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Benefits from using Kalman filter in forward and inverse groundwater modelling

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1. Introduction

In groundwater applications, Kalman filter has been applied in both forward and inverse modelling. The use of Kalman filter in inverse modelling can be direct or indirect (Eigbe et al., 1998). In the direct inverse modelling, the filter automatically calibrates the model parameters based on the deviation of the measurements from the current state estimates (e.g. Eppstein and Dougherty, 1996). In the indirect inverse modelling (e.g. Van Geer and Te Stroet, 1990), estimates of the model parameters are obtained by an off-line procedure (an independent optimization algorithm) that involves minimization of the differences between actual head measurements and those predicted from the filter (a.k.a. Kalman filter innovations).
2. Benefits from Kalman filter in forward modelling

In simple worlds, Kalman filter is a method to synthesize the incoming information from observations and the knowledge of the system behaviour as it is expressed by the model. The higher the confidence in the model the less the observations are taken into account and vice versa.

- $Q_{ii} = 0.0025$ for a reliable model.
- $Q_{ii} = 0.04$ for a less reliable model (here the model produces a constant output)
3. Benefits from Kalman filter in inverse modelling

According to Van Geer et al. (1991) the advantages of Kalman filter innovations (used in the formulation of the objective function) are:

- The variance of the Kalman filter innovations is smaller than the variance of the deterministic innovations (i.e. the algebraic differences between model results and observations).*
- The Kalman filter innovations are uncorrelated in time whereas the deterministic innovations show a time correlation. **

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*This means that scattering of innovations about the mean in case of the Kalman filter is smaller and consequently the mean, which should be equal zero for a well calibrated model, can be estimated more accurately.
**This means that in the deterministic case the estimate of the mean value is biased, in particular for relatively short measurement series compared to the correlation length of the deterministic innovations.
4. Study scope

The basic parameters of Kalman filter are the covariance matrix of the process-noise \((Q)\) and the covariance matrix of the measurements’ noise \((R)\). Specifying numerical values for these matrices is notoriously difficult, in particular, for the former (Eigbe et al., 1998). Furthermore, in cases of indirect inverse modelling, the process-noise changes (is hopefully reduced) with the calibration of the model and, thus, the matrix \(Q\) should also change. In this study we investigate the effects of the Kalman filter parameters on the efficiency of the filter, concerning its application in both forward and inverse modelling.
5. Case study

The case study is based on a real application of a multi-cell groundwater model (Rozos and Koutsoyiannis, 2006, 2010) in a complex water-basin of Greece (Nalbantis et al., 2011).
6. Synthetic measurements / models

Synthetic “measurements” were derived from the multi-cell model by corrupting the corresponding simulated timeseries using the formula \( M_i = S_i (1 + e_i) \), where \( M_i \) the synthetic “measurement” at time step \( i \), \( S_i \) the value of the simulated time series at step \( i \) and \( e_i \) a random number that follows normal distribution with zero mean and standard deviation equal to 0.1. Two models were used along with the Kalman filter: (a) the multi-cell model as provided by Nalbantis et al. (2011) with ill-calibrated spring conductances (the **good** model) and (b) a model that returns a constant value equal to the mean of the corresponding simulated time series (the **bad** model).
7. Implementation of Kalman filter

The integration of the groundwater models with the Kalman filter was implemented in GNU Octave, the open source equivalent of Matlab. The groundwater model is written in C (to maximize speed) and was compiled into a Matlab executable (MEX) whereas the Kalman Filter was implemented in an m-file based on the equations provided by Welch and Bishop (2006). The matrix $R$ was chosen diagonal with all diagonal elements equal to 0.01 m$^2$. The matrix $Q$ was also diagonal with all diagonal elements ($Q_{ii}$) being equal. The filter was applied with four different $Q_{ii}$ values (0.04, 0.01, 0.0025 and 0.0001 m$^2$). The $R_{ii}$ was kept constant equal to 0.01 m$^2$. 
8. Overview of the Kalman filter effect

$Q_{ii} = 0.01$

- Kalman filter significantly improves the performance of the bad model, especially with larger $Q_{ii}$ values.

$Q_{ii} = 0.0025$

- When applied on the good model, the Kalman filter is less influenced by $Q_{ii}$. 
9. Kalman filter in forward modelling

To highlight the benefits of Kalman filter in groundwater simulations the calibrated multi-cell model of Nalbantis et al. (2011) was considered as the perfect model that describes the real conditions. Then, the RMS of the measurements, the bad model and the good model are 4.174, 6.731 and 3.999 m respectively. Note that the RMS of the measurements at this location is higher than the RMS of the good model.

<table>
<thead>
<tr>
<th>$Q_{ii}$ (m$^2$)</th>
<th>Bad model RMS (m)</th>
<th>Good model RMS (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0001</td>
<td>6.6639</td>
<td>3.2564</td>
</tr>
<tr>
<td>0.0025</td>
<td>5.4317</td>
<td>2.2497</td>
</tr>
<tr>
<td>0.01</td>
<td>3.922</td>
<td>2.767</td>
</tr>
<tr>
<td>0.04</td>
<td>3.5733</td>
<td>3.5019</td>
</tr>
</tbody>
</table>

Performance has improved! Best improvement with $Q_{ii}$=0.0025.
10. Kalman filter in indirect inverse modelling

To highlight the benefits of Kalman filter in indirect inverse groundwater modelling, the deterministic innovations of the two models were compared with the Kalman filter innovations for different $Q_{ii}$ values. The Kalman filter innovations tend to make more distinguishable the difference between the performances of the good and the bad model.

<table>
<thead>
<tr>
<th>$Q_{ii}$ (m²)</th>
<th>Bad model innovation (m)</th>
<th>Good model innovation (m)</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0001</td>
<td>7.9165</td>
<td>4.7953</td>
<td>1.651</td>
</tr>
<tr>
<td>0.0025</td>
<td>6.3965</td>
<td>3.0836</td>
<td>2.074</td>
</tr>
<tr>
<td>0.01</td>
<td>3.9978</td>
<td>1.9732</td>
<td>2.026</td>
</tr>
<tr>
<td>0.04</td>
<td>1.5991</td>
<td>0.9124</td>
<td>1.753</td>
</tr>
<tr>
<td>Deterministic</td>
<td>7.9957</td>
<td>5.4248</td>
<td>1.474</td>
</tr>
</tbody>
</table>

Greater ratio achieved with $Q_{ii}=0.0025$.

Deterministic innovation has the lowest ratio.
11. Conclusions

In our case study, Kalman filter benefited both forward and inverse groundwater modelling. In forward modelling, the Kalman filter improved the model performance even in cases where the measurements had higher RMS than the model. This improvement is desirable in applications where the knowledge of present conditions is important (e.g. stochastic forecast). In the indirect inverse modelling the filter, through Kalman filter innovations, made more distinguishable the difference between the bad and the good models, which most probably will facilitate the optimization algorithm. In both forward and inverse modelling there was an optimum covariance matrix of the process-noise ($Q$; the same for both cases) that maximized the benefits of the Kalman filter.
12. References

- Welch, G. and Bishop, G. (2006). An Introduction to the Kalman Filter, TR 95-041, Department of Computer Science University of North Carolina at Chapel Hill Chapel Hill, NC 27599-3175.