ARTICLE IN PRESS

JGLR-00720; No. of pages: 15; 4C:

Journal of Great Lakes Research xxx (2014) xxx–xxx

Contents lists available at ScienceDirect

Journal of Great Lakes Research

journal homepage: www.elsevier.com/locate/jglr

Accommodating environmental thresholds and extreme events in hydrological models: A Bayesian approach

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ARTICLE INFO

Article history:
Received 14 June 2013
Accepted 12 February 2014
Available online xxxx

Communicated by Ram Yerubandi

Index words:
SWAT model
Bayesian inference
Uncertainty analysis
Extreme events
Runoff estimation
Hamilton Harbour

ABSTRACT

Extreme events appear to play an important role in pollutant export and the overall functioning of watershed systems. Because they are expected to increase in frequency as urbanization and recent climate change trends continue, the development of techniques that can effectively accommodate the behavior of watersheds during extreme events is one of the challenges of the contemporary modeling practice. In this regard, we present a Bayesian framework which postulates that the watershed response to precipitation occurs in distinct states. Precipitation depth above a certain threshold triggers an extreme state, which is characterized by a qualitatively different response of the watershed to precipitation. Our calibration framework allows us to identify these extreme states and to characterize the different watershed behavior by allowing parameter values to vary between states. We applied this framework to SWAT model implementations in two creeks in the Hamilton Harbour watershed of Redhill Creek, an urban catchment, and Grindstone Creek, an agricultural one. We found that our framework is able to coherently identify watershed states and state-specific parameters, with extreme states being characterized by a higher propensity for runoff generation. Our framework resulted in better model fit above the precipitation threshold, although there were not consistent improvements of model fit overall. We demonstrate that accommodating threshold-type of behavior may improve the use of models in locating critical source areas of non-point source pollution.

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Introduction

Hydrology has long been concerned with extreme events in the form of floods (Gumbel, 1954). Recent developments in the field have suggested that extreme events may play an important role in the overall functioning of watershed systems, despite their relatively low frequencies of occurrence (Macrae et al., 2007; Shields et al., 2008). In particular, extreme hydrological events have been found to significantly contribute to the overall export of nitrogen and phosphorus in agricultural (Macrae et al., 2007) as well as urban systems (Duan et al., 2012; Shields et al., 2008). There is evidence that both urbanization (Duan et al., 2012; Shields et al., 2008) and climate change (Kunkel et al., 2013) will make extreme hydrological and nutrient export events more common in the future.

Watershed modeling can play a key role in advancing our understanding of the likely effects of an increased frequency of extreme events on water quality (Rode et al., 2010). For instance, Michalak et al. (2013) used the Soil-Water Assessment Tool (*SWAT*) to estimate the unusually high nonpoint source soluble phosphorus inputs associated with the largest algal bloom in Lake Erie's history. However, continuous watershed models typically focus on the processes or variables responsible for the "average" system behavior. Due to their infrequency, extreme events and any processes (or dynamics) associated with them will usually not be considered in the model development process and are often relegated to the role of "outliers". This is perhaps why hydrological model parameter studies often find that the ideal parameter set for modeling high flow conditions is different from that used when modeling the entire range of flows (e.g., Cibin et al., 2010; Zhang et al., 2011). There is empirical evidence that this is not an artifact of mathematical models, but a genuine reflection of the thresholds which do in fact operate in hydrological systems at the hillslope and watershed scales. As mentioned previously, extreme events can represent a significant proportion of annual fluxes of water or materials out of a watershed and should be better considered by continuous models.

Empirical work in hydrology has found that extreme events can result from different flow mechanisms than more common events. McDonnell (1990), for instance, found that flow through the soil matrix was responsible for small runoff events, whereas macropore flow tended to be responsible for larger events. Subsequent empirical work has found that the initiation of macropore flow tended to occur when the soil was close to saturation (Zehe et al., 2001). While an explicit

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http://dx.doi.org/10.1016/j.jglr.2014.04.002
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Please cite this article as: Wellen, C., et al., Accommodating environmental thresholds and extreme events in hydrological models: A Bayesian approach, J Great Lakes Res (2014), http://dx.doi.org/10.1016/j.jglr.2014.04.002

introduction of this two-domain conceptualization of flow into numerical watershed models did prove to be feasible, doing so required prohibitively extensive field data (Zehe et al., 2001). Other environments, such as the Canadian Shield, are characterized by "fill-and-spill" mechanisms where certain cascading storages in bedrock depressions must be filled before the catchment as a whole is able to export significant water volumes (Ali et al., 2013; Oswald et al., 2011). In many watersheds of management interest, threshold behavior may be at work in differentiating the response to extreme precipitation events; yet, obtaining a detailed process understanding and explicitly representing this behavior in our mathematical models is typically not feasible. We are focused on such cases in this paper.

In a review of threshold behavior of hydrological systems, Zehe and Sivapalan (2009) identified two strategies for accommodating threshold behavior in watershed models. The first strategy is explicit through the model equations, as done, for instance, by Zehe et al. (2001) with their two-domain model of soil water movement. The second, less commonly pursued, strategy is to assume that, as we do here, the system operates in multiple states or modes of behavior, the identification of which is a component of the model calibration process. Our novel contribution to the study of extreme events in watershed modeling is an example of this second strategy. We posit that extreme events may be modeled as a different response of a system to precipitation inputs above a threshold. That is, the system may be thought of as having distinct states of response to precipitation. This approach to extreme events is in agreement with empirical and theoretical developments in the field (Ali et al., 2013; Zehe and Sivapalan, 2009; Zehe et al., 2001).

