processes, we can transfer process knowledge to any watershed with a flow gauge (McMillan, 2020). The link between signatures and watershed processes is the basis for several applications described in later sections, such as using signatures to quantify similarity between watersheds, and evaluating physical realism of hydrologic models.

Sometimes the link between watershed processes and signatures is clear, such as when winter snowfall causes a spring snowmelt peak, or when karst geology causes high baseflow. McDonnell et al. (2007) argue that both watershed descriptors and hydrologic signatures should focus on how watersheds function. Currently, this is not the case and many signatures such as low flow frequencies are only weakly related to watershed function. A useful test of the relationship is how well signatures can be predicted from watershed attributes. Eng, Grantham, Carlisle, and Wolock (2017) tested 612 signatures and found that only 40% could be reliably predicted from U.S. watershed attributes. Signatures describing mean flows and high flows are typically well-predicted, while signatures describing low flows are poorly predicted (Addor et al., 2018; Eng et al., 2017; Zhang, Vaze, Chiew, Teng, & Li, 2014).

A compelling explanation for differences in signature predictability is that climate descriptors (e.g., aridity, snow fraction) provide most of the predictive power, while watershed descriptors (e.g., soil type, forest cover, slope) provide little predictive power (Figure 3; Addor et al., 2018; Merz & Blöschl, 2009). Therefore, signatures that relate closely to climate characteristics are well predicted. At the seasonal scale, wet or impermeable watersheds transfer climate variability almost directly into hydrologic variability, explaining why seasonal, high flow signatures are more easily predicted (Gnann, Howden, & Woods, 2020). However, by focusing on situations where expert knowledge suggests that hydrology is more important than climate, relationships can be uncovered. For example, watershed drainage pattern helps to predict flood signatures (Oppel & Schumann, 2020), and information on surface waterbodies helps to predict baseflow signatures (Beck et al., 2013).

The weak relationship between watershed descriptors and signatures contradicts extensive field evidence that shows how watershed features control streamflow responses. Therefore, there is great potential to create new watershed descriptors that better characterize hydrologic behavior and flow signatures (Gnann, McMillan, Woods, & Howden, 2020). In turn, this would allow for better predictions of the flow regime in ungauged watersheds.

2.2.1 | Defining similarity between watersheds

Analyzing hydrologic similarity enables us to transfer information between similar watersheds. We might use insights from a similar watershed to design monitoring networks or models in a new watershed, or to estimate the impacts of land use or climate change (Wagener et al., 2007). Similar watersheds will have similar ecology and can benefit from similar conservation efforts and environmental flow regulations (Kennard, Pusey, et al., 2010). Similarity measures can also pick out watersheds that behave differently, such as Australia and southern Africa that have more extreme flows relative to mean flow than on other continents (McMahon, Vogel, Peel, & Pegram, 2007). Often, a similarity measure is used to define clusters (also called classes) of similar watersheds. Many generic clustering algorithms are available, such as hierarchical clustering, *k*-means clustering, or Bayesian mixture modeling (Jain, Murty, & Flynn, 1999). Using signatures as the similarity measure creates clusters that are hydrologically similar in terms of flow regimes, instream ecosystem, and watershed processes. Although clustering can be based on physical watershed attributes instead (topography, land cover, etc.), this produces substantially different groupings (Ali, Tetzlaff, Soulsby, McDonnell, & Capell, 2012).

Similarity in signatures implies a combination of climate similarity and process similarity. This creates clusters that are largely geographically compact (climate influence), but with some geographical spread (process influence). For example, Kennard, Pusey, et al. (2010) use signatures to cluster Australian watersheds. They find compact clusters influenced by seasonal timing of flow, flood magnitude, and baseflow magnitude, but some outliers such as highly intermittent streams, which are driven more strongly by process and have a wide geographical distribution (Figure 4). Climate typically dominates clusters derived directly from signature similarity (Coopersmith, Yaeger, Ye, Cheng, & Sivapalan, 2012; Sawicz, Wagener, Sivapalan, Troch, & Carrillo, 2011). Therefore, Knoben, Woods, and Freer (2018) recommend separating climatic and hydrological similarity when deriving clusters.

