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Optimization model for management of ground-water survey

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Abstract

An integrated ground-water management model is formulated as nonlinear optimization problem. To simulate the physical and chemical processes occurring within a leaky confined aquifer system, the finite-difference forms of the flow and transport equations are embedded in the management model. The Hooke-Jeeves method, a nonlinear programming technique, in conjunction with the exterior penalty function method is used to solve this management model. The suitability and capability of this method to solve the management problems for study areas of different sizes and different numbers of management periods are demonstrated. The performance evaluation of this proposed methodology establishes its potential applicability for the solutions of different kinds of ground-water management problems. The developed methodology also demonstrates the suitability of the embedding technique to solve a dimensionally large nonlinear ground-water management problem. The proposed methodology does not require the linking of simulation and optimization models externally. It is shown that global optimality of obtained solutions is dependent on the extensive identification of local optimal solutions and the accuracy in prescribed characteristics.

Keywords: Optimization model, management, ground-water survey

Introduction

The objective of managing groundwater in contaminated areas is to either remove the plume of polluted water, contain it within a specified zone, or control its flow away from wells, streams, and lakes in which water quality is to be protected. These objectives can be attained by inserting curtain walls into the aquifer between the plume and the zone to be protected, or by digging up and removing the polluted soil, but more usually by installing and operating pumping and/or recharge wells so as to control the flow field. Planning and operation of such remediation schemes is aided by simulation and optimization models. Simulation allows the investigation of "what if" questions, which allow the comparison of alternative schemes. Optimization models are designed to find the solution that is best according to a specified objective, usually economic, while satisfying a set of stated physical, technological, legal, and other constraints.

In this paper we present an optimization model for (1) locating pumping and recharge wells within an aquifer and then (2) operating them, in steady state, so as to control groundwater gradients and thus keep a plume of polluted water from entering a protected zone. The primary innovation of the approach presented in this paper is that the optimal solution is sought under uncertainty about the hydraulic conductivities in the aquifer. In this paper we focus on the uncertainty about aquifer properties, for several reasons. First, aquifer properties (such as hydraulic conductivities) can never be known with certainty. Hydraulic conductivities are measured from pumping tests or by taking soil samples (cores) from the site and measuring these samples in the laboratory, but these methods provide only local or at best zonal data. In principle, other uncertain parameters such as boundary conditions and locations of contaminants could be determined without completely disrupting the site. Secondly, once a problem has been formulated that includes the uncertainty in the aquifer parameters, many of the other sources of uncertainty can be considered without additional conceptual difficulty.

We use a stochastic optimization method, which incorporates the uncertainties and their economic consequences explicitly into the objective function and into the relevant constraints.

In the method presented in this paper, stochastic programming with recourse, the form of the penalties will affect the frequency and the extent of constraint violations. Recourse models are often much larger that the corresponding deterministic models, and require different solution techniques. However, due to advances in both stochastic optimization methods and in computer technology, useful stochastic optimization problems can be formulated and solved without excessive computer resources.

This paper will discuss a number of formulations of a stochastic programming model for managing groundwater quality under uncertainty. The formulations vary in the degree of complexity; in general, the more complex formulations allow greater realism and modeling flexibility.

In the next section we provide a brief review of the literature relevant to this problem and to the background of stochastic programming. We then present the stochastic optimization model developed for this problem, analyze the value of information, and finally show results for a sample problem.

Method of solution

In this problem the decision variables are the pumping rates (w_j). The violations ($v_{i \cdot \omega}$) are completely specified by these pumping rates, and can be thought of as dependent variables. Thus the problem actually involves only a moderate number of decision variables. However, there remains the necessity of having a set of violation constraints for each realization included in the problem, leading to an extremely large number of constraints. Thus due to its size, this full optimization problem could not be solved easily.

Rockafellar and Wets [1986a, b] [17]. Have developed the finite generation algorithm (FGA) for solving convex linear quadratic stochastic optimization programming problems with recourse. The FGA solves the dual problem, which has a large number of decision variables but a moderate number of constraints, by using decomposition in the dual space to obtain an approximation to the dual problem that is much smaller than the original. Each iteration of the FGA involves the solution of this small dual approximation and updating of the approximated terms. In the implementation of the extended FGA used in this paper, in each iteration a convex nonlinear optimization sub problem is solved using GAMS (version 2.02)/MINOS (version 5) [*Brooke et al, 1988*]. Solution of the largest optimization problem considered in this paper could be solved in about 1 hour on a PC clone.

