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Abstract

In this paper we consider two model problems in groundwater supply optimization, implement the objective functions and constraints with MODFLOW, a widely-used production code, and solve the problems with the implicit filtering algorithm. These constraints and objective functions are discontinuous and have multiple local minima. Our objectives are not only to show how the problems can be formulated and solved, but also to make the data and codes available to the community. We provide the data for our formulation and solution on the web.

1 Introduction

The objectives of this paper are to show how a class of model problems in groundwater supply optimization can be formulated and solved, and to make the codes that generate our results publicly available, as test problems for both the optimization and hydrology communities. While considerable work has been done in optimal desing of subsurface systems (see [1, 21] and the papers cited therein), this paper is unique in that we enable the reader to easily modify our approach to formulation, simulation, and optimization by exchanging the simulator or the optimization code, or by formulation the optimization problem in a different way.

The objective functions that we consider in this paper are, as we formulate them, nonconvex and discontinuous. The discontinuity arises from the requirement that the wells be located at grid points of the simulator. This is the most significant difficulty and influences our choice of optimization algorithm, as does the likely presence of local minima that are not satisfactory solutions of the

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problem. A lesser issue is that errors in the flow simulator produce low-amplitude noise, but that noise is not an issue in this paper. The discontinuities and nonconvexity can cause cause a gradient-based optimizer to fail, either in the attempt to differentiate a non-differentiable function or by entrapment in a local minimum that is far from a useful result.

It is natural to approach this problem with a method that does not use derivative information. Global optimization methods such as genetic and evolutionary algorithms [2, 16, 25, 27], simulated annealing [20, 26], and tabu search [31] have been have been applied to many subsurface remediation problems (see [21] for many more references).

In this paper we take the view that there is enough structure in the problem to use a deterministic sampling method. These methods are designed to solve problems with difficult, but not violently oscillatory optimization landscapes, such as the ones in Figures 8.4, and 8 in § 8. The Nelder-Mead [24], Hooke-Jeeves [15], MDS [9, 30], DIRECT [17], and implicit filtering [12, 13, 18] are examples of discrete sampling methods.

We begin with a description of the model problems that is independent of any implementation. We then show how we built tractable formulations of the problems. This process included choosing the underlying simulator, optimization method, formulation of constraints, and the approach to handling the location and number of wells.

Managing a subsurface system includes making decisions about water resources and contaminated site cleanup requiring optimal design for problems involving groundwater flow and transport. Formulation and solution of such an optimal design problems requires

- development of a conceptual model for the physical phenomena,
- formulation of the governing equations and closure relations as a well-posed problem,
- using this formulation to develop an objective function and constraints,
- realization of the objective function and constraints via simulation, and
- solution of the optimization problem.

In [21, 22] a suite of test problems is proposed for the purpose of benchmarking and comparing optimizers. In this work we describe an implementation of a subset of the applications proposed in [21], and present optimization results obtained with a FORTRAN implementation [7] of the implicit filtering [18] algorithm.

The remainder of the paper follows the steps above, intending to lead the reader though the formulation and solution of the problems. We have made the numerical data and codes available at

http://www4.ncsu.edu/˜ctk/community.html

so that the reader may implement the problems with a different simulator, another formulation of the optimization problem, or a different optimization algorithm.

2 Conceptual Model

An aquifer is a fully saturated, water-bearing region and is considered confined if bounded on both the top and the bottom by essentially impermeable material. An unconfined aquifer has the water table as its upper bound. The main difference between the two geological formations is that the saturated thickness of an unconfined aquifer can vary as the hydraulic head varies, thus leading to a nonlinear free boundary value problem.

We consider a well-field design problem. The hydrological settings are homogeneous confined and unconfined aquifers aquifers in three dimensions. For the problems considered a set of wells is distributed in the domain. Each well is allowed either to inject or extract water. Well-field design problems involve the selection of well locations and pumping rates to minimize the cost of water production. The cost of supplying water typically involves the cost to drill, equip, and connect wells to a treatment or distribution system, and the cost to pump the water and maintain the well. In turn, the cost to pump groundwater depends upon the energy needed to lift the water from its level below the ground surface to the discharge point and to supply sufficient discharge pressure to achieve the desired flow. Since groundwater supplies the drinking water needs of about 50% of the population of the U.S., this sort of application occurs routinely.

