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Advances in Water Resources 29 (2006) 719–734
Advances in Water Resources
www.elsevier.com/locate/advwatres

Calibration framework for a Kalman filter applied to a groundwater model

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Received 27 April 2004; received in revised form 22 February 2005; accepted 7 July 2005
Available online 29 August 2005

Abstract

The paper presents a novel approach to the setup of a Kalman filter by using an automatic calibration framework for estimation of the covariance matrices. The calibration consists of two sequential steps: (1) Automatic calibration of a set of covariance parameters to optimize the performance of the system and (2) adjustment of the model and observation variance to provide an uncertainty analysis relying on the data instead of ad-hoc covariance values. The method is applied to a twin-test experiment with a groundwater model and a colored noise Kalman filter. The filter is implemented in an ensemble framework. It is demonstrated that lattice sampling is preferable to the usual Monte Carlo simulation because its ability to preserve the theoretical mean reduces the size of the ensemble needed. The resulting Kalman filter proves to be efficient in correcting dynamic error and bias over the whole domain studied. The uncertainty analysis provides a reliable estimate of the error in the neighborhood of assimilation points but the simplicity of the covariance models leads to underestimation of the errors far from assimilation points.

Keywords: Groundwater; Automatic calibration; Ensemble Kalman filter; Uncertainty estimation; Bias; Latin hypercube sampling

1. Introduction

Groundwater modeling faces the problem of modeling an invisible asset. There are generally few locations where observations are available, and the geological structure of the aquifer is only partially known. Even though groundwater models manage to reproduce the dynamics of the variation of the piezometric heads, they tend to be biased. To circumvent this, it is possible to include the additional information contained in the observations by using data assimilation. Kalman filtering is the most popular approach to data assimilation in hydrological modelling because of its simplicity of implementation and the development of a number of suboptimal schemes that can be used to deal with high dimensional systems (see for example [22,25,1,2] and a literature review [7]).

In most Kalman filter applications, the covariance matrices that define the model and the observations uncertainties are chosen arbitrarily, either to provide a correction that does not drive the model to instability, or according to rules. A more advanced approach is proposed by Van Geer et al. [24]. They parameterize the covariance matrices and include the parameters to the list of model parameters that have to be calibrated. One of their calibration objectives includes an accurate model uncertainty estimate based on statistical analysis of the innovation. Following the same philosophy, Dee [4] uses adaptive estimation of the covariance parameters to make the covariance matrices vary with the statistical properties of the problem.

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doi:10.1016/j.advwatres.2005.07.007

In this paper, we provide a novel approach to Kalman filter setup and calibration that not only improves the model performance in the root mean square error sense but also provides an uncertainty estimate that is coherent with the observed errors over the domain studied. Given a model setup, we parameterize the covariance matrices and calibrate the parameters in two steps:

- A calibration of the expected value of the state of the system, where the main objective is to improve the match between the model and the observations without overfitting at the assimilation points.
- A calibration of the covariance matrices that fits the estimated uncertainty to the observed errors.

This method is applied to an ensemble implementation of the colored noise Kalman filter (ColKF) [5] that uses lattice sampling instead of the traditional Monte Carlo sampling. It is tested on an artificial setup of a groundwater model.

Section 2 describes the Kalman filter implementation used in this paper. Section 3 presents the setup of the numerical experiments. Section 4 compares different sampling techniques and implementations for the ensemble approach. Section 5 describes the automatic calibration algorithm and the multi-objective approach. Section 6 presents the results of the proposed calibration procedure on the groundwater model setup.

2. Colored noise Kalman filter (ColKF)

We provide here a summary of the colored noise Kalman filter method that can be used to correct biased model forecast. For more details, refer to [5].

In the rest of the paper, n denotes the number of variables in a state vector and q the number of observations. It is also assumed that the observations are unbiased, so that the model bias is equal to the bias between the model and the observations.

2.1. Filter derivation

The colored noise Kalman filter uses an autoregressive model of order 1 (AR1) to describe the model noise. For a linear system, the stochastic model propagation equation is written as follows:

$$\begin{bmatrix} \mathbf{x}_k \\ \boldsymbol{\eta}_k \end{bmatrix} = \begin{bmatrix} \mathbf{M}_k & -\mathbf{I} \\ \mathbf{0} & \boldsymbol{\Lambda}_k \end{bmatrix} \begin{bmatrix} \mathbf{x}_{k-1} \\ \boldsymbol{\eta}_{k-1} \end{bmatrix} + \begin{bmatrix} \mathbf{B}_k\mathbf{u}_k \\ \mathbf{0} \end{bmatrix} + \begin{bmatrix} \boldsymbol{\mu}'_k \\ \boldsymbol{\mu}_k \end{bmatrix} \tag{1}$$

with $\mathbf{x}_k$ the state vector, $\boldsymbol{\eta}_k$ the model error, $\mathbf{M}_k$ the linear model operator, $\boldsymbol{\Lambda}_k$ the autoregressive model operator, which is a diagonal matrix containing the coefficients of the AR1 model, $\mathbf{u}_k$ the model forcing, $\mathbf{B}_k$ the transition matrix from the forcing space to the state space, $\boldsymbol{\mu}_k$ and $\boldsymbol{\mu}'_k$ two uncorrelated sources of zero-mean, time-uncorrelated Gaussian noise with covariances $\mathbf{Q}_k$ and $\mathbf{Q}'_k$ respectively.

