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Contaminant source reconstruction by empirical Bayes and Akaike's Bayesian Information Criterion

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ABSTRACT

The objective of the paper is to present an empirical Bayesian method combined with Akaike's Bayesian Information Criterion (ABIC) to estimate the contaminant release history of a source in groundwater starting from few concentration measurements in space and/or in time. From the Bayesian point of view, the ABIC considers prior information on the unknown function, such as the prior distribution (assumed Gaussian) and the covariance function. The unknown statistical quantities, such as the noise variance and the covariance function parameters, are computed through the process; moreover the method quantifies also the estimation error through the confidence intervals. The methodology was successfully tested on three test cases: the classic Skaggs and Kabala release function, three sharp releases (both cases regard the transport in a one-dimensional homogenous medium) and data collected from laboratory equipment that consists of a two-dimensional homogeneous unconfined aquifer. The performances of the method were tested with two different covariance functions (Gaussian and exponential) and also with large measurement error. The obtained results were discussed and compared to the geostatistical approach of Kitanidis (1995).

1. Introduction

Contaminant release history identification has received considerable attention in the literature over the past several decades. Although a number of reasonable approaches have been developed during this time no panacea has yet emerged. This is in part due to its ill-posed nature, and frequently, either the data stream is of insufficient length, contains missing data points, or is inaccurate. The reader is referred to Atmadja and Bagtzoglou (2001); Michalak and Kitanidis (2004); Sun et al. (2006) or Cupola et al. (2015) for extensive reviews of this specific problem in groundwater hydrology.

Interest in this area continues because it is a good representative of an inverse problem in hydrology. Since mathematical inversion is a cornerstone-problem in geophysics, the impact of any successful works will be high. Inverse theory, in its truest sense, is different from standard parameter estimation problems in statistics in that the unknowns sought are functions and not a small set of numbers (Parker, 1977; Tarantola, 1987; Ulrych and Sacchi, 2005). This means that in principle, there is an infinite number of variables sought. A variety of approaches exist and there are two main avenues to take. One of these deals with the ideal case of an infinite amount of exact data and the unknowns sought are continuous functions. For example, a Fourier transform and its inverse. This is the realm of the applied mathematician and these approaches tend to be analytic or quasi-analytic in nature. Analytic techniques are sensitive to the way data are collected

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and to noise present. Nevertheless these approaches are useful for their results concerning uniqueness, stability and so on (see also Tarantola, 2005, Ch 5, functional space inversion). The other main avenue relates to the practical problems encountered in the geophysical sciences where the model is "parameterized" into a finite set of parameters and involves the collection of incomplete and noisy data. One could on purpose propose a small number of structures such that more data than unknowns are present. It is in this area where the vast majority of efforts in groundwater are concentrated and a variety of approaches are possible. The more computationally demanding, and perhaps interesting problems are those in which the parameterization is done so that a high degree of resolution is possible, if one is willing to tolerate the ambiguity of the result (e.g. Woodbury and Ulrych, 2000; Painter et al., 2007). Stability in the presence of noise is always an issue, as is uniqueness which is difficult to prove. The technique that permits unique and stable inverse solutions by introducing prior information is called regularization. The widely used Levenberg–Marquardt method imposes "smoothness" to the model. This is essentially the basis for the well known PEST wrap-around code. In fact, Tikhonov showed that once an ill-posed problem becomes properly regularized it becomes stable. For these reasons, parameterized inverse problems are stabilized by weighting with error terms and are regularized to achieve some measure of uniqueness under one norm, or a variety of norms. The validity of the regularization terms becomes apparent, and perhaps justified when the inverse problem is approached from Bayesian or maximum entropy perspectives (Ulrych and Sacchi, 2005).

Specifically, in our review of the literature on this subject (see the above references) suggests that improvements are needed in terms of a reliable procedure, one that is easy to implement, with only few hyperparameters to estimate, and is able to evaluate confidence intervals. For these reason the purpose of this work is to propose an empirical Bayesian approach combined to the Akaike's Bayesian Information Criterion (ABIC) to estimate the contaminant release history, and to demonstrate its effectiveness.