Bayesian inference provides an approach to model calibration, which is uniquely suited to the problem of identification of latent states (Gelman et al., 2004; Prado and West, 2010). Applications of Bayesian inference techniques to accommodate different states of a watershed system have typically focused on one of two techniques: mixture likelihoods and time varying parameters. Employing mixture likelihood explicitly accounts for multiple watershed states by assuming the model residuals represent different populations with different statistical properties. Yang et al. (2007a), for instance, showed that the residuals from (pre-specified) dry and wet seasons have distinct variances and temporal correlation patterns, while Schaefli et al. (2007) showed that the class membership of particular residuals could be identified as part of the model training exercise. The main advantage of mixture likelihoods is to essentially weight different residuals more or less strongly, which serves to quantitatively express an expectation that the model would not perform consistently well throughout its temporal domain, e.g., we expect that a model would not reproduce the high flow periods as closely as the baseflow conditions (Yang et al., 2007a). In doing so, we avoid both biasing the model calibration in favor of the more uncertain states of the system and overestimating the residual variance of the states which are characterized by lower uncertainty.

While useful and statistically coherent, mixture likelihoods do not allow us to accommodate the different processes, which may be operating in the different members of the mixture of the residuals. In fact, Schaefli et al. (2007) found that the use of a mixture likelihood led to a higher residual variance for large events. This would serve to decrease the impact of these events on the overall likelihood function value, leading to a model calibration which would tolerate very large residuals during the extreme events instead of reducing them, precisely the opposite of what we here aim to do. A second strategy to accommodate extreme events is to allow the model parameters to vary in time. This type of approach has mainly opted for a continuous evolution of parameter values through time, either in a manner analogous to the Kalman filter (Kalman, 1960), where parameter values are adjusted at each time step to allow a better correspondence of the model and the data, or with a type of random walk, where parameter values may change significantly at each time step. Such approaches may be stationary (Reichert and Mieleitner, 2009) or non-stationary (Lin and Beck, 2007). While suitable for tracking gradual changes in watershed functioning, such approaches may not sensibly identify a number of distinct states of watershed functioning; especially, if we consider that using different parameters for every time step likely results in an over-parameterization of the model.

In this study, we take a state-specific approach, founded upon a multivariate Bayesian approach, which effectively balances the need to relax rigid model structures but does not introduce the complexity typically entailed by continuous parameter evolution in time (Arhonditsis et al., 2008a,b; Wellen et al., 2012). We discuss the mathematical details of our approach in the methodology section, but we essentially posit that a threshold of precipitation exists above which the watershed is characterized by different parameter values relative to those used to parameterize the model below the threshold. However, the values of a particular parameter are not independent between the two watershed states or modes of behavior but are characterized by a covariance structure to be identified during model calibration. Finally, we critically discuss the prospect of the present methodological framework to offer an effective means for reproducing watershed dynamics during extreme events.

Methodology

Incorporating threshold behavior in model parameter estimation

We may think of a deterministic hydrological model as a function, which connects a time series of environmental inputs with a time series of streamflow outputs:

$$Y = f(\gamma, \theta) \tag{1}$$

where Y indicates the time series of model predictions (e.g., streamflow, chloride concentration), f indicates the model, γ indicates the various time series of environmental inputs (e.g., precipitation, temperature, wind speed, crop rotations), and θ indicates the vector of model parameters. Because both the watershed model and the measurements from the system are subject to substantial uncertainty, we typically introduce a term to describe their mismatch, and so we re-write Eq. (1) as:

$$Y = f(\gamma, \theta) + \varepsilon, \tag{2}$$

where ε indicates the time series of model residuals, defined as the difference between measurements and model predictions. The statistical treatment of the ε time series has been the subject of considerable work in hydrology — the emerging consensus is that it is typically autocorrelated and non-Gaussian (Schoups and Vrugt, 2010; Sorooshian and Dracup, 1980; Yang et al., 2007b). The error characterization can guide us in drawing statistically sound inference, and the mismatch of model predictions and system measurements is mainly due to the simplifications employed when constructing models of highly complex natural systems, such as watersheds. Thus, reducing the model structural error, a significant component of the ε time series, requires creating better models. While ultimately better models must be arrived at by using systems of equations which more accurately represent the environmental system in question, we contend that a significant step in this direction can be made by relaxing the assumptions made by the inference procedure. Namely, we relax the assumption that the vector of model parameters (θ) is constant for all time steps.

Frameworks for relaxing this assumption have been proposed before, but all of them tend to favor either the replacement of a subset of the parameter vector θ with a stochastic process in time (e.g., Reichert and Mieleitner, 2009; Wellen et al., 2012) or the relaxation of a subset of the parameter vector θ to evolve in time (e.g., Lin and Beck, 2007). We here postulate that rather than a gradual evolution or a continuum of system responses to climate forcing, watersheds can be thought of as characterized by multiple discrete states of response. We take an approach philosophically similar to a class of models called Markov-

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