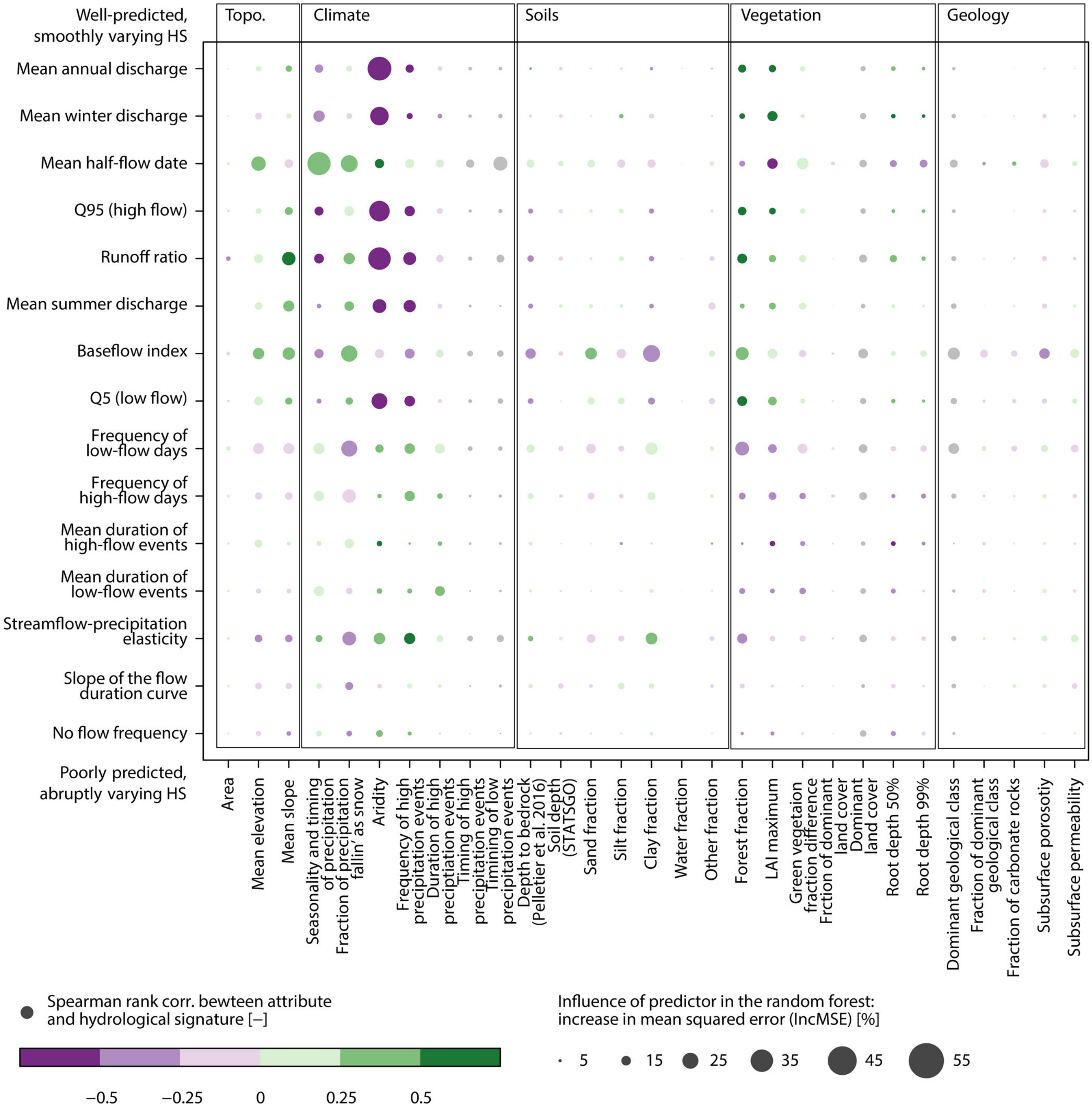

FIGURE 3 Comparison of the influence of catchments attributes (*x* axis) used to predict hydrological signatures (*y* axis) with a random forest method for 671 U.S. watersheds with minimal human influence. Large, brightly colored circles imply strong correlations and high influence. The signatures are ordered with better predicted signatures at the top. The strongest relationships are between climate attributes and mean or high flow signatures, with topography, soils, vegetation and geology having low predictive power (Reprinted with permission from Addor et al. (2018). Copyright 2018 Wiley)

An alternative to signature-based clusters is to use climate or watershed descriptors to derive clusters, and look for similarities in signature values in each cluster. Climate-based clusters such as the Köppen–Geiger classes produce different patterns to signature-based clusters (Jehn, Bestian, Breuer, Kraft, & Houska, 2020). However, climate descriptors can be targeted towards creating hydrology-relevant clusters, by using descriptors such as aridity that is related to the water balance (Berghuijs, Sivapalan, Woods, & Savenije, 2014). Instead of looking at signature values within in a cluster, a recent proposal is to use hydrological archetypes. These are graphs of the median annual hydrograph of all

