

THE ADJOINT METHOD AND LATIN HYPERCUBE SAMPLING IN GROUNDWATER MODELING

Adjoint sensitivity analysis has been used by DOE contractors in regional groundwater flow modeling for some of the potential HLW repository sites. The purpose of this note is to briefly describe what the adjoint method is, what it is used for, and how it compares with other sensitivity analysis techniques, including Latin hypercube sampling.

Summary

The adjoint method can be classified as an analytic method while Latin hypercube sampling is a special form of direct sampling used during Monte Carlo simulation. These methods are summarized in Table 1.

The adjoint method is computationally efficient for calculating the sensitivities (or sensitivity coefficients) of one performance measure of a model's output to the entire parameter field. It is much more efficient than the direct (differentiation) method when the number of parameters of interest (e.g. porosities) is much larger than the number of performance measures (head values, for instance). The direct method is more efficient when the number of parameters is much less than the number of performance measures, for example when the sensitivities of all head values to one conductivity is desired. The adjoint method is particularly useful in identifying crucial areas where additional resolution of the parameter field is warranted. Neither the adjoint nor direct method generates the actual head values or other performance measures in the process of calculating the sensitivities. Monte-Carlo simulation allows estimation of sensitivity coefficients from a large number of deterministic solutions with different input parameter sets. This technique generates the distribution of model output (head values) resulting from the

TABLE 1

COMPARISON OF ANALYTIC AND MONTE CARLO METHODS

ANALYTIC METHODS - Calculating Sensitivities

Direct and Adjoint Methods

- Local sensitivities deterministically calculated from governing equations
- Sensitivities for only small region of parameter range
- Must be incorporated into numerical model of interest
- Does not generate multiple model outputs
- Does not include any information on parameter ranges or correlations

Direct Method

- Computationally efficient when number of parameters is small

Adjoint Method

- Computationally efficient when number of parameters is large

MONTE CARLO METHODS - Direct Sampling, Latin Hypercube Sampling, Regression

- Sensitivities estimated from multiple deterministic model output
- Sensitivities for entire parameter range
- External to numerical model of interest
- Generates multiple model outputs
- Generates unbiased probability distribution functions
- Includes parameters ranges, pdf's and correlations
- Computationally burdensome

Latin Hypercube Sampling

- Reduces number of model runs required for statistical accuracy

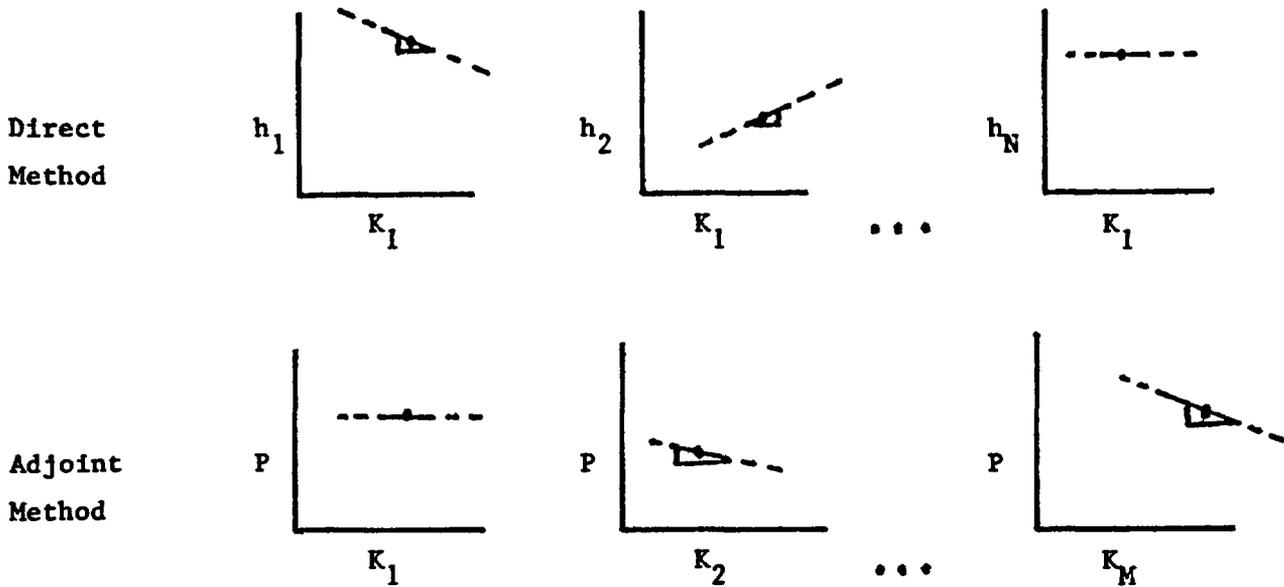
range of input parameters. For many problems, Latin hypercube sampling (LHS) minimizes the number of solutions required by selecting input values from a partitioned parameter distribution. Parametric sensitivity analysis also generates multiple model outputs, which directly show changes due to limited parameter changes and can be used to estimate sensitivities. This technique, however, involves fewer parameter changes and does not always include important relationships between parameters. Figure 1 illustrates the different output from these techniques.