Representation of the Hydraulic Conductivities

The hydraulic conductivities for each realization were obtained by using a turning bands program to generate a realization of the random hydraulic conductivity field [*Tompson et al, 1987*]. This turning band program generates spatially correlated variables from a normal distribution with mean of 0 and standard deviation of 1. The program can produce output from a normal distribution with user specified mean and standard deviation by linear transformation of of the variables, as well as from a lognormal distribution by taking the log of the normally distributed variables.

These variables are spatially correlated in two dimensions according to the stationary exponential correlation function:

$$C(\varepsilon) = \sigma^2 \exp\left\{-\left[\left(\frac{\varepsilon_1}{\lambda_1}\right)^2 + \left(\frac{\varepsilon_2}{\lambda_2}\right)^2\right]^{1/2}\right\} \qquad (1)$$

Where

$C(\varepsilon)$ Stationary anisotropic covariance for two points separated by vector ε

σ^2 Variance of the random field

ε_i Separation along dimension i (i = 1, 2)

λ_i Correlation scale along dimension i

Each run of the turning bands program produces a realization of the hydraulic conductivities for each cell: realization from separate runs are independent. Thus each realization is equally likely. So $\pi_\omega = 1/\Omega$.

One additional step is needed to use the hydraulic conductivity values in the finite difference equations. The hydraulic conductivities generated by the turning bands program are for cell centers. However, in the finite difference equations, we require the hydraulic conductivity that will give the correct flow between the centers of the two elements. To find the "average" or effective hydraulic conductivity between the two elements, we employed the common approach of using the harmonic average:

$$K_{eff} = \frac{2(K_i K_i)}{K_i + K_j} \qquad (2)$$

These hydraulic conductivities are incorporated into the F matrices, as described in Appendix A. These matrices were inverted before they were incorporated in the optimization programs, using a FORTRAN program for LU decomposition [*Press et al.1986*] [14].

The Value of Information in the Decision-Making Process

The value of the information about the hydraulic conductivities depends on when in the decision-making process the information is obtained and to what extent this information can affect further decisions. To examine the value of information, we will develop a number of different stochastic optimization formulations based on the framework developed above, and use their solutions to define measures of the value of information.

The best case for a decision maker is when there is no uncertainly at all, and the problem is deterministic. We examine this case by solving the deterministic problem of (1) subject to (2)-(4), with all hydraulic conductivities set to their expected value. In our case, the site is then homogeneous, since the hydraulic conductivity distributions are all assumed to have the same mean. In the next case examined, the gradient constraints across the capture curve are treated, not as hard constraints, but as constraints which may be violated at some cost. This penalty cost for constraint violations is included in the objective function. This case is the closest to the following formulations of the stochastic problems, and is therefore used for comparison. We define EV as the value of the optimal solution to the problem with all data set to their expected values.

Madansky [1960] has shown that for a linear program with uncertain right-hand sides the following inequalities hold:

$$\text{EV} \le \text{WS} \le \text{RP} \le \text{EEV} \qquad (3)$$

We shall examine the actual values obtained in our example to see whether these inequalities hold for our nonlinear convex and nonlinear non convex sample problem.

Birge [1982b] has defined the value of the stochastic solution

$$\text{(VSS) as} \text{VSS} = \text{EEV} - \text{RP} \qquad (4)$$

Which is the difference between the expected total costs (including recourse) for the solution from the model not explicitly considering uncertainty (the expected value model), and the model that did explicitly consider uncertainty (the full recourse model).

Results

In this section, a sample problem of determining a pumping plan to contain an area of groundwater contamination is described. This problem is then solved using the above stochastic programming formulations, and the results of the different formulations are compared.

Description of the Sample Problem

The sample contaminant containment problem used in this paper, is a smaller version (10 x 11 cells) of a sample problem examined by Gorelick (1987) [8]. Measuring from the bottom of the aquifer, the confining layer is at 100 m and the surface at 150 m. A 1% gradient is imposed by constant head boundarian of 110 m to the north and 100 m to the south. To the east and west are no-flow boundaries. The capture curve (show in the figure) has 17 "edges" and there are 23 possible pumping wells.