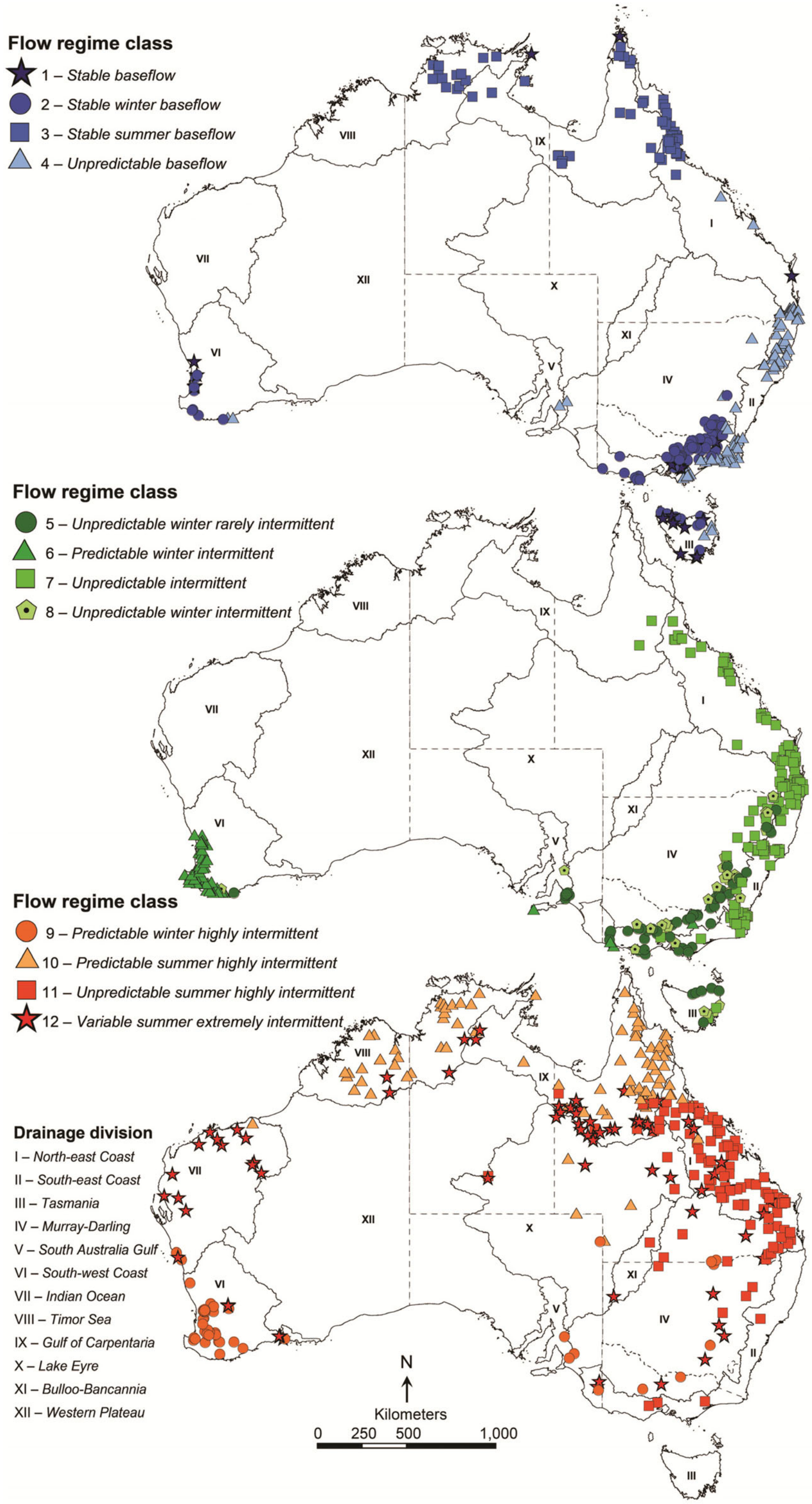

FIGURE 4 Flow regime classes for 830 stream gauges in Australia, clustered using 120 hydrologic signatures. The signatures describe mean and variance in the streamflow magnitude (average, low, high), frequency (low, high), duration (low, high), timing and rate of change. Note that some classes are geographically compact (e.g., 2) while some are dispersed (e.g., 12) (Reprinted with permission from Kennard, Pusey, et al. (2010). Copyright 2010 Wiley)

watersheds in the cluster, with upper and lower percentiles, giving an overview of the hydrological behavior. These visual representations integrate the information in multiple signatures in an intuitive way (Lane et al., 2018).

An important application of hydrologic similarity is to estimate how vulnerable watersheds are to climate or land use change. We can already see the impacts of climate change on flow signatures, as watersheds move between clusters over time as their climate changes (Sawicz et al., 2014). When planning for future impacts, watersheds with similar signature values are assumed to react similarly to climate changes. We can predict future watershed behavior using space-for-time substitution, that is, looking for similar watersheds that already have climates similar to future predictions in the area of interest (Sivapalan, Yaeger, Harman, Xu, & Troch, 2011).

2.3 | Modeling

As signatures can quantify hydrologic function, it is a natural progression to use signatures in the pursuit of models that accurately represent hydrologic function. Signatures are used at all stages of the modeling process, from model structure selection, through calibration and evaluation.

2.3.1 | Calibration

The first uses of signatures for modeling were for calibration. In calibration, parameters are adjusted manually or automatically to optimize model performance. Manual calibration procedures are often complex and link parts of the hydrograph to different parameters, for example using baseflow periods to set baseflow parameters (Boyle, Gupta, & Sorooshian, 2000). Automatic calibration procedures are usually simpler, aiming to optimize a performance measure. Performance measures are commonly based on the sum of squared errors between observed and modeled flows, such as the Nash–Sutcliffe efficiency (Nash & Sutcliffe, 1970). However, these performance measures are criticized because they lack a clear link to hydrologic function, and so it is unclear which parameters should be changed to improve performance. By replacing the sum-of-squared errors measure with a measure composed of one or more signatures, we can improve the link to watershed function in an automatic calibration procedure.

Drawing on manual calibration expertise, hydrologists have long incorporated flow regime signatures into automatic calibration. Sugawara (1979) used hydrograph volume and recession slope as performance measures, while Refsgaard and Knudsen (1996) combined flow duration curves and annual maximum flow signatures with NSE and visual comparison of hydrographs. Hogue, Sorooshian, Gupta, Holz, and Braatz (2000) mimic a complex multi-objective manual approach in an automatic procedure, and signatures from multiple data sources can complement flow series during calibration (Hay et al., 2006; Hingray, Schaefli, Mezghani, & Hamdi, 2010). More generally, Gupta, Sorooshian, and Yapo (1998) argue that multi-objective calibration is necessary given trade-offs between a model's ability to match different parts of the hydrograph. Building on this, Gupta, Wagener, and Liu (2008) state that given the high dimensionality of the data available for calibration and the model parameter space, this information should not be compressed into a one-dimensional performance measure. Instead, they recommend model calibration against multiple signatures, each related to specific parameters. Kavetski, Fenicia, Reichert, and Albert (2018) name the approach "signature-domain calibration," in contrast to "time-domain calibration."

The call for model calibration using flow signatures was widely taken up, with several adaptations. Some studies use signatures to evaluate the modeled flow regime when data are scarce, or when precipitation and flow data are available for different time periods. These studies choose signatures that summarize the flow regime such as the flow duration curve (Westerberg et al., 2011) or spectral density of the flow signal (Montanari & Toth, 2007; Winsemius, Schaefli, Montanari, & Savenije, 2009).

