A comparison between Monte Carlo and first-order approximation methods in capture zone design

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Abstract Monte Carlo analysis is a versatile method that can easily be implemented and used for representing parameter uncertainty in stochastic processes. It has been extensively and successfully used in stochastic well-capture zone design. Although still computationally viable, in terms of CPU times, for unconditional simulations, it requires huge amounts of CPU time for conditional simulations. Conditioning hydraulic parameters on state variables, e.g. head, pore water velocity or concentration, requires solution of the inverse problem. This can be computationally intensive by itself. Here, we investigate first-order approximation as an alternative uncertainty propagation method to Monte Carlo analysis. A comparison between the two methods, in terms of the statistics produced of state variables from pore water velocity and particle tracking models, is performed.

Key words first-order approximation; Monte Carlo analysis; stochastic analysis; well-capture zone design

INTRODUCTION

In stochastic well-capture zone design, the mean capture zone and its associated confidence interval are required. A stochastic framework for designing well-capture zones is essential because of uncertainties in hydraulic parameters, boundary conditions and conceptual models. The Monte Carlo (MC) method has been used extensively in stochastic well-capture zone uncertainty analysis (e.g. Van Leeuwen et al., 1998, 2000; Guadagnini & Franzetti, 1999; Varljen & Shafer, 1991). As none of these studies considered conditioning on state variable measurements, i.e. head and travel time, this approach was feasible in such analyses. However, conditioning on state variables by solving the stochastic inverse problem (Bakr, 2000) is very CPU demanding. Consequently, using the MC method in capture zone design, when conditioning on state variable measurements, will be even more CPU demanding.

Another approach that is also used in uncertainty analysis is the first-order (FO) approximation method (Dettinger & Wilson, 1981). The method, in general, requires less CPU time. It is based on Taylor’s series expansion in which second and higher order terms are ignored. The success of the method in approximating the mean and variance of the variable of interest depends on the significance of the ignored terms. If this approximation is achievable, then under the assumption of normality, the calculated mean and variance of the capture zone can be used to approximate its confidence interval.
In this paper we investigate the FO method as an alternative to MC for uncertainty propagation in stochastic well-capture zone design, through comparison of particle tracking state variable and pore water velocity statistics generated by the two methods. The main particle tracking state variable compared is the particle end point (hence trajectory). We use backward particle tracking, hence a particle start point is at the well and its end point presents a point in the capture zone. The estimation of an accurate mean and variance for particle end points would enable us to delineate mean capture zones and their associated confidence interval, provided that the end point, in terms of x- and y-coordinates or a surrogate function of these variables, are normally distributed. Normality of end point coordinates is examined by plotting commutative probability functions of the end point coordinates.

As a crucial component, in terms of accuracy, in calculating second moments of pore water velocity and particle end points, the sensitivities of these variables with respect to transmissivity are calculated using adjoint equations (Ahlfeld et al., 1988; Sun, 1994). Verification of these sensitivity coefficients is carried out using a perturbation method.

SENSITIVITY COEFFICIENTS

Calculating travel time and particle end points requires identification of head distribution in an aquifer of interest. Once the head distribution is determined, Darcy’s law can be used to calculate pore water velocity in the x- and y-directions. They can then be used to track a conservative particle within the aquifer. The location of a particle at any time \( t \) can be given by:

\[
x' = x'^{-1} + u_{xa} \Delta t
\]

(1)

and

\[
y' = y'^{-1} + u_{ya} \Delta t
\]

(2)

where \( u_{xa} \) and \( u_{ya} \) are average pore water velocity in the x- and y-directions, respectively. Sensitivity coefficients of a particle location at time \( t \) with respect to \{\( Y \)\}, logarithmic transformation of transmissivity \( T \), are obtained by differentiating equations (1) and (2) with respect to \{\( Y \)\}. This gives:

\[
\frac{dx'}{d\{Y\}} = \frac{dx'^{-1}}{d\{Y\}} + \frac{du_{xa}}{d\{Y\}} \Delta t
\]

(3)

and

\[
\frac{dy'}{d\{Y\}} = \frac{dy'^{-1}}{d\{Y\}} + \frac{du_{ya}}{d\{Y\}} \Delta t
\]

(4)

