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A new approach to simulating stream isotope dynamics using Markov switching autoregressive models

Christian Birkel [a,*], Roberta Paroli [b], Luigi Spezia [c], Sarah M. Dunn [d], Doerthe Tetzlaff [a], Chris Soulsby [a]

[a] Northern Rivers Institute, School of Geosciences, University of Aberdeen, Aberdeen, United Kingdom
[b] Dipartimento di Scienze Statistiche, Università Cattolica SC, Milano, Italy
[c] Biomathematics & Statistics Scotland, Aberdeen, United Kingdom
[d] James Hutton Institute, Aberdeen, United Kingdom

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ABSTRACT

In this study we applied Markov switching autoregressive models (MSARMs) as a proof-of-concept to analyze the temporal dynamics and statistical characteristics of the time series of two conservative water isotopes, deuterium (δ^2H) and oxygen-18 ($\delta^{18}O$), in daily stream water samples over two years in a small catchment in eastern Scotland. MSARMs enabled us to explicitly account for the identified non-linear, non-Normal and non-stationary isotope dynamics of both time series. The hidden states of the Markov chain could also be associated with meteorological and hydrological drivers identifying the short (event) and longer-term (inter-event) transport mechanisms for both isotopes. Inference was based on the Bayesian approach performed through Markov Chain Monte Carlo algorithms, which also allowed us to deal with a high rate of missing values (17%). Although it is usually assumed that both isotopes are conservative and exhibit similar dynamics, $\delta^{18}O$ showed somewhat different time series characteristics. Both isotopes were best modelled with two hidden states, but $\delta^{18}O$ demanded autoregressions of the first order, whereas δ^2H of the second. Moreover, both the dynamics of observations and the hidden states of the two isotopes were explained by two different sets of covariates. Consequently use of the two tracers for transit time modelling and hydrograph separation may result in different interpretations on the functioning of a catchment system.

1. Introduction

Conservative tracers of streamflow sources and temporal dynamics have been widely used in hydrology to characterize catchment systems and their integrated process dynamics. Isotopic tracers in particular have provided revolutionary insights into the mechanisms of water movement, storage and mixing in the translation of precipitation to runoff [1,2]. In the era of novel laser spectroscopy, long-term and high-resolution (daily and sub-daily) time series of both deuterium (δ^2H) and oxygen-18 ($\delta^{18}O$) as stable water isotopes can provide insights into both the rapid mobilization and slower long-term release (up to around 4 years of mean transit time) of solutes at the catchment scale, aiding applied management issues such as estimation of clean-up times for diffuse pollution [3,4]. Traditionally, stable isotope tracers have been used to estimate the parameters of travel time distributions and resulting water age by applying lumped, time-invariant convolution methods to either deuterium or oxygen-18 time series [5,6]. More recently, isotope tracers have been directly incorporated into lumped, conceptual rainfall-runoff models used to help in model identification and evaluation through testing of hypotheses of the dominant transport and mixing processes [7,8].

Despite the merits of these approaches, a range of issues such as unknown boundary conditions of catchments, parameterization uncertainties and scaling effects have been found to make process representation surprisingly difficult, given the over-simplified assumptions needed when translating a perceptual model into a conceptual rainfall-runoff model [9,10]. However, catchment systems can also be examined as complex stochastic systems that may exhibit non-Normal, non-linear and non-stationary rainfall-runoff and solute dynamics. It is increasingly recognized that rainfall-runoff and tracer dynamics exhibit heavy-tailed and/or multimodal distributions (e.g. discharge data). These dynamics also present asymmetric cycles or hysteresis in the sequence of data (e.g. storm flow) which decrease at a rate different from that they increase (e.g. [11,12]). Finally they appear with non-constant mean and/or variance for all times (non-stationarity). Non-stationary solute transport has been theoretically and experimentally identified by e.g. McGuire et al. [13], Hrachowitz et al. [14] and Rinaldo et al. [15]. This reflects the influence of short and long-term environmental variability [16]. It remains an open question as to how

* Corresponding author.
E-mail address: c.birkel@abdn.ac.uk (C. Birkel).

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best tackle such complex natural systems in a suitable model framework.

In this study, we adopt a novel approach to analyzing stream isotope dynamics. This follows recommendations by Sivapalan et al. [10] to utilize the characteristics of measured time series data as means of inferring system characteristics (e.g. non-linearity) and process dynamics (e.g. short and long-term, wet and dry, etc.). The class of Markov Switching Autoregressive Models (MSARMs) provide a useful and versatile tool to analyze complex time series which can capture features that produce non-Normality, non-linearity, and non-stationarity. MSARMs utilize pairs of stochastic processes, one observed and one unobserved, or hidden. We model the unobserved process as a finite state Markov chain and assume that the observed process, given the hidden Markov chain, is conditionally autoregressive, which means that the current observation depends on its recent past. MSARMs are widely used within the econometric community following seminal work by Hamilton [17–19], but they are rarely exploited elsewhere. We are aware of just two papers using MSARMs in hydrology, which were applied to streamflow forecasting: Lu and Berliner [20] and Gelati et al. [21]. MSARMs have many similarities with Normal Hidden Markov Models (NHMMs), which are more widely applied in hydrology to precipitation and streamflow forecasting, and more recently to water quality data [22–25]. The critical difference is that NHMMs do not account for the conditional autoregressive process what indicates a potential memory affecting the system.

