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Research paper

Water Residence Time estimation by 1D deconvolution in the form of a l_2-regularized inverse problem with smoothness, positivity and causality constraints

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ABSTRACT

The Water Residence Time distribution is the equivalent of the impulse response of a linear system allowing the propagation of water through a medium, e.g. the propagation of rain water from the top of the mountain towards the aquifers. We consider the output aquifer levels as the convolution between the input rain levels and the Water Residence Time, starting with an initial aquifer base level. The estimation of Water Residence Time is important for a better understanding of hydro-bio-geochemical processes and mixing properties of wetlands used as filters in ecological applications, as well as protecting fresh water sources for wells from pollutants. Common methods of estimating the Water Residence Time focus on cross-correlation, parameter fitting and non-parametric deconvolution methods. Here we propose a 1D full-deconvolution, regularized, non-parametric inverse problem algorithm that enforces smoothness and uses constraints of causality and positivity to estimate the Water Residence Time curve. Compared to Bayesian non-parametric deconvolution approaches, it has a fast runtime per test case; compared to the popular and fast cross-correlation method, it produces a more precise Water Residence Time curve even in the case of noisy measurements. The algorithm needs only one regularization parameter to balance between smoothness of the Water Residence Time and accuracy of the reconstruction. We propose an approach on how to automatically find a suitable value of the regularization parameter from the input data only. Tests on real data illustrate the potential of this method to analyze hydrological datasets.

1. Introduction

The hydrological *Water Residence Time distribution* (named in this article simply as residence time) is a measure allowing the analysis of the transit of water through a given medium. Its estimation is necessary when using wetlands as a natural treatment plant for pollutants that are already in the water Werner and Kadlec (2000), to better manage and protect drinking water sources from pollution Cirpka et al. (2007), to study the water transport of dissolved nutrients Gooseff et al. (2011). For a more comprehensive application range, including deciphering hydro-bio-geochemical processes or river monitoring, the review done in McGuire and McDonnell (2006) is a useful starting point. We call here the residence time the linear response of the aquifer system. In this context it refers to wave propagation of the water dynamics, not to the actual molecular travel time Botter et al. (2011).

To obtain the residence time, one can distinguish two families of methods: active and passive. The active methods are carried out by releasing tracers at the entrance of the system at a given time, like artificial dyes, and then by tracing the curve while measuring the tracer levels at the exit of the system Dzikowski and Delay (1992); Werner and Kadlec (2000); Payn et al. (2008); Robinson et al. (2010). Although robust, this methodology involves high effort and high operational costs. It could also perturb the water channel and this may lead to biased results. The passive methodology consists of recording data at the inlet and outlet of the water channel by specific water isotopes McGuire and McDonnell (2006), water electrical conductivity Cirpka et al. (2007) or by simply recording the rainfall levels at high altitude grounds and the aquifer levels at the base Delbart et al. (2014). In the passive case, the residence time is not measured directly but must be retrieved by deconvolution. Some authors also use deconvolution in the active methodology when the release of tracer cannot be considered as instantaneous McGuire and McDonnell (2006); Cirpka et al. (2007); Payn