Equations (3) and (4) are based on the assumption that \( \Delta t \) is not a function of \{\( Y \)\}. Similarly, we can obtain the sensitivity coefficients of a particle travel time, \( t \), between its start and end points. These sensitivity coefficients are dependent on sensitivity of the heads with respect to \{\( Y \)\}. The sensitivity coefficients with respect to \{\( Y \)\} are obtained by differentiating the discrete groundwater flow equations.
FIRST-ORDER ANALYSIS

FO approximation is based on Taylor’s series expansion, which can be stated as:

$$\sigma = \bar{\sigma} + \frac{\partial \sigma}{\partial \rho} (\rho - \bar{\rho}) + \frac{1}{2} \frac{\partial^2 \sigma}{\partial \rho^2} (\rho - \bar{\rho})^2 + \cdots$$  \hspace{1cm} (5)

where $\sigma$ is a state variable (e.g. pore water) that is function of parameter $\rho$ (e.g. transmissivity); $\bar{\sigma}$ is the prior mean of $\sigma$; $\bar{\rho}$ is the prior mean of $\rho$. Ignoring the second and higher order terms and taking the expectation of equation (5), gives:

$$E[\sigma] = \bar{\sigma}$$  \hspace{1cm} (6)

since the expectation of $(\rho - \bar{\rho})$ is 0. However, if we only ignore terms higher than the second term we get:

$$E[\sigma] = \bar{\sigma} + \frac{1}{2} \frac{\partial^2 \sigma}{\partial \rho^2} E[(\rho - \bar{\rho})^2]$$  \hspace{1cm} (7)

The last term on the right-hand side is the variance of the parameter $\rho$.

Similarly, we can obtain estimation for the variance of $\sigma$, by taking the expectation of $(\sigma - \bar{\sigma})^2$, which can be obtained from equation (5):

$$E[(\sigma - \bar{\sigma})^2] = \left(\frac{\partial \sigma}{\partial \rho}\right)^2 E[(\rho - \bar{\rho})^2]$$  \hspace{1cm} (8)

This assumes that the variance of the parameter is small enough to ignore the second and higher order terms. However, we should keep in mind that this is not a sufficient condition, although it is necessary, to have the second and the higher terms in Taylor’s series small enough to be ignored. This is because the existence of the second and higher derivatives of $\sigma$ with respect to $\sigma$, which we generally assume to be small enough to ignore.

Note that equations (5)–(8) consider a scalar state variable and a scalar parameter. Extending these equations to a vector state variable and a vector parameter is straightforward.

Monte Carlo method

The MC method proceeds by generating a number of statistically likely realizations of the parameter(s). A forward model is then used to obtain a prediction of the state variables, which are then statistically analysed. In this case, the whole statistical distribution can be estimated; not only the first and the second moment (see Van Leeuwen et al., 2000).

NUMERICAL EXAMPLE

In the following sections we shall investigate the accuracy of the calculated sensitivity coefficients of head, pore water velocity and particle end points using the perturbation method. Also, a comparison between FO and MC methods, in terms of the statistics
produced of the state variables from pore water velocity and particle tracking models, is performed. A confined aquifer of 1000 m (from -200 m → 800 m) × 1000 m (-500 m → 500 m) with a pumping well, which pumps at rate 200 m$^3$ day$^{-1}$ at the origin, is considered. The model has a grid size of 10 m and boundary conditions of constant heads at the east and west boundaries, and no flow boundary conditions at the north and south boundaries. The transmissivity field has an exponential model with a log mean of 3.91, variance of 0.5 and correlation length of 30 m in the x- and y-directions.

**VERIFICATION OF SENSITIVITY COEFFICIENTS**

Calculation of accurate sensitivity coefficients is very important to produce a good estimation of the variance of a state variable. The sensitivity coefficients of particle end points are a function of the sensitivity coefficients of pore water velocity, which, in turn, is a function of the sensitivity coefficients of the head state variable.

Table 1 shows sensitivity coefficients of head and pore water velocity at the centre of an arbitrarily chosen element (element number 4236) with respect to logT at the nodes of the element corners as calculated using perturbation and adjoint methods. As seen in this table, the sensitivity coefficients are almost identical. We should bear in mind that perturbation length used in the perturbation method should be adjusted to obtain accurate sensitivity coefficients using this method. This table verifies the accuracy of the sensitivity coefficients that are calculated using the adjoint equations. A similar test is performed to verify the sensitivity coefficients of particle end points with respect to nodal logT. Figure 1 shows the derivative of x- and y-coordinates of five particles, evenly distributed around the well and backtracked to their start points, with respect to logT at nodes 4464 (left) and 4573 (right), these nodes are also arbitrarily chosen. The first five ordinates on the x-axis of each of the graph in this figure are for the x-coordinates of the five particles, while the last five ordinates are for the y-coordinates. Although that the sensitivity coefficients calculated using the adjoint and the perturbation methods are not identical, they are very close apart from a small number of discrepancies. These discrepancies could be related to the inaccuracy of the perturbation method.