Several studies use signature-based calibration to search for models that achieve "hydrologic consistency," that is, that reproduce multiple flow signatures (Martinez & Gupta, 2011; Pechlivanidis, Jackson, McMillan, & Gupta, 2014; Pokhrel, Yilmaz, & Gupta, 2012; Sahraei, Asadzadeh, & Unduche, 2020; Shafii & Tolson, 2015). The hope is that these models provide a realistic representation of a range of hydrologic processes. For example, He et al. (2018) use signature-based calibration to produce stable and realistic model parameters in a glaciated basin, and Shafii, Basu, Craig, Schiff, and Cappellen (2017) use signatures based on the L'vovich partitioning framework to create models with realistic partitioning between quick and slow flow, infiltration, and evapotranspiration. If the selected signatures capture all the information in the flow signal, they are referred to as "sufficient statistics" (see section 5.3.1 in Kavetski et al., 2018).

The opposing view to sufficiency is that careful selection of signatures enables us to match some parts of the hydrograph, while ignoring parts that are less important or have known errors (e.g., timing errors). In this way, the user controls the weighting of different aspects of model performance. Signatures can focus the calibration on just one part of the hydrograph, such as high flows (Mizukami et al., 2019) or low flows (Pfannerstill, Guse, & Fohrer, 2014). When the model aim is to predict an ecologically relevant signature, the signature should be included in the calibration, as using a statistical performance measure may bias signature predictions by up to 25% (Pool, Vis, Knight, & Seibert, 2017). We can also calibrate a model using a structured approach, starting with signatures at annual or longer timescales, and progressing to shorter timescales (Shamir, Imam, Gupta, & Sorooshian, 2005). Note that none of the studies above apply signature calibration in the way that Gupta et al. (2008) suggested—by matching signatures to individual parameters. A recent example that does achieve that type of calibration is a manual, signature-based recalibration of the distributed J2000 model (Horner, 2020). One reason that such studies are rare is that correspondences between parameters and signatures differ between watersheds, complicating transferability of the method (Guse et al., 2017).

When calibrating models against signatures, we often want to account for model uncertainties, to create probabilistic streamflow predictions. Many of the studies described above use approaches similar to the generalized likelihood uncertainty estimation framework (Beven & Freer, 2001). In this framework, simulations are accepted (and/or weighted) if the modeled signatures lie within some tolerance of the observed signatures. This approach has been criticized because it does not conform to a strict statistical definition of a likelihood function. More recently, the approximate Bayesian computation (ABC) technique has been proposed to calculate probabilistic parameter distributions without the need to compute a likelihood function. This is beneficial for signature-domain calibration, as it would be difficult to create signature likelihood functions. Kavetski et al. (2018) provide clear guidance on how to apply ABC for signature-domain calibration, and Fenicia, Kavetski, Reichert, and Albert (2018) investigate practical questions such as the impacts of number of signatures and length of data series, and the ability of signature-domain calibration to cope with model deficiencies.

2.3.2 | Evaluation of model structure and parameters

Signatures can be used to design hydrologic model structure, often in a multi-model framework such as FUSE (Clark et al., 2008) or SUPERFLEX (Fenicia, Kavetski, & Savenije, 2011). These frameworks offer a mix-and-match approach to build a model from pre-designed components. In some cases, signature values can be directly mapped to model decisions, such that a given signature value implies a given model choice. For example, signatures based on flow, precipitation, and soil moisture data were targeted at specific model decisions in the FUSE framework (McMillan et al., 2014; McMillan, Clark, Bowden, Duncan, & Woods, 2011), with model tests confirming the data analysis (Clark, McMillan, Collins, Kavetski, & Woods, 2011).

A model can be chosen from a set of possible structures, by running each one and evaluating its ability to reproduce multiple signatures (e.g., Gunkel, Shadeed, Hartmann, Wagener, & Lange, 2015). Here, signatures provide an independent test of whether the model is physically realistic. Example applications are to evaluate sequentially more complex SUPERFLEX models (Euser et al., 2013), to investigate why different models succeed in watersheds with different hydrologic characteristics (Kavetski & Fenicia, 2011), and to compare geology versus topography discretizations in a distributed model (Fenicia, Kavetski, Savenije, & Pfister, 2016). Testing for realistic signature values helps avoid excessive model complexity where unrealistic parameter values compensate for one another (Hrachowitz et al., 2014), while retaining the complexity needed to reproduce streamflow dynamics (Farmer, Sivapalan, & Jothityangkoon, 2003; Jothityangkoon, Sivapalan, & Farmer, 2001). Using signature evaluation to progress from simple, large scale models to more complex models including finer-grained processes embodies the “downward” approach to model development proposed by Klemeš (1983).

After a model is built and calibrated, it may still predict inaccurate flows. Analysis of how well the model reproduces different signatures can help identify which parts of the model are failing. This draws from previous studies that identify which model decisions influence which signatures. For example, Coxon, Freer, Wagener, Odoni, and Clark (2014) show which FUSE model decisions influence water balance and flow duration curve signatures, across a range of watershed types from flashy to baseflow-driven. The baseflow parameterization was usually the most influential. In karst systems, model storage constants in fast flow and groundwater reservoirs affect high- and medium-flow flow duration curve slopes, respectively (Hartmann, Weiler, et al., 2013). Large differences in signature values between calibration and validation periods provide additional clues if the model struggles to reproduce changing dynamics (Jayathilake & Smith, 2019). A new use for signatures is to evaluate hydrologic models based on machine learning, such as long short-term memory (LSTM) networks. Signatures can assess predictive accuracy, and assess whether internal model components are physically meaningful, by testing whether watersheds that activate similar parts of the LSTM network have similar signature values (Kratzert et al., 2019).