Both analytic and statistical sampling methods are important in sensitivity and uncertainty analysis. Analytic methods, including the adjoint method, are useful in parameter identification, local sensitivity calculations, and stochastic models. Monte Carlo simulations, with direct or Latin hypercube sampling, generate probability distribution functions for model output corresponding to the entire range of parameter values with associated probabilities and correlations.

Sensitivity Analysis

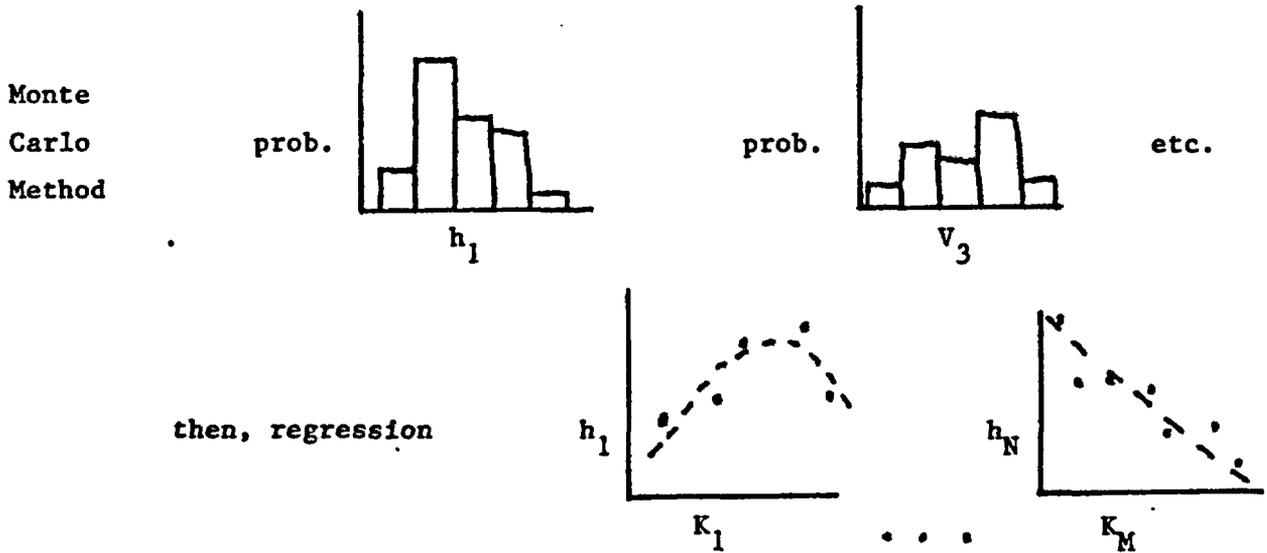
Due to our imperfect knowledge, groundwater flow (and transport) assessments are uncertain. Areas of uncertainty include field data collection and interpretation, conceptual model development, model parameter estimation, and probability estimation. In assessing the impact of this uncertainty, it is often beneficial to have a quantitative understanding of how the predicted flow system is affected by errors in individual or groups of input parameters. For example, how much would the predicted flow velocity change if the hydraulic conductivity changed? Or, which porosity values are most important in determining the velocity at a certain location? These questions are

FIGURE 1 OUTPUT FROM ANALYTIC AND MONTE CARLO METHODS



for example
 $P = (h_1 + h_2) / 2$

then, stochastic model for variance



addressed through sensitivity analysis. Calculating sensitivities is a major portion (but not all) of sensitivity analysis.

