Using Bayesian inverse modelling in real-world projects: opportunities and challenges

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Abstract Since a few years ago, TNO has had an efficient representer-based inverse algorithm operational for practical applications. This paper discusses the advantages that are encountered by using the inverse algorithm in real-world groundwater modelling studies. We also discuss problems we encounter in real-world groundwater modelling studies that are related to convergence problems for nonlinear, nondifferentiable packages of the groundwater model, especially drains.

Keywords calibration; drains; inverse modelling; practical applications, representer-based Bayesian method

INTRODUCTION

For a number of years, TNO has had an efficient representer-based Bayesian inverse algorithm operational for practical applications. The algorithm minimizes the sum of measurement residuals and deviations of model parameters from their prior mean. These penalty terms are weighted by the inverse of the measurement error and model parameter covariance matrix, respectively. A short overview of the inverse algorithm is given in the next section of this paper. A more extensive overview of the inverse algorithm is given in Valstar (2001) and Valstar *et al.* (2004).

The algorithm has the advantage that it does not require a user-defined parameterization, such as zonation, which is often applied in groundwater studies (Cooley, 1977; Carrera & Neuman, 1986; Hill *et al.*, 2000). The inverse model has the flexibility to update model parameters where the information from the measurement tells them to do so. In order to run realistic real world problems, we upscale the model before the inverse model and downscale it again afterwards. This paper first introduces the Bayesian estimation method and then we discuss the merits and problems that are encountered by using the inverse algorithm in real world groundwater modelling studies.

BAYESIAN ESTIMATION METHOD

The inverse method is based on the Bayesian estimation theory in which all uncertain model parameters and model errors are supposed to have a random distribution.

The forward model is a discretized, linear steady-state groundwater flow equation:

$$A(\alpha)h = q + w \tag{1}$$

where A is the transition matrix, which is a function of the model parameters α ; h the head vector; q the deterministic driving force vector and w the model error vector.

The measurements are given by:

$$z = M(h) + \varepsilon \tag{2}$$

where z is the measurement vector and M the head vector of maps to the predicted measurement values, while ε is the measurement error vector.

Assuming that all model parameters, model errors and measurement errors are not mutually cross-correlated and are normally distributed with known covariances, we arrive at the following objective function:

$$J = \left\{ \left[z - M(h) \right]^T C_{\varepsilon}^{-1} \left[z - M(h) \right] \right\} + \left\{ \left[\alpha - \overline{\alpha} \right]^T C_{\alpha}^{-1} \left[\alpha - \overline{\alpha} \right] \right\} + w^T C_w^{-1} w$$
(3)

where the matrices C denote the prior covariances and $\overline{\alpha}$ denotes the prior mean value of the model parameters.

For a large number of model parameters and model errors, this objective function can be minimized efficiently using the following basis function expansions:

$$\alpha = \overline{\alpha} + \sum_{i=1}^{Nmeas} b_i \Psi_i \tag{4}$$

$$h = h_F + h_{correction} + \sum_{i=1}^{Nmeas} b_i \Xi_i$$
(5)

where Ψ_i and Ξ_i are, respectively, the parameter and head representer for the *i*th measurement; *b*, a vector of coefficients (the only independent unknown parameters); h_F , the first guess estimate of the heads (obtained from the model using the prior mean model parameters and no model errors); and $h_{correction}$ the head correction term that corrects for the nonlinear relationship between the heads and model parameters.

Valstar (2001) shows that these terms can be obtained from the following equations:

$$\Psi_i = C_{\alpha} \left(\Phi_i \frac{\mathrm{d}A(\alpha)}{\mathrm{d}\alpha} h \right) \tag{6}$$

$$A\Xi_{i} = \Psi_{i} \frac{\mathrm{d}A}{\mathrm{d}\alpha} h + C_{w} \Phi_{i}$$
⁽⁷⁾

$$A(\alpha)h_{correction} = q + \left(\frac{\mathrm{d}A(\alpha)}{\mathrm{d}\alpha}(\alpha - \overline{\alpha})\right)h - A(\alpha)h_{F}$$
(8)

$$(M(\Xi) + C_{\varepsilon})b = (z - h_F - h_{correction})$$
⁽⁹⁾

with

$$A\Phi_i = \frac{\mathrm{d}M_i(h)}{\mathrm{d}h} \tag{10}$$

After coefficients b are calculated in equation (9); the parameters are updated using equation (4). Updating the parameters results in changes to equations (6)–(9) and therefore it needs to be solved iteratively. The straightforward implementation of the

optimization algorithm does not always converge. We stabilized the search by introducing a line search. As we cannot always analyse the objective function for large scale models as we cannot store the covariance matrix of the model parameters and invert it, we perform the line search by comparing the modelled heads with the linear expansions of equation (5).