<table>
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<tr>
<th>LogT at node</th>
<th>Head $u_x$</th>
<th>Head $u_y$</th>
<th>$u_x$</th>
<th>$u_y$</th>
</tr>
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<td></td>
<td>FD</td>
<td>ADJ</td>
<td>FD</td>
<td>ADJ</td>
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<td>4379</td>
<td>-0.8885E-02</td>
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<td>-0.4009</td>
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</tr>
<tr>
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<td>-0.3706</td>
<td>-0.3705</td>
</tr>
</tbody>
</table>

**First-order analysis vs Monte Carlo method**

This section presents a comparison between the FO analysis and MC method to calculate the mean and variance of pore water velocity and particle end points. Figure 2
Comparison of Monte Carlo and first-order approximation methods in capture zone design

Fig. 1 Sensitivity coefficients of particle end point (in terms of $x$- and $y$-direction) with respect to log $T$ at nodes 4464 (left) and 4573 (right) as calculated using adjoint and perturbation methods.

Fig. 2 Average (left) and variance (right) of pore water velocity in the $x$-direction calculated using FO vs MC methods.

shows the average and variance of pore water velocity in the $x$-direction, as calculated using the FO and MC methods. The figure shows identical values calculated from the FO and MC methods for the average $x$-direction pore water velocity. Similar results are concluded for the variance of the pore water velocity, except in the vicinity of the pumping well where some differences are observed. Results for the pore water velocity in the $y$-direction show similar agreement.

Figure 3 shows the average and variance of the $x$-coordinate of particle end points that are calculated using the FO and MC methods. The figure shows higher discrepancies of the calculated average and variance using the two methods. A higher discrepancy in the variance is generally observed. Less discrepancy was obtained in the $y$-direction. It is also noted that higher discrepancies in the mean produce higher discrepancies in the variance.
Normality of particle end points

In this section the normality of particle end points is examined. This is done by visually inspecting the frequency distribution and cumulative probability of $x$- and $y$-coordinates of particle end points. Figure 4 shows the cumulative probability distributions of the $x$-
and \( y \)-coordinates of two particles out of five equally distributed around the pumping well and tracked in a backward direction for 30 days. The figure shows the results of particle \#1, which has a zero angle with the pumping well, and particle \#4. The two particles show the best conformity and the worst conformity, respectively, to normality. The results showed that the average \( x \)-coordinate of particle \#4 (and also particle \#3) are the smallest, which indicates that they have travelled in a very low velocity field close to the well stagnation point.

**SUMMARY AND DISCUSSION**

Accurate calculation of sensitivity coefficients of head and pore water velocity is crucial for the FO method and can be obtained using the adjoint method. Verification of these coefficients with the perturbation method shows, in general, good agreement.

A comparison between the FO and MC methods for mean and variance of pore water velocity shows a good agreement (Fig. 2). For the mean and variance of particle end point, less agreement between the FO and MC methods was obtained (Fig. 3). It can be seen that at the points where there is more discrepancy in the calculated mean, a higher discrepancy in the calculated variance is observed. We relate these discrepancies to the inaccuracy of the FO method in approximating the mean and the variance of the particle end points. This means that a higher order approximation is required, e.g. equation (7) for estimating a second-order approximation of the mean.

Finally, the normality of particle end points was examined (Fig. 4). Although some particle end points followed a normal distribution, others did not. These results suggest that, although it is possible to use the FO method as an alternative to the MC method in well-capture zone design, it is only valid for some of the particles at the front of the capture zone. A better approximation of the mean and the variance of particle end points is possible using second-order approximation at the expense of more CPU time. Meanwhile, even with a better approximation of the mean and variance of particle end points, the method cannot be used for all of the particle end points because of the violation of the end points normality for many of the tracked particles. Finally we should keep in mind that these results are obtained using a small variance of log \( T \). This actually means that worse results are expected with higher variances of log \( T \).

**REFERENCES**