The sensitivity (or sensitivity coefficient) is the first-order partial derivative of the solution curve with respect to a parameter. For example, if we plotted the piezometric head at one location versus the hydraulic conductivity of one unit, the sensitivity would be the slope of that curve. From this illustration, two important points can be made. The first is that that curve may not necessarily be straight, and hence the sensitivity may not be constant over the entire range of that parameter. That is, the second-order derivative may not be zero. Secondly, this curve is developed holding all other parameters constant. If those other parameters change independently, or change in response to a change in the parameter of interest, the sensitivity would change. Thus, combining these points, the sensitivity at a point is a function of all parameters of the system, including the parameter to which the sensitivity of the solution is desired.

Sensitivity coefficients are used in several sensitivity and uncertainty analysis procedures. The actual change in output values can be estimated by multiplying the calculated sensitivity (first-order derivative) by a step change in the parameter. This is only an estimate in that the sensitivity coefficient may not be constant over that step range. The sensitivity can also be used during model calibration or parameter identification. Part of the calibration procedure is minimizing error in model output, based on measured values, by changing parameter values. The sensitivities provide the gradient in this optimization procedure [e.g. Carrera and Neuman 1984]. Sensitivities for an entire parameter field indicate the relative importance of different parameters. This may be very useful in optimizing data collection activities [e.g. Doctor et al. 1982]. Sensitivities can also be useful in directly

relating uncertainty in model output to uncertainty in input parameters [e.g. Sagar and Clifton 1983]. For example, given an estimated uncertainty in conductivity, the corresponding uncertainty in head calculations and the effect of that uncertainty on the mean head can be determined. These determinations require sensitivity coefficients, but also include procedures which are beyond the scope of this paper [see e.g. Townley 1984].

For many groundwater flow problems which have closed form solutions, the sensitivity can be evaluated directly. That is, the solution can be directly differentiated with respect to a parameter. That calculated sensitivity is a direct function of the parameters input. This exercise can identify important properties of general flow solutions [e.g. Wilson and Dettinger 1979]. Unfortunately, many real heterogeneous groundwater flow systems cannot be adequately described with analytical solutions, and we must resort to numerical solutions.

The general concepts of sensitivity analysis also apply to numerical models. In this case, rather than having one or two values of hydraulic conductivity, a system may be modeled with hundreds of different conductivity values for different areas. As above, it is possible to solve certain sensitivity problems directly, even for complicated numerical models. The numerical representation of the solution, typically a set of simultaneous equations, can be directly differentiated with respect to a parameter. However, when the sensitivity to a large number of parameters is desired, these computations can be burdensome. The adjoint method has arisen as an efficient computational technique for problems where the sensitivities of a single output value (or a single combination of output values) to a large number of parameters are desired. Another technique for sensitivity analysis is called direct sampling or Monte-Carlo simulation, and involves generating numerous

solutions to the flow equations with ranges of the parameters of interest. These output are statistically evaluated to estimate sensitivities. Latin hypercube sampling is a parameter set generation technique which reduces the number of solutions required for many direct sampling problems. These techniques are discussed in more detail below.

The Direct Differentiation Method

For discussion, consider a numerical solution to a steady state groundwater flow problem. This problem is solved using a distributed parameter technique, such as finite element or finite difference. Numerically, this problem is the solution of a set of linear simultaneous equations represented in matrix form by:

$$\underline{\underline{K}} \underline{h} = \underline{F} \quad (1)$$

where $\underline{\underline{K}}$ is the system stiffness matrix, \underline{h} is the vector of unknown heads, and \underline{F} is the forcing vector. The stiffness matrix contains conductivity and geometric terms relating the nodal head values to each other. The forcing vector contains the boundary condition terms, including distributed recharge/discharge. Equation (1) can be differentiated with respect to a scalar parameter of interest, α , yielding:

$$\underline{\underline{K}} \frac{\partial \underline{h}}{\partial \alpha} = - \frac{\partial \underline{\underline{K}}}{\partial \alpha} \underline{h} + \frac{\partial \underline{F}}{\partial \alpha} \quad (2)$$

Note that (2) is the derivative with respect to only one parameter. The forward problem, (1), is solved once, and the sensitivity of all head values to

the parameter of interest is determined by solving (2). All terms in (2) can be directly calculated or are available from the solution of (1), except of course $\partial h / \partial \alpha$ which are the desired sensitivity coefficients. Calculating sensitivities directly is appropriate when the number of head values of interest is much greater than the number of parameters of interest. If however, sensitivities to several parameters, say the conductivities of 20 elements, are desired, (2) would have to be solved once for each element conductivity.