Given increasing interest in national- to global-scale hydrologic models, signatures are useful to diagnose how model performance varies, or how model structure needs adaptation, for diverse climates or environments. Global signature databases, such as the Global Streamflow Indices and Metadata archive of 30,000 basins, make this possible (Gudmundsson, Do, Leonard, & Westra, 2018). In their comparison of 12 global hydrologic models, Beck et al. (2017) use signature-based evaluation to understand how models in different Köppen–Geiger climate regions perform in predicting water balance, flow magnitude, seasonal timing and flashiness. At national scale, McMillan, Booker, and Cattoën (2016) use signature-based evaluation to test how model performance varies with watershed area, wetness, and groundwater influence (Figure 5). Alternatively, signatures can be used to summarize which flow regimes are easy or difficult for models to simulate. In the United Kingdom, Topmodel and PRMS were preferable for flashy watersheds (low baseflow index), while the Sacramento model was preferred for groundwater-driven watersheds (high baseflow index) (Lane et al., 2019). After model structural changes, signatures can show which types of watersheds see an improvement. For example, de Boer-Euser, McMillan, Hrachowitz, Winsemius, and Savenije (2016) test a new method to set model soil depth based on co-evolution theory that estimates plant rooting depth, and use signatures to evaluate its success across wet and dry watersheds.

2.3.3 | Signature regionalization for predictions in ungauged basins

Hydrologic signatures provide a powerful tool for predicting flow in ungauged basins. Previous methods relied on regionalizing model parameters—estimating parameters for the ungauged basin by transferring parameters from nearby or physically similar watersheds, or regressing parameter values on watershed attributes. However, these methods were often unsuccessful (Oudin, Andréassian, Perrin, Michel, & Le Moine, 2008). Instead, signatures can be used in a three-part method (Figure 6): (a) relate watershed attributes to signatures in gauged basins, using regression on watershed attributes, (b) use that relationship to estimate (regionalize) signature values for the ungauged basin, and (c) use the regionalized signatures as a performance metric to calibrate a model for the ungauged basin. This method works because watershed attributes are more closely related to signatures than model parameters, and because signature regionalization is independent of the choice of model and model structural error. The method saw significant development and success during the predictions in ungauged basins (PUB) decade (Hrachowitz et al., 2013; Wagener & Montanari, 2011).

Steady progress has been made in advancing the signature regionalization method. The choice of signatures is guided by research into which signatures vary more smoothly across space and are more accurately predicted from watershed attributes (Addor et al., 2018). The regionalization method has advanced from regression to machine learning methods such as artificial neural networks (Beck, De Roo, & van Dijk, 2015) or random forests (Prieto, Vine, Kavetski, García, & Medina, 2019; Zhang, Chiew, Li, & Post, 2018). Many studies stress the importance of including uncertainty estimation at all stages of the process, from data uncertainty affecting the signature values (Westerberg et al., 2016), to using a probabilistic regionalization model (Prieto et al., 2019), to retaining an ensemble of models that adequately predict the regionalized signatures (Yadav, Wagener, & Gupta, 2007).

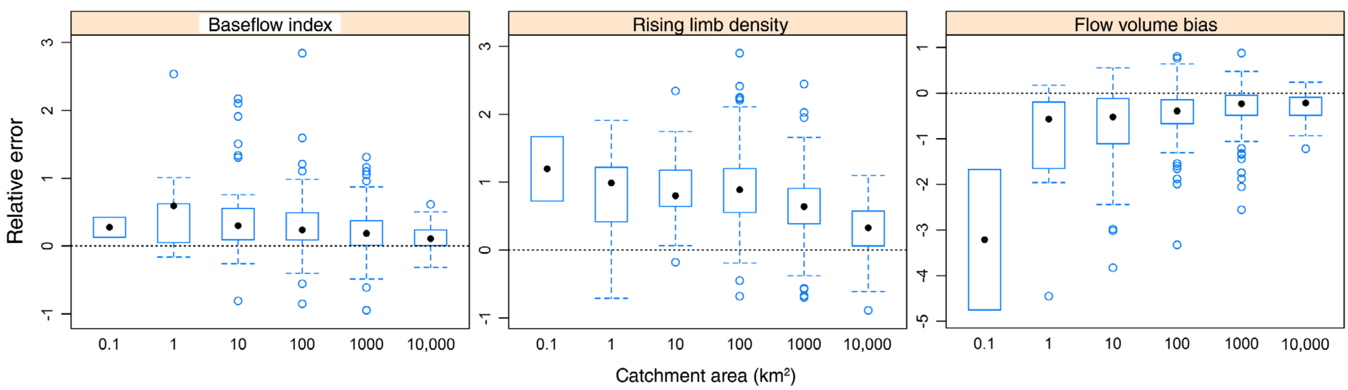

FIGURE 5 Model bias error when a national model is used to simulate three signatures (baseflow index, rising limb density, flow volume), using data from 485 watersheds in New Zealand. These graphs are used to test hypotheses about how model performance varies with watershed area. Bias in all three signatures is lower for large watersheds (Reprinted with permission from McMillan, Booker, et al. (2016). Copyright 2016 Elsevier)

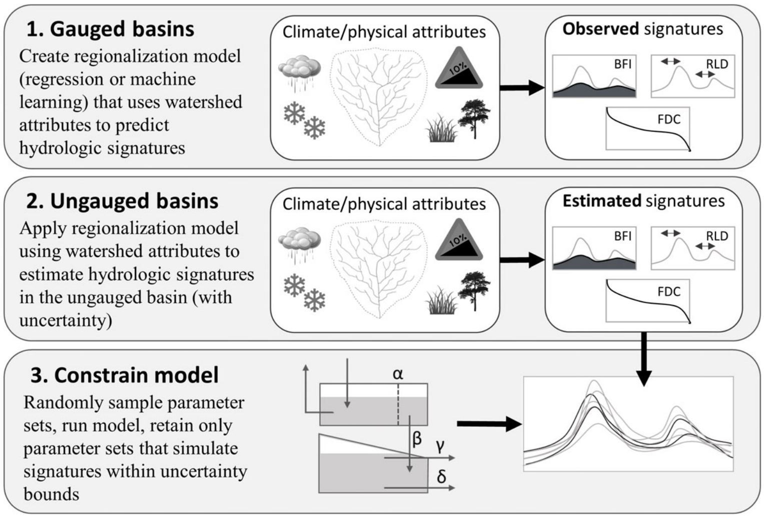

FIGURE 6 Schematic illustration of how hydrologic signatures are used in regionalization. Signatures are regionalized to an ungauged basin, and then those signatures are used to condition a hydrologic model for the ungauged basin