The daily cost of pumping (A_1) was set to \$13.824 $m^{-3}m^{-1}d^{-1}$. This figure is based on 0.0032 kWh of energy ti lift 1 m^{-3} of water a height of 1 m and \$0.05 kWh^{-1} for electricity. In all formulations, two sets of problems were run, on set including no benefit of water ($A_2 = 0$) and the other set with the benefit $A_2 = 500(m^3)^{-2}d^{-1}$.

The maximum pumping rate ($\overline{w}$) was set to 0.1 $m^3s^{-1}$for all wells. The maximum is quite high, and was rarely an active constraint.

The mean hydraulic conductivity was taken from *gorelick* [1987] [8]. To be 0.0004 ms^{-1}, giving a transmissivity of 0.04 m^2s^{-1}. To generate realizations of heterogeneous hydraulic conductivities, the turning bands program requires the (geometric) mean hydraulic conductivity value of the lognormal hydraulic conductivity distribution and the standard deviation of the underlying normal distribution. A standard deviation of 1 was used. Thus 95% of the in K values should fall between -8.82 and -6.82, corresponding to a range of K values of 0.000147 to 0.000108 ms^{-1}. For all cases, the hydraun conductivities were assumed to be isotropic and exponentially correlated with the correlation scale equal to 10 m.

On hundred realizations of the hydraulic conductivities were generated ($\Omega = 100$). Ideally, a different set of realizations would be run for each formulation, but due to the time involved in inverting the F matrices, both the "wait and see" and the same 100 realizations.

For all cases, the parameter values were $p = 0.1$ $q = 10$. Problems with a single realization such as the expected value problem and the individual "wait and see" problems were solved directly using GAMS (version 2.02)/MINOS (version 5) [Broke *et al.*, 1988]. The recarsue problem was solved using the extended finite generation algorithm [Wagner, 1988] [20].

Expected Value Problem Results

If we set all the hydraulic (0.0004 ms^{-1}), we obtain a deterministic problem with homogeneous soil. We can model this problem two ways: (1) with the gradient restrictions allowed but penalized in the objective function. The non linier program with the gradient restrictions as "hard" constraints.

$$\text{Min} \sum_i A_1 w_i \left(s - \sum_j \overline{F}^{-1}_{i,j} [w_j - f_j\} \right) - A_2 \left(\sum_i w_i \right)^2$$

Subject to

$$\sum_j \overline{G}_{I,j} \{w_j - f_i\} \le 0 \qquad \forall j$$

$$0 \le w_i \le \overline{w} \qquad \forall i \tag{5}$$

Where $\overline{F}^{-1}$ and $\overline{G}$ domain the expected values of the F^{-1} and G matrices.

The nonlinear program with the gradient restrictions as "soft" constraints is

EV=min

$$\sum_i A_1 w_i \left(s - \sum_j \overline{F}^{-1}_{i,j} [w_j - f_j\} \right) + \sum_i \rho(v_j) - A_2 \left(\sum_i w_i \right)^2$$

Subject to

$$v_j = \sum_j \overline{G_{i,j}} \{w_j - w_j\} \le 0 \qquad \forall j$$

$$0 \le w_i \le \overline{w} \qquad \forall i \tag{6}$$

The first problem involves no benefit of water ($A_2 = 0$) and the so is convex. The second problem does involve a benefit of water ($A_2 = 500$) and is not a convex problem. As expected, the cost is lower and optimal pumping rates are higher for the case when benefit is obtained from the water. When the gradient restrictions are treated as "soft" constraints the total cost is less, again as expected. All results show symmetry, also as expected.

The expected value problem with the penalized gradient constraints is the closest formulation to the subsequent problems, and can best be used for comparison. Thus from these runs EV = \$169.71 for the no-benefit case and EV = \$131.71 for the benefit case.

Distribution problem results

If we were able to repeatedly "wait and see" what the hydraulic conductivities were and subsequently solve the optimization problem, we would obtain a distribution of optimal pumping costs. In order to approximate the "wait and see" distribution we solved 100 deterministic problems (one for each realization of the hydraulic conductivities) and then analyzed the statistics of the outcomes. The "wait and see" problem is

WS_A=min

$$\sum_i A_1 w_i \left(s - \sum_j \overline{F}^{-1}_{i,j,k} [w_j - f_j\} \right) + \sum_i \rho(v_{i,k}) - A_2 \left(\sum_i w_i \right)^2$$