The results of the direct method are the solution of the flow problem (1), and the sensitivities of each head value to the single parameter of interest. This technique does not result directly in different solutions of the flow problem. That is, it does not actually calculate heads which would result from different values of the parameter of interest. Sagar and Clifton [1983] use direct differentiation techniques in a stochastic flow model. This model results in the mean head solution, and the variance of the mean solution due to variance in the conductivity field.

The advantages of the direct method are that sensitivities are calculated directly from the governing equations rather than estimated from model output data, and the method is efficient when the number of parameters is less than the number of performance measures. Directly calculated sensitivities are required for some sensitivity and uncertainty analysis techniques, such as stochastic models. Sagar and Clifton [1983] also compute second order derivatives directly in their stochastic flow model. The disadvantages of the direct method are that the distribution of model output is not computed, the method is computationally burdensome when the number of parameters is much greater than the number of performance measures, and the computed sensitivities may apply to only a small region of the parameter range. Numerical

implementation of the direct method is internal to any particular computer program; it cannot be applied a posteriori.

The Adjoint Method

When the number of parameters of interest is larger than the number of performance measures of interest, the adjoint method may be appropriate. First, a performance measure for the forward problem (1) is defined. For example, that function may be:

$$P = \int_V \underline{g} \cdot \underline{h} \, dV = \int_V f \, dV \quad (3)$$

where P is the scalar performance measure, \underline{h} is the vector of heads, \underline{g} is a vector of weighting functions, and f is the weighted head, a function of location. The integral is over the entire domain. The weighting functions simply specify how the model output is combined to form a scalar performance measure. For a simple case, \underline{g} could contain a 1 at one node and 0's at all other locations. For this case, P would equal the head value at the node of interest. The performance measure could include several heads, or even velocities. The sensitivity of this performance measure to any one parameter is calculated from [INTERA 1983a]:

$$\frac{dP}{d\alpha} = \int_V \left[\frac{\partial f}{\partial \alpha} + \underline{\psi}' \frac{\partial \underline{Q}}{\partial \alpha} - \frac{\partial \underline{\psi}'}{\partial x_i} \frac{\partial T_{ij}}{\partial \alpha} \frac{\partial h}{\partial x_j} \right] dV \quad (4)$$

$$+ \left\{ \text{boundary condition terms} \right\}$$

Terms in (4) are defined by INTERA [1983a]. Suffice to say that (4) contains only known terms and derivatives which can be calculated directly, except for \underline{h} , which is the solution to the forward problem (1), and $\underline{\Psi}'$, which is called the adjoint state, or the adjoint state sensitivity, or an importance function. The adjoint state, $\underline{\Psi}'$, "represents the change in the value of the performance measure caused by a unit volume influx of water at any point x in the domain" [INTERA 1983a]. Plotting the adjoint state for an entire area shows the numerical impact of additional influx at each location on the performance measure. Solving (4) for a particular sensitivity does not require solution of simultaneous equations. The adjoint state vector, $\underline{\Psi}'$, is determined by solution of the adjoint problem:

$$\underline{K}' \underline{\Psi}' = - \frac{\partial f}{\partial h} \quad (5)$$

which is a system of simultaneous equations. However, equation (5) is solved only once for a given performance measure, and then the sensitivity of that performance measure to any parameter can be calculated from (4). When the sensitivities of one performance measure to many parameters are desired, this is much more efficient than solving (2), which is a system of simultaneous equations, for each parameter.

The numerical values of sensitivity calculated using the direct method (equations (1) and (2)) and those calculated using the adjoint method are identical. There are no simplifying or approximating assumptions made in the adjoint method for calculating first-order derivatives. It is simply an efficient calculation technique for problems with a large number of parameters

of interest. Of course, if the performance measure (3) changes, the adjoint problem (5) must be re-solved, and this method loses its attractiveness.