The method can be scaled up globally, both for the signature regionalization (Beck et al., 2013, 2015), and the model calibration (Yang et al., 2019), and is particularly valuable in locations lacking a dense network of streamflow gauges (Kapangaziwiri, Hughes, & Wagener, 2012; Ndzabandzaba & Hughes, 2017; Visessri & McIntyre, 2016). Where available, the regionalized signatures can be combined with local, expert knowledge of watershed dynamics (Bulygina, Ballard, McIntyre, O'Donnell, & Wheater, 2012; Kelleher, McGlynn, & Wagener, 2017) and previously regionalized signatures, for example, the soil infiltration curve number, or baseflow index predicted from soil types in the United Kingdom (Almeida, Vine, McIntyre, Wagener, & Buytaert, 2016). Overall, regionalization of signatures is a robust, generalizable tool for PUB (Zhang, Wagener, Reed, & Bhushan, 2008).

3 | METHODS IN USING HYDROLOGIC SIGNATURES

3.1 | Choosing signatures

So far, we have discussed generalized uses of hydrologic signatures. However, any application must choose which signatures to use. The choice of signatures is important to: (a) ensure individual signature accuracy and robustness; (b) create a complete and independent set of signatures; and (c) choose signatures relevant to the specific application. We will discuss each in turn.

Individual signature choice (a) plays a role because there are often multiple signatures that capture a given aspect of the flow regime. For example, several common signatures quantify the frequency and duration of high flow events, using different thresholds to define "high flow" based on flow quantiles, or multiples of the mean or median flow. There are often additional choices in the signature definition, such as the data timestep to use (Westerberg & McMillan, 2015). To assist signature choice, Shamir, Imam, Morin, Gupta, and Sorooshian (2005) recommend choosing signatures that are *consistent*, that is, produce similar values for different time periods, and *distinguishable*, that is, produce different values for watersheds with different hydrologic functioning. McMillan, Westerberg, and Branger (2016) extend these recommendations to five desirable signature properties, including low uncertainty, low sensitivity to measurement design and watershed scale, and ability to discriminate between different hydrologic responses. Schaefli (2016) adds that signatures used in model evaluation should have the *discriminatory power* to constrain the range of acceptable model parameters.

When choosing sets of signatures (b), the signatures should cover all required aspects of the watershed function, while limiting redundancy or overlap. Previous studies commonly select signatures to cover a range of flow behavior (Westerberg et al., 2016), range of timescales (Sawicz et al., 2014), or range of watershed functions (Yilmaz, Gupta, & Wagener, 2008); and may reuse previous sets of signatures (Coxon et al., 2014). A selection of 5–10 signatures to summarize the flow regime is typical (e.g., Euser et al., 2013). Redundancy can be avoided by calculating the correlation between signature values for a large set of watersheds, and selecting independent signatures with low correlations.

Principal component analysis (PCA) is often used to avoid the need for a priori selection of signatures out of a large potential set. PCA can identify combinations of signatures that explain a high proportion of variability between watersheds, while remaining relatively independent (Clausen & Biggs, 2000; Olden & Poff, 2003; Prieto et al., 2019). Avoiding or accounting for highly correlated signatures improves outcomes when conditioning models on the signature values (Almeida et al., 2016).

When selecting signatures for an application (c) the choice of signatures can impact the data analysis, modeling, or calibration outcomes. Preferred signatures may depend on location, and may need to be adapted when transferring between sites. For example, McMillan and Srinivasan (2015) adapt a signature describing runoff generation thresholds by adding the antecedent wetness condition as an extra predictor controlling runoff. In modeling, the best signatures to constrain the model predictions depend on the watershed characteristics (Coxon et al., 2014). Signatures describing the water balance constrained parameters more strongly in groundwater-dominated watersheds, while signatures describing timeseries dynamics and the flow duration curve constrained parameters more strongly in rainfall-driven watersheds. Choosing signatures that span the range of model function is important for calibration, for example choosing signatures based on the L'vovich partitioning framework can improve calibration results (Shafii et al., 2017).

3.2 | Scaling

A little-explored aspect of flow signatures is how their interpretation changes with scale, and how signature values aggregate or change along a river network. For example, when two tributaries meet, how do signature values in the downstream reach relate to the values in the tributaries? In general, hydrologic function shows complex scaling behavior: dominant processes often change with scale, and emergent behavior at watershed scales is not easily modeled as the accumulation of smaller-scale behavior (Blöschl, 2001). Signatures have the potential to identify scale-independent dynamics, for example they have been used to identify soil moisture dynamics that are consistent beyond the small scale of soil moisture sensors (Branger & McMillan, 2019). In ecology, flow signatures are used to group watersheds into scale-independent classes according to their dynamics, before developing within-class relationships between flow alteration and ecological responses (Kennard, Pusey, et al., 2010; Poff & Ward, 1989). However, signatures can sometimes be sensitive to scale, such as modeled future changes in signatures that depend on climate model scale (Maina, Siirila-Woodburn, & Vahmani, 2020; Mendoza et al., 2016).