PRACTICAL EXPERIENCE

A first advantage is the fact that errors in the model concept are revealed easily using the inverse model. As the inverse model has the flexibility to update parameters strongly at locations where measurements tell them to, the inverse model will immediately do so if measurement residuals are large due to errors in the model concept. Analysis of the results of the inverse model can then lead to significant improvements in the model concept. In fact, clients are usually directly involved in the calibration process with the inverse model, as their knowledge of the (local) groundwater system often plays a key role in understanding the behaviour of the residuals.

Secondly, regional or local trends in parameters can be revealed with the representer-based inverse algorithm can. For example, in one case we obtained evidence of an unanticipated—at least by us—regional trend in the hydraulic conductivity of a model layer. Geological research revealed a sound geological explanation for this regional trend. If we had used an inverse model with a predefined zone for this layer, we would not have discovered this property.

A third advantage that we address is that the uncertainty of the modelled state variables can be verified, based on the information in the measurements, by using a straightforward cross-validation. Consequently we can produce reliability maps which are extremely valuable for a.o. optimization of monitoring networks.

CONVERGENCE PROBLEMS FOR NONLINEAR GROUNDWATER MODELS

Problems we encounter in real world groundwater modelling studies are often related to convergence problems for nonlinear, nondifferentiable packages of the groundwater model, especially drains. Whether or not a drain is discharging may give a totally different behaviour of the groundwater model and the sensitivity of some model parameters. In one inverse iteration the model parameters are updated strongly by some measurements (parameters are sensitive when drains do not discharge), whereas in the next iteration the parameters are insensitive because the drains are discharging strongly. Consequently, the prior model terms want to keep these parameters close to their prior mean. The resulting oscillation strongly reduces the inverse algorithm's efficiency. As a first solution of this problem, we extended the drain package by incorporating a quadratic relation between heads and discharge for a small trajectory, which improved the efficiency. Currently, we also use time-variant inverse models, which may overcome these efficiency problems.



Fig. 1 Schematization of illustrative example.

Here we illustrate the disturbing behaviour of drains by a simple 1-D example with a constant recharge of 1 mm day⁻¹ to an aquifer with a constant conductivity, Fig. 1. Variations of the saturated thickness of the aquifer are negligible compared to the thickness of the aquifer. Thus transmissivity can be assumed constant.

The left boundary is a constant head boundary with a value 0 m, and the right boundary at a distance of 100 m is a no-flow boundary which also has a drain with a drainage level of 1 m and an infinitely large drainage conductance. Depending on the value of the transmissivity T, the drain is active or not active. When we are estimating the lnT of this aquifer using the Bayesian objective function with a head measurement at the right boundary of 1.05 m and a standard deviation of 0.1 m; a prior mean of ln $T = \ln 6 \text{ m}^2 \text{ day}^{-1}$ and a standard deviation of 1.0, the objective function is as shown in Fig. 2.



Fig. 2 Value of the objective function as a function of ln*T*.

The objective function has a minimum value for $\ln T$ of about 1.6. In this minimum the objective function is not differentiable due to the nonlinear behaviour of the drain.

When performing an optimization with any second order optimization algorithm, it will not arrive at this minimum. If arrived at a lower estimate of $\ln T$, the optimization

algorithm predicts an optimum at $T = 6 \text{ m}^2 \text{ day}^{-1}$: The sensitivity of the head is zero as the drain is active and the optimization algorithm wants to go back to the prior mean of $\ln T$. If it arrives at an estimate of $\ln T$ that is higher than the optimum, the optimization algorithm estimates the optimum value at approximately $\ln 4.8$ as the drain is not presently active. Therefore the optimization algorithm will oscillate around its minimum but never arrive there. Performing a line search will improve the search, but can never find a minimum in which the gradient is zero or in which any linearization tells us we have arrived at the optimal head value.

In practice, we found that this oscillating phenomenon is very annoying for our optimization algorithm. When building a model, we often put drains with large conductance at the surface level in order to prevent simulating heads to be above surface level. During our optimization, which includes a line search, very small steps are made within the line search as a result of this oscillating behaviour. At different parts of the model, large improvements were still to be made but progress was very slow due to the small steps taken in the line search.

After analysing this behaviour we obtained two possible ways to prevent this slow improvement of the inverse algorithm. The first is to make our model time variant as it is likely that during part of the simulation period heads are above and below the drainage level, which prevents sensitivities becoming zero. The second way is to replace the nondifferentiable drain function by a similar differentiable drain function.

DISCUSSION

The Bayesian estimation method discussed in this paper is a very promising tool for improving groundwater flow models using measurements of hydraulic heads. The method has the advantage that it does not need a user-defined parameterization and it balances the uncertainty from model parameters and measurement errors consistently. In real world model studies the measurement errors are often considerable and when they are not handled correctly, the inverse model results are often questionable.

Nonlinear groundwater flow problems may cause trouble for the inverse procedure. In this paper an example is given of the nondifferentiable drain function in which the objective function may not be differentiable in its optimum. In such cases any inverse algorithm based on a zero gradient of the objective function with respect to the model parameters will show convergence problems.

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