The stochastic observation equation is

$$\mathbf{y}_k^{\mathrm{o}} = [\mathbf{H}_k \quad \mathbf{0}] \begin{bmatrix} \mathbf{x}_k \\ \boldsymbol{\eta}_k \end{bmatrix} + \boldsymbol{\varepsilon}_k \tag{2}$$

with $\mathbf{y}_k^{\mathrm{o}}$ the observations, $\mathbf{H}_k$ the observation operator for the state vector alone, and $\boldsymbol{\varepsilon}_k$ the observation noise with covariance $\mathbf{R}_k$.

The fact that the colored noise and the state are concatenated in an augmented state vector ensures that the noise source seen by the Kalman filter fulfills the original assumptions of the filter [13], i.e., time-uncorrelated zero-mean Gaussian noise.

We define the augmented state

$$\mathbf{X}_k = \begin{bmatrix} \mathbf{x}_k \\ \boldsymbol{\eta}_k \end{bmatrix} \tag{3}$$

and the augmented observation operator

$$\mathbf{H}'_k = [\mathbf{H}_k \quad \mathbf{0}] \tag{4}$$

The covariance matrix of the augmented state is denoted $\boldsymbol{\Phi}_k$. The ColKF is identical to the classical Kalman filter applied to the augmented state. The deterministic propagation equation is

$$\mathbf{X}_k^{\mathrm{f}} = \mathbf{M}'_k\mathbf{X}_{k-1}^{\mathrm{a}} + \begin{bmatrix} \mathbf{B}_k\mathbf{u}_k \\ \mathbf{0} \end{bmatrix}, \quad \mathbf{M}'_k = \begin{bmatrix} \mathbf{M}_k & -\mathbf{I} \\ \mathbf{0} & \boldsymbol{\Lambda}_k \end{bmatrix} \tag{5}$$

where the superscript $(\cdot)^{\mathrm{f}}$ denotes the forecast value before assimilation and $(\cdot)^{\mathrm{a}}$ the analyzed value, i.e., the value corrected by the filter.

The propagation equation of the covariance matrix of the augmented state is

$$\boldsymbol{\Phi}_k^{\mathrm{f}} = \mathbf{M}'_k\boldsymbol{\Phi}_{k-1}^{\mathrm{a}}\mathbf{M}_k'^{\mathrm{T}} + \begin{bmatrix} \mathbf{Q}'_k & \mathbf{0} \\ \mathbf{0} & \mathbf{Q}_k \end{bmatrix} \tag{6}$$

The innovation is defined as the difference between the observations and the forecasted value of the state projected onto the observation space

$$\mathbf{d}_k = \mathbf{y}_k^{\mathrm{o}} - \mathbf{H}'_k\mathbf{X}_k^{\mathrm{f}} \tag{7}$$

The analysis equations for the augmented state and its covariance matrix are

$$\mathbf{X}_k^{\mathrm{a}} = \mathbf{X}_k^{\mathrm{f}} + \mathbf{K}_k \cdot \mathbf{d}_k \tag{8}$$

$$\boldsymbol{\Phi}_k^{\mathrm{a}} = \left(\mathbf{I} - \mathbf{K}_k\mathbf{H}'_k\right)\boldsymbol{\Phi}_k^{\mathrm{f}} \tag{9}$$

The Kalman gain $\mathbf{K}_k$ is derived from the constraint that the analyzed state $\mathbf{X}_k^{\mathrm{a}}$ should be the minimum variance estimate of $\mathbf{X}_k$ given the observations $\mathbf{y}_k^{\mathrm{o}}$.

$$\mathbf{K}_k = \boldsymbol{\Phi}_k^{\mathrm{f}}\mathbf{H}_k'^{\mathrm{T}}\left[\mathbf{R}_k + \mathbf{H}'_k\boldsymbol{\Phi}_k^{\mathrm{f}}\mathbf{H}_k'^{\mathrm{T}}\right]^{-1} \tag{10}$$

2.2. Remarks

The estimate of the bias is given by the mean of the model error

$$\mathbf{b}_k = \mathrm{E}\{\boldsymbol{\eta}_k\} \tag{11}$$