There is limited information about whether relationships between flow signatures and watershed processes change with scale. Most of these relationships are derived from studies in small, experimental watersheds, and may not apply in large basins. Some signatures become less meaningful at larger scales where flow dynamics represent a mixture of upstream tributaries. For example, diurnal cycles in flow indicate snowmelt and evapotranspiration processes, but mixing out-of-phase cycles from different tributaries blurs the signal. Faster water velocities preserve in-phase fluctuations throughout the stream network to produce strong cycles, but slower water velocities in the late summer cause out-of-phase fluctuations and weaker cycles (Wondzell, Gooseff, & McGlynn, 2007).

Other processes show the same blurring of signature values with scale. At small scales, watershed aspect controls patterns of snowmelt and therefore creates differences in flow signatures, but these dynamics converge at larger scales as aspects average out (Comola et al., 2015). Similarly, when using isotopic signatures of water age, mean transit times tend to converge for larger watersheds that aggregate diverse upstream watersheds (Hrachowitz, Soulsby, Tetzlaff, & Speed, 2010). For one standard method to determine water age based on seasonal tracer cycles in precipitation and streamflow, aggregation is a greater concern as mixes of tributary waters of different ages do not return the correct mean value (Kirchner, 2016). However, using an alternative formulation for age calculation can reduce the aggregation bias (Danesh-Yazdi, Botter, & Foufoula-Georgiou, 2017).

In some cases, downstream changes in signature values successfully provide information on how processes change with scale. For example, where diurnal cycles are preserved downstream, cycles with peaks later in the day suggest that the snowline is higher or further upstream (Lundquist & Cayan, 2002). Instead of blurring at larger scales, some processes become more complex as multiple flow sources enter a river. For example, recessions become more nonlinear as hillslope-scale, watershed-scale and riparian aquifer flows are added downstream (Clark et al., 2009; Harman, Sivapalan, & Kumar, 2009). Alternatively, the extent of blurring may indicate how model structure should change with scale, for example as thresholds between antecedent wetness and runoff generation weaken at large scales (McMillan, 2012). In summary, caution is advised when using signatures to understand processes at very different scales to those for which the signatures were developed. There remains great scope to use well-instrumented watersheds to study how relationships between signatures and processes change with scale, and to use signatures to more accurately understand upstream processes.

3.3 | Uncertainties

Any signature calculated from hydrologic data is impacted by inherent data uncertainty. Sources of uncertainty in flow data occur in measurement techniques for individual gaugings, and in using those gaugings to create a stage-discharge rating curve (Kiang et al., 2018). Signatures using precipitation data are additionally subject to errors in interpolating that data to the watershed scale. All of the signature applications discussed in this paper—ecology and habitat assessment, process understanding, and modeling—are affected by signature uncertainty. Ignoring uncertainty can lead to biased model parameters, unreliable predictions, and poor management decisions (McMillan et al., 2017; McMillan, Westerberg, & Krueger, 2018; Renard, Kavetski, Kuczera, Thyer, & Franks, 2010). Therefore, to improve the reliability of these applications, uncertainty should be explicitly accounted for in the signature methods (Juston et al., 2012).

A general method for estimating uncertainty in a signature value is by using a Monte Carlo approach (Westerberg & McMillan, 2015). First identify the dominant sources of uncertainty in the underlying flow and/or rainfall data, perhaps by creating a perceptual model of uncertainty (Westerberg, Di Baldassarre, Beven, Coxon, & Krueger, 2017). Next, estimate the magnitude and distribution of each uncertainty component, using dedicated experiments or information from the literature. Repeatedly draw samples of each measurement (flow and/or precipitation) including uncertainty, and use the sample to calculate the signature. If there is no uncertainty information for the watershed, simulated measurement uncertainty (e.g., adding random errors or multiplicative bias to the flow) is a good alternative. Uncertainty magnitudes can be taken from the literature (e.g., McMillan, Krueger, & Freer, 2012), or from a watershed with similar gauge type and channel stability where uncertainties are known (e.g., choosing one or more watersheds from Westerberg et al., 2016 or Coxon et al., 2015, 2020). Using a large number of samples, aggregate the resulting signature values to find the estimated distribution of the signature: an example is shown in Figure 7, with signature uncertainties commonly exceeding ±20%. Mean and standard deviation of the signature can be calculated if needed. This process may in itself suggest methods for reducing the uncertainty. If extreme high flows are most uncertain due to out-of-bank events, then signatures might be adjusted to avoid those values, for example by adjusting the quantiles used to calculate the flow duration curve slope.

Beyond uncertainty in rainfall and flow data, signature uncertainty can occur due to a short flow record (Kennard, Mackay, Pusey, Olden, & Marsh, 2010), flow data that is only available at coarse temporal scales (Poff, 1996), and uncertainty in the precise method used to calculate the signature (Dralle, Karst, Charalampous, Veenstra, & Thompson, 2017). To estimate the signature uncertainty resulting from these factors, the flow time series can be split into (possible overlapping) subsamples and the signature calculated for each one to obtain a range or distribution of