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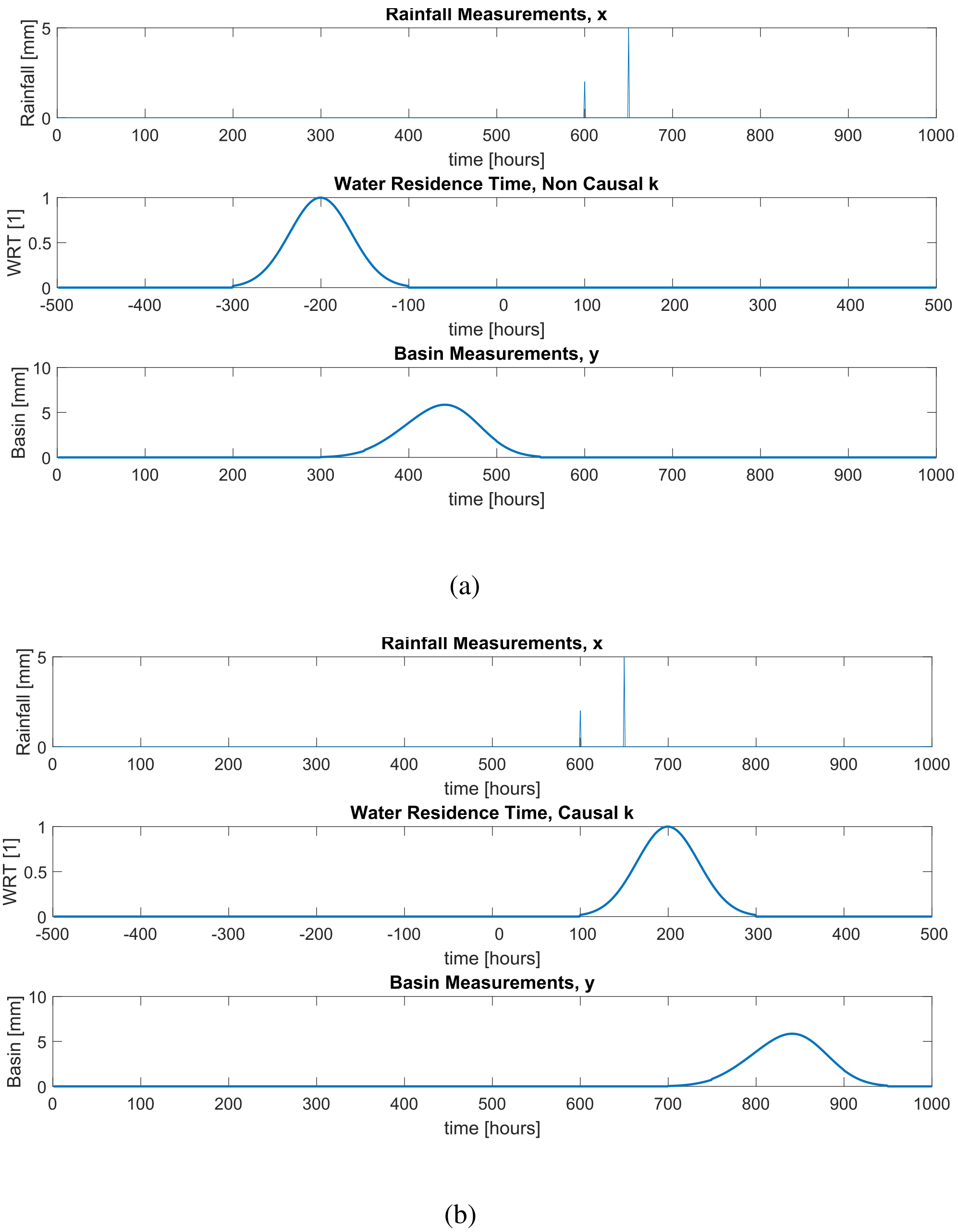

Fig. 1. Enforcing causality while doing the convolution in the Fourier Domain needs to include the negative time domain interval of the residence time.

et al. (2008). The residence time can then be approximated as the impulse response of the system and this in turn can be estimated by deconvolution Neuman et al. (1982); Skaggs et al. (1998); Fienen et al. (2006). The method can also be used for enhancing geophysical models, although not targeted explicitly for Water Residence Time estimation Zuo and Hu (2012). Deconvolution methods can be parametric Neuman and De Marsily (1976); Long and Derickson (1999); Etcheverry and Perrochet (2000); Werner and Kadlec (2000); Luo et al. (2006); McGuire and McDonnell (2006) or non-parametric Neuman et al. (1982); Dietrich and Chapman (1993); Skaggs et al. (1998); Michalak and Kitanidis (2003); Cirpka et al. (2007); Fienen et al. (2008); Gooseff et al. (2011); Delbart et al. (2014).

Parametric methodology has the advantage of always providing a result with expected properties such as correct shape and positiveness but with the caveat of being insensitive to unexpected results for real data (for instance a second peak in the residence time). The non-parametric deconvolution has the advantage of being ”blind”, meaning that no strong *a priori* are being set on the estimated curve, but in the absence of adapted mathematical constraints, the results may not reflect the physics of the residence time curve (these are sometimes negative or non-causal).

Our method is non-parametric and takes into account limitations of previous methods from the same category: variable-sized rainfall time series as input compared to Neuman et al. (1982), a more compact direct model formulation than in Neuman et al. (1982); Cirpka et al. (2007), less computational effort and less time consuming than for a Bayesian Monte-Carlo inverse problem methodology Fienen et al. (2006, 2008), strictly using a passive method with respect to mixed methods like the ones in Gooseff et al. (2011). In contrast to the cross-correlation Vogt et al. (2010); Delbart et al. (2014) we avoid the unrealistic hypothesis that the rain signal can be considered as white noise. In fact, rainfall datasets have long range memory properties and therefore we simulate the input rainfall for synthetic tests as a multifractal signal Tessier et al. (1996). One important difference from other non-parametric deconvolution methods is that we enforce causality explicitly through projection.