The advantages of the adjoint method are that sensitivities are calculated directly from the governing equation and the method is efficient when the number of parameters is much greater than the number of performance measures. Calculated sensitivities are required for some sensitivity and uncertainty analysis techniques, such as stochastic models. The disadvantages of this method are the same as the direct method (see above), except that the adjoint method is not efficient when the number of performance measures is larger than the number of parameters. The adjoint method computes the sensitivity of one performance measure to all parameters. Each time the performance measure is changed (for example, head at a different location), the adjoint problem must be resolved. Harper [1983] argues that the major disadvantage of the adjoint method is the required familiarity with the computer code which is to be 'adjointed'. Thomas [1982] considers the direct and adjoint methods as "analytical methods" and finds them "superior to the statistical sampling method in logical rigor and numerical accuracy." These comparisons are made on the basis of calculating sensitivity coefficients, and not on the basis of use of the methods in a comprehensive sensitivity and uncertainty analysis.

The adjoint method has been used at the SALT HLW sites [INTERA 1983a, 1984a, 1984c]. The adjoint method was developed in the nuclear engineering field [Oblow 1978a, 1978b] but has received little attention outside that field.

Monte Carlo Methods

Monte Carlo simulation techniques are related to parametric sensitivity analysis. As stated above, one objective of sensitivity analysis is to quantitatively assess the change in model output due to changes in model input. A simple procedure for assessing this impact would be to actually re-solve the model equations using the new parameter set of interest. These results could then be directly compared with results using the initial parameter set. The sensitivity could then be estimated by dividing the change in model output by the change in model input. Running a model with different parameters is called a parametric sensitivity analysis and has been used in both the HLW [Ertec 1983; INTERA 1983b, 1984b] and LLW [e.g. Oztunali et al. 1983] programs.

Monte Carlo techniques are an extension of parametric sensitivity techniques. However, Monte Carlo techniques are much more powerful because they incorporate parameter sets representing the entire range of possibilities, and because they incorporate the probabilistic and interdependent nature of real properties. Each parameter of interest is defined by a probability distribution function. In addition, the relationship between parameters can be defined by covariance functions. Multiple parameter sets are generated, choosing each parameter randomly. The word 'random' here means that the actual value used for each model run is not known a priori, but is picked from the available distribution at random. It is also implied that the technique for picking these random values results in parameter values for the entire set of multiple simulations which correspond to that parameter's probability distribution function, and to applicable correlations with other parameters. This results in a multitude of model outputs corresponding to 'realizations' of the parameter set which reflect the statistics of the

individual parameters. These output can then be statistically analyzed to determine sensitivities. In addition, these output directly show the ranges of model outputs.

The advantages of Monte Carlo simulation are that actual output values are calculated which directly show effects of different parameters over the entire parameter range, that deterministic models of any process can be used (the Monte Carlo technique is external to the particular simulation model), and that all relationships between parameters and output, including nonlinear effects, are incorporated. The disadvantages of this technique are computational burden (often hundreds of simulations are required to assure statistical accuracy), sensitivities are estimated by statistical analysis of the model output as opposed to directly calculated, and results may not be directly reproducible. That is, since the technique incorporates parameter selection using, typically, some sort of random number generator, and since the results analysis may be performed with different statistical tools, results may not be identical from computer to computer. This latter point may be especially important to regulatory actions. Townley [1983, 1984] compares results from Monte Carlo simulation and from stochastic flow models using adjoint sensitivity. He considers the Monte Carlo simulation as the 'correct' result and relates the observed differences in the results to nonlinear or higher order effects which are not included in his stochastic model.

Latin Hypercube Sampling

Latin hypercube sampling (LHS) [Iman et al. 1980a] reduces the computational burden of Monte Carlo simulation by partitioning the probability distribution for each parameter into smaller ranges. For example, when

generating two parameter values using LHS, one value will be chosen (randomly) from each half of that parameters distribution. Using this technique, the statistics of the model output converge to a constant value with lower numbers of parameter sets, and hence solutions. Monte Carlo simulation with LHS has been used extensively by Sandia [e.g. Iman et al. 1980b] and by the staff in its rationale for Part 60 [NRC 1983]. Strictly speaking, LHS is only the generation of the parameter sets which are used in the Monte Carlo simulation. It does not includes the statistical analysis (regression) of the model output [see Iman et al. 1980; Iman and Conover, 1982].

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