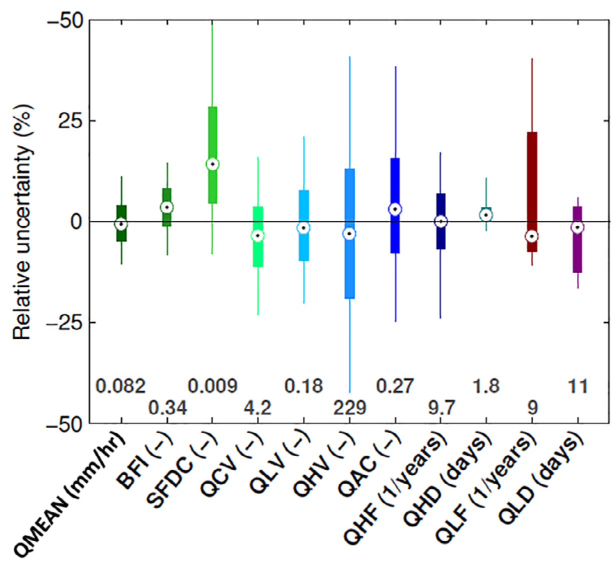

FIGURE 7 Relative uncertainty in 11 hydrologic signatures caused by uncertainty in the stage-discharge rating curve, for a watershed in New Zealand. The boxplot whiskers extend to the 5 and 95 percentiles, and the box covers the interquartile range. Signatures are as follows: BFI, base-flow index; QAC, flow autocorrelation; QCV, overall flow variability; QHD, high-flow event duration; QHF, high-flow event frequency; QHV, high-flow variability; QLD, low-flow event duration; QLF, low-flow event frequency; QLV, low-flow variability; QMEAN, mean flow; SFDC, slope of the normalized flow duration curve (Reprinted with permission from Westerberg and McMillan (2015). Copyright 2015 Copernicus Publications)

signature values (Schaefli, 2016; Vogel & Fennessey, 1994). A similar approach for data from multiple locations is to subsample the data in space (Blazkova & Beven, 2009).

Estimates of signature uncertainty should then be incorporated into signature applications. The applications discussed throughout this paper vary in their development of uncertainty methods. When using signatures to understand watershed processes, uncertainty has been recognized but not incorporated into our methods. Unquantified data uncertainty contributes to abrupt variations of signatures in space, and makes it harder to relate landscape characteristics with signature values (Addor et al., 2018). For eco-hydrologic assessment, uncertainty estimation has been incorporated into methods for detecting hydrologic change. Long streamflow records are needed to overcome natural variability and detect changes in the number and duration of exceedances of high- and low-flow thresholds: 40-years for high flow and 60-year for low flow (Huh, Dickey, Meador, & Ruhl, 2005). The perceptual model of uncertainty sources is important: treatment of streamflow errors as random versus non-random can make the difference as to whether deforestation-induced changes in a flow duration curve over time can be detected (Juston, Jansson, & Gustafsson, 2014).

In modeling, signature uncertainty methods are more fully developed. When signatures are used for model evaluation, a "limits of acceptability" approach is commonly used, where model runs are accepted if they simulate signature values within estimated uncertainty bounds (Blazkova & Beven, 2009). Model runs can be scored according to the size of model signature errors compared to the width of the uncertainty bounds (Westerberg, Sikorska-Senoner, Viviroli, Vis, & Seibert, 2020). In signature regionalization, uncertainty methods are common and were previously discussed in Section 2.3.3. Accounting for uncertainty avoids over-conditioning the regionalized model and produces more reliable results (Westerberg et al., 2016). When quantifying signature uncertainty for modeling applications, it is useful to check for unrealistic signature values. For example, unrealistic runoff ratio values may indicate errors in basin area or precipitation undercatch (Kauffeldt, Halldin, Rodhe, Xu, & Westerberg, 2013). These "disinformative" data periods should be removed to prevent corruption of the modeling process (Beven & Westerberg, 2011). Given the significant potential for data errors in large-sample datasets such as from the Global Runoff Data Centre, this signature-based check provides valuable error identification.

4 | SUMMARY AND CONCLUSIONS

Hydrologic signatures are metrics that extract and summarize the information contained in streamflow. They range from simple statistics of the flow series, to complex descriptors of flow dynamics that relate to watershed processes. Signatures are commonly categorized according to whether they describe the magnitude, timing, frequency, duration, or rate of change of flow.

This review described three main areas of application for hydrologic signatures:

1. *Ecohydrology, environmental flows and hydrologic alteration*. Signatures provide an easy way to summarize the flow regime of a river. The flow regime controls the suitability of instream habitat for different species, with flow extremes and flow variability being particularly important. Species requirements can be encoded as signatures that must lie in defined ranges. The signatures and ranges are determined by establishing relationships between signatures and species abundance across large numbers of sites. Using these relationships, changes in signatures over time describe how river environments have been altered, and how these changes impact freshwater species.
2. *Watershed processes*. Signature values are related to upstream watershed processes. By relating signatures to the occurrence and strength of different processes, we can transfer process knowledge between basins. Conversely, by relating watershed attributes to signature values via regression relationships, we can estimate flow regimes in ungauged basins. These regression relationships are strongest between climate-related attributes and signatures of mean and high flow magnitudes. Similarity in signature values is used to define clusters of hydrologically similar watersheds, that can share strategies for designing monitoring networks or models, and might react similarly to land use or climate change.
3. *Modeling*. Signatures are used as performance measures in calibration, to require models to reproduce components of flow dynamics that relate to watershed function. Multi-objective calibration against a range of signatures is typical. These calibration methods incorporate uncertainty by allowing for errors in the signature values. Signatures can be used to create hydrologic models for ungauged basins, by regionalizing signatures based on their relationship with watershed attributes, and then using the signatures for calibration. Signatures are used to design and test model

structure and complexity, which is particularly useful in global models where spatial differences in model structure may be necessary.

Extending from this wide range of signature applications, there remain multiple unsolved problems and avenues for development. In modeling, we lack thorough knowledge of the correspondences between model parameters and flow signatures, with therefore few examples where signature-domain calibration reduces the dimensionality of parameterization methods. It would be beneficial to design signatures with stronger relationships to watershed processes and model parameters, as current signatures typically relate to multiple processes. Overall, the ability to share and build on knowledge of signatures would be enhanced by greater consistency of signature choice between studies. Despite current limitations, new uses of signatures across different hydrologic data types and for data-rich applications in global modeling and machine learning, suggest an expanding role for signatures in hydrology.

CONFLICT OF INTEREST

The author has declared no conflicts of interest for this article.

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