In this paper we use MSARMs to analyze the temporal characteristics of two stream isotope time series, δ^2H and $\delta^{18}O$, recorded at daily intervals for two years in a small catchment in eastern Scotland. We present a fully Bayesian analysis based on Markov Chain Monte Carlo (MCMC) algorithms for model selection. Hereby, the autoregressive order and the dimension of the hidden Markov chain state-space are selected by a Bayesian model choice technique. Then identifiability constraint specification, variable selection, and parameter estimation follow. Missing values are also restored by the MCMC sampler [26]. The hidden states of the Markov chain represent unobserved levels of variability in the observed process that result from complex interactions of meteorological and hydrological conditions. The hidden Markov chain is non-homogeneous and the transition probabilities are modelled via logit functions of some covariates. Additional meteorological and hydrological time series are also used as covariates to the autoregressive structure of the model along with a yearly periodic component to identify seasonal components in the isotope time series. Even though the memory retained by the chemical composition of streamflows from past chemical disturbances is long-lasting (e.g. expressed by the long tail of travel time distribution models [27]), we considered contemporary covariates for model selection only. This is due to the fact that MSARMs are able to represent stochastic, non-linear and non-stationary changes in process dynamics (e.g. short and long-term, wet and dry, etc.), described by the Markov switching between various hidden states. This may ultimately provide a useful alternative to describe long

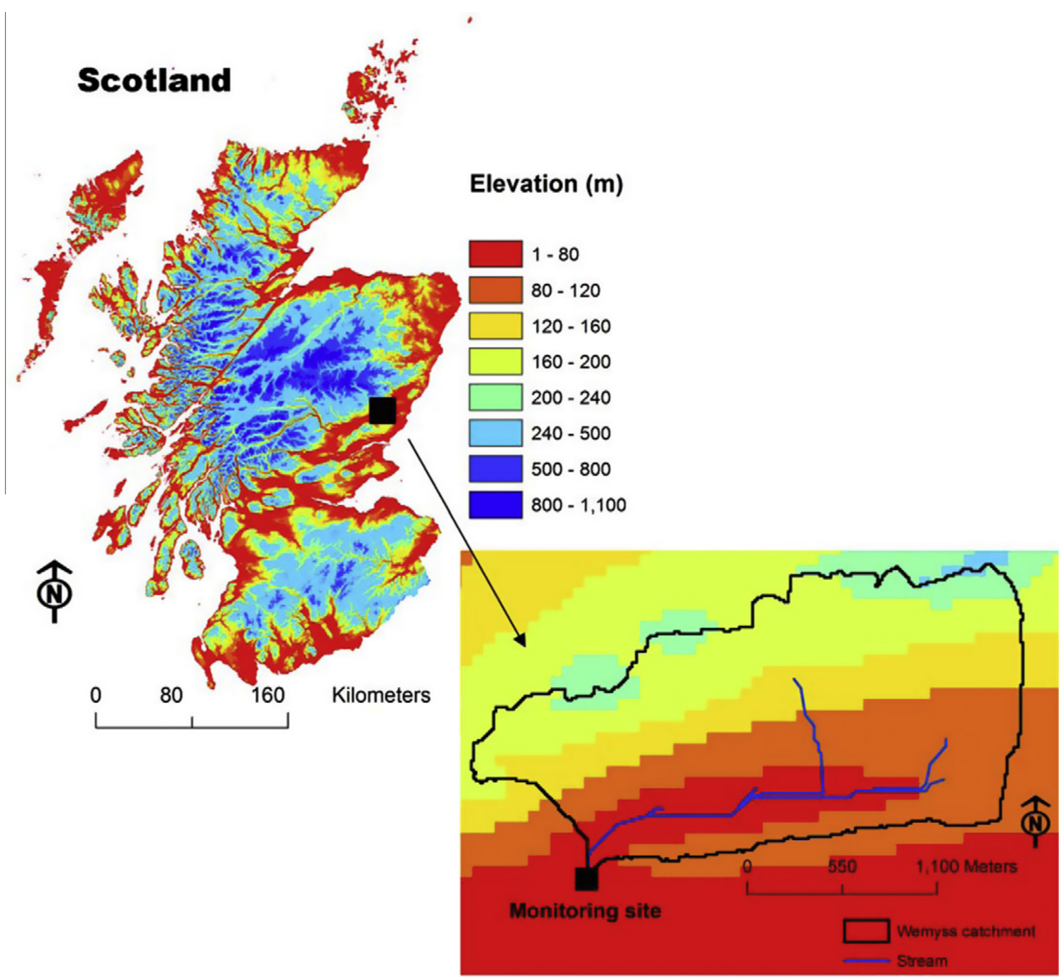

Fig. 1. Location and elevation of the Wemyss study catchment in eastern Scotland.