Subject to

$$v_{i,k} = \sum_j G_{I,j,k} \{w_j - f_j\} \qquad \forall l$$

$$0 \le w_i \le \overline{w} \qquad \forall i \tag{7}$$

We then estimate the expected value of the distribution by taking the mean of mean these solutions:

$$WC \sum_{k=1}^{\Omega} v_k WC_k \tag{8}$$

The first set of runs was intended to examine the convex problem, where no benefit is derived from the water that is pumped from the site. One hundred scenarios were run, producing a minimum cost ranging from \$46.90 to \$437.53, with an average of \$171.54. A histogram of the results is shown in figure 3. About 83% of the total costs were between \$150 and \$250. The penalty cost ranging from \$2.73 to \$302.85. These penalty costs represent between 6% and 70% of the total cost with an average of 44% over all 100 outcomes. The optimal number of well used for these scenarios ranged from a minimum of two to a maximum of five wells, with 93% of the outcomes using two, three, or four wells. The 11 interior wells were never used. Of the remaining 12 wells, the wells at the beginning and the and of the fifth row were used 79% and 77% of the time, respectively. In the second set of runs we included benefit obtained from the water pumped from the site ($A_2 = 500$). Minimum total cost ranged from -\$6914.45 to \$409.25. (Only two outcomes had negative costs, indicating that enough benefit could be obtained from the pumped water so as to make a profit. Far there two ounces, the optimal pumping plan included some of the wells being pumped at their maximum

rates, leading to unrealistic head gradients. Thus these two pumping plans are neglected in the subsequent calculations. About 78% of the outcomes had minimum total cost of between \$100 and \$ 200. The average minimum total cost of the plans with positive cost was \$152.55. This average cost is less than the no-benefit case (\$171.54) since the revenues from the water pumped out can be used to reduce the total cost of operation. The percent of total cost of operation that is due to the penalty cost had a range of between 0% and 73% with an average of 34%. The number of well used ranged from a minimum of two to a maximum of 12, with 92% of the outcomes using two, three, of four wells. As in the run with no benefit from the water, the 11 interior wells were never used. Again the wells at the beginning and the end of the fifth row were the most widely used, 72% and 65% respectively.
From these runs, WS = \$171.54 for the no-benefit case and WS = \$152.55 for the benefit case.

Recourse Problem Results

The recourse problem includes a number of realizations of the hydraulic conductivities. The solution to the recourse problem provides the pumping plan that minimize the expected total cost (including recourse cost) over these realizations. For these problems, 100 sets of hydraulic conductivity realizations were used. This problem (developed previously) can be stated as

$$RP = \min \sum_{\omega} \pi_{\omega} \left[\sum_{i} A_1 w_i \left(s - \sum_{j} \overline{F}^{-1}_{i,j,\omega} \{w_j - f_j\} \right) + \sum_{i} \rho(v_{l,\omega}) \right] - A_2 \left(\sum_{i} w_i \right)^2 {}_2$$

Subject to

$$v_{l,\omega} = \sum_{j} G_{I,j,\omega} \{w_j - f_j\} \qquad \forall l \forall \omega$$

$$0 \le w_i \le \overline{w} \qquad \forall i \tag{9}$$

Again, two cases were run, one with and one without benefit of water. The expected total cost for the case with no benefit of water was \$217.51, which included 51% for expected recourse costs. The total costs over the 100 outcomes ranged from \$108.34 to \$508.33. A histogram of the results is shown in Figure 4. The total pumping in this case was 0.181 m^3s^{-1}. The expected total cost for the case including benefit of water was \$196.96, which included 48% for expected recourse costs. The total costs over the 100 outcomes ranged from \$103.07 to \$436.18. The total pumping in this case was 0.216 $m^3 s^{-1}$.
In both of these solutions only four or five wells, out of a possible 23, are to be used. These wells are on the "edges" of the pumping area. We also note that the pumping pattern is no longer symmetrical. Over one realization with heterogeneous soil we would, in fact, not necessarily expect the pumping plan to be symmetry may indicate that more than 100 realization should be used in the model. *Gorelick* [1987] [8]. Also obtained asymmetric optimal pumping plans. From these runs, RP = \$217.51 for the no-benefit case and RP = \$196.96 for the benefit case. The problem for the case benefit of water is convex, so the finite generation algorithm will converge [*Rockafellar and Wets, 1986 a,b*] [17]. And it will converge to the global minimum. For the non-convex case (with benefit of water) we have no such assurances. To test the convergence of the solutions and the robustness of this solution, the optimal solution obtained from the recourse problem was perturbed by first adding and then subtracting a small value to each possible pumping well in turn. The expected costs of these perturbed solutions were then computed. For very small perturbations (±0.001) some perturbed solutions did have slightly lower expected costs than reported "optimal" solution, indicating that the algorithm had not quite converged. However, perturbing the solutions by ($\perp$ 0.05) did result in all expected costs from the perturbed solutions being higher than unperturbed solution. Indicating that the reported solution is indeed quite close to an actual (at least) local minima.
We find that the EEV for the non-benefit case has an expected cost (including recourse) of \$262.71, with 40% of this cost due to recourse costs. For the case including benefit, EEV is \$230.45, with 46% due to recourse costs.
We also see that the form of the solutions is somewhat different when uncertainty is explicitly included. The recourse solutions call for less pumping than the expected value solutions. In a sense, the solutions from the recourse formulations can be thought of as reserving some of the budget available "here and now" to pay "wait and see" recourse cost.
In summary, for the no benefit of water case,