This work estimates the temporal contaminant release history of a point source with the following simplifying assumptions: the solute is conservative, it is a 1-D or 2-D problem, the source location is known, the flow is uniform and steady, and the transport parameters are known at each point of the domain. These assumptions are necessary for the development and testing of the current methodology. Further, the release concentration is uncertain and its probability density function is assumed multivariate Gaussian. Specifically, we adopt a probabilistic approach to the inversion, assume a Gaussian likelihood and Gaussian prior to the problem, and seek the solution that minimizes Akaike's Bayesian Information Criterion, the ABIC. We propose an important extension to the algorithm that constrains solutions to only positive models and we test the method out on three test cases: the classic Skaggs and Kabala (1994) source, a "midnight dump" example that consists of three delta-like sources and lastly a laboratory experimental dataset, consisting of two measurement points spatially but with synoptic observations, obtained from a laboratory equipment, that reproduces the response of a 2-D unconfined aquifer.

2. Theory

2.1. Contaminant transport in groundwater

The following Eq. (1) describes the transport process in an aquifer reacting to the injection of a non-sorbing, non-reactive solute at a point source (Bear and Verruijt, 1987):

$$\frac{\partial(\varphi C(\mathbf{x},t))}{\partial t} = \nabla\cdot[\varphi\mathbf{D}(\mathbf{x})\nabla C(\mathbf{x},t)] - \nabla\cdot[\varphi\mathbf{u}(\mathbf{x},t)C(\mathbf{x},t)] + m(\mathbf{x}_0,t)\delta(\mathbf{x}-\mathbf{x}_0) \qquad (1)$$

where: φ [−] is the effective porosity, $\mathbf{u}(\mathbf{x},t)$ [LT^{-1}] is the effective velocity at location $\mathbf{x}$ and time t [T], $\mathbf{D}(\mathbf{x})$ [L^2T^{-1}] is the dispersion tensor, $C(\mathbf{x},t)$ [ML^{-3}] is the concentration, $m(\mathbf{x_0},t) = c_{in}(t)\cdot q_{in}(\mathbf{x_0},t)$ [MT^{-1}] is the amount of pollutant per unit time injected into the aquifer through the source located at $\mathbf{x_0}$, $c_{in}(t)$ [ML^{-3}] is the concentration of the released contaminant at time t and $q_{in}(\mathbf{x_0},t)$ [L^3T^{-1}] is the injection flow rate.

Eq. (1), considering uniform porosity, can be rewritten as:

$$\varphi\frac{\partial C(\mathbf{x},t)}{\partial t} = \nabla\cdot[\varphi\mathbf{D}(\mathbf{x})\nabla C(\mathbf{x},t)] - \nabla\cdot[\varphi\mathbf{u}(\mathbf{x},t)C(\mathbf{x},t)] + m(\mathbf{x}_0,t)\delta(\mathbf{x}-\mathbf{x}_0). \qquad (2)$$

The solution of Eq. (2) when associated with the initial and boundary conditions: $C(\mathbf{x},0) = 0$; $C(\infty,t) = 0$, is given by the convolution integral:

$$C(\mathbf{x},t) = \int_0^t m(\mathbf{x}_0,\tau)g(\mathbf{x},t-\tau)d\tau \qquad (3)$$

where $g(\mathbf{x},t-\tau)$ [L^{-3}] is the Kernel function that describes the effects at $\mathbf{x}$ at time t [T] by an impulse injection occurring at $\mathbf{x_0}$ at time τ.

Under simple flow conditions (such as homogeneous, isotropic, absence of withdrawal or recharge) the Kernel functions can be determined analytically, for instance for 1-D flow

$$g(x,t-\tau) = \frac{x}{2\sqrt{\pi D(t-\tau)^3}}\exp\left[-\frac{(x-v(t-\tau))^2}{4D(t-\tau)}\right]. \qquad (4)$$

In non-uniform flow field it is necessary to employ numerical approaches, such as the Stepwise Input Function procedure methodology developed by Butera et al. (2006, 2013), that is a numerical strategy for Kernel functions calculation. The time derivative of Eq. (3), considering a constant and known input function $m(\mathbf{x}_0,t) = F_0\cdot H(t)$, where $H(t)$ [−] is the Heaviside step function and $F_0 = c_0\cdot q_{in}(\mathbf{x_0},t)$ [MT^{-1}] is the amount of pollutant per unit time injected into the aquifer with constant and known concentration c_0, results in:

$$g(\mathbf{x},t) = \frac{1}{F_0}\frac{\partial C(\mathbf{x},t)}{\partial t} = \frac{1}{c_0 q_{in}(\mathbf{x}_0,t)}\frac{\partial C(\mathbf{x},t)}{\partial t} \quad t>0. \qquad (5)$$

Eq. (5) shows that it is possible to compute the Kernel functions at a generic point $\mathbf{x}$ by processing the concentration history (breakthrough curve) at the same location due to a