$$(EV = \$169.71) \le (WS = \$\ 171.54) \le (RP = \$\ 217.51) \le (EEV = \$262.71). \tag{10}$$

And for the case when benefit of water is included,

$$(EV = \$131.71) \le (WS = \$152.55) \le (RP = \$196) \le (EEV = \$230.45). \tag{11}$$

We see that Madansky's inequalities do hold for these non linier problems. The value of the stochastic solution (EEV – RP) is \$15.20 for the no benefit cost and \$22.12 for the benefit case. Thus, ignoring the uncertainty in the model formulations (by using the EV solutions and then paying recourse) increases the expected costs by 21% in the no-benefit case and 17% in the benefit case. Aquifer remediation programs are often extremely expensive; thus savings in the range of 20% could be quite significant.
It is also interesting to compare the expected costs of the recourse solution with the expected "wait and see" cost. The " wait and see" cost is 21% less than the expected recourse cost for the no benefit case and 23% less in the benefit case. Thus we estimate that we are paying a penalty of about 20% due to the fact that we must determine a pumping plan without knowing the heterogeneous hydraulic conductivities.

Conclusions

Uncertainty in aquifer parameters affects the management of groundwater quality. Solutions from models that explicitly incorporate uncertainty are different from those that only use the expected values of uncertain parameters, and models that incorporate uncertainty can lead to savings, at least in the expected value sense.
Stochastic optimization can be used to explicitly incorporate uncertainty in management models. These techniques, although sophisticated, can be used without extensive computer resources. Small problems can be solved using PCs; larger problems could be solved on workstations.
The simple recourse formulation is useful for incorporating uncertainty and can, we believe, be used to model fairly realistic situations. The extended finite generation algorithm is available to solve nonlinear and non-convex problems (with possibly only locally optimal solutions). This model allows

considerable flexibility to the decision maker in the representation of and managerial response to uncertainty.

There are a number of possibilities for extensions of this work. Larger and more realistic containment problems could be solved using this technique. Presently the most time-consuming step, and the step requiring the most computer resources, is the inverting of the F matrices. The current inversions were done using a fairly time-efficient algorithm, but no attempt was made to save space by exploiting the special banded structure of the F matrix. More sophisticated matrix storage and inversion routines would allow faster preprocessing of the data to the extended finite generation algorithm and so would allow considerably larger problems to be solved. In the actual optimization step, the size of the problem is determined only by the number of possible pumping wells, not by the number of finite elements considered, so the size of the area studied need not be of great concern.

Chance constraints could also be included in the finite generation algorithm, with no additional work, by including the deterministic equivalents as "hard" constraints in the recourse model. This approach was used with the finite generation algorithm for convex problems by *Eigerand Shamir* [1991] for a problem of managing reservoir operations. Additionally, measurements of hydraulic conductivities taken at the site can be incorporated into this procedure, and thus reduce the uncertainty in these values. Using a method developed by *Wagnerand Gorelick* [1989] the realizations of the hydraulic conductivities generated for use in the optimization problem could be made conditional upon available measurements.

The solution methods could also be extended in a number of ways. Some preliminary work has been done in including concentration variables so as to directly manage the water quality [*Wagner,* 1988]. It would also be interesting to see if the model could be extended to a dynamic case, in order to examine the transient behavior of gradients and contaminants under possible containment and remediation plans.

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