The decision variables for this type of problem are the pumping rates $\{Q_i\}_{i=1}^n$ (m^3/s) at the n wells in the model and the locations $\{(x_i, y_i)\}_{i=1}^n$ of the wells. Pumping rates can be constant or variable in time depending upon the application.

3 Formulation

Flow in saturated porous media can be described by

$$S_s \frac{\partial h}{\partial t} = \nabla \cdot (K \nabla h) + \mathcal{S}, \tag{1}$$

where S_s (1/m) is the specific storage coefficient, the unknown h (m)is the hydraulic head, K (m/s) is the hydraulic conductivity. Here the source term $\mathcal{S}$ is a model of the wells, a sum of δ-functions, for example, that satisfies

$$\int_\Omega \mathcal{S}(t) d\Omega = \sum_{i=1}^{n} Q_i. \tag{2}$$

Ω is the spatial domain.

For the confined aquifer, we use the following boundary and initial conditions:

$$\left.\frac{\partial h}{\partial x}\right|_{x=0} = \left.\frac{\partial h}{\partial y}\right|_{y=0} = \left.\frac{\partial h}{\partial z}\right|_{z=0} = 0, t > 0 \tag{3}$$

$$q_z(x, y, 30, t > 0) = -1.903 \times 10^{-8} \text{(m/s)} \tag{4}$$

$$h(1000, y, z, t > 0) = 50 - 0.001y \text{(m)} \tag{5}$$

$$h(x, 1000, z, t > 0) = 50 - 0.001x\text{(m)} \tag{6}$$

$$h(x, y, z, 0) = h_s \tag{7}$$

Here

$$q_z = -K\frac{\partial h}{\partial z}$$

is the Darcy flux out of the domain, a negative sign in eqn (4) thus represent flow into the aquifer or recharge that could be the result of rainfall infiltration or leakage from an overlying aquifer, and h_s is the steady state solution to the flow problem prior to the addition of wells. We use $S_s = 10^{-6}$ (1/m). For the unconfined aquifer, (4), (5) and (6) are replaced with

$$q_z(x, y, h, t > 0) = -1.903 \times 10^{-8}\text{(m/s)}, \tag{8}$$

$$h(1000, y, z, t > 0) = 20 - 0.001y\text{(m)}, \tag{9}$$

and

$$h(x, 1000, z, t > 0) = 20 - 0.001x\text{(m)}. \tag{10}$$

$S_s = 2.0 \times 10^{-1}$ is the specific yield of the unconfined aquifer. For the homogeneous applications, $K = 5.01 \times 10^{-5}$ (m/s).

The physical domain is $\Omega = [0, 1000] \times [0, 1000] \times [0, 30]$ m with the ground elevation at $z_{gs} = 60$ m for the confined aquifer and $z_{gs} = 30$ m for the unconfined aquifer.

4 Objective Function

We consider a capital cost f^c and an operational cost f^o seeking to minimize $f^T = f^c + f^o$. The objective function depends on the pumping rates $\{Q\}_{i=1}^n$ and locations $\{(x_i, y_i)\}_{i=1}^n$ of n operating wells. Note that $Q_i < 0$ means the well is extracting water, and $Q_i > 0$ means the well is injecting water. For this work, we begin with a virtual fixed well field containing N wells with the number of operating wells $n \leq N$.

A well is considered operating if $|Q_i| > 0.0001$. Once the pumping rate falls below this level, the well is no longer changing the flow field significantly. In that case, we remove the well from the objective function and no longer considered it installed. This may lead to a well being turned off during the optimization, and we did observe that in a six well optimization.

Our simulations were over a time of $t_f = 5$ (years).

The objective function is given by

$$f^T = \underbrace{\sum_{i=1}^{n} c_0 d_i^{b0} + \sum_{Q_i < -.0001} c_1 |Q_i^m|^{b_1} (z_{gs} - h^{min})^{b_2}}_{f^c} + \tag{11}$$

$$\underbrace{t_f\left(\sum_{i,Q_i<-.0001} c_2 Q_i (h_i - z_{gs}) + \sum_{i,Q_i>.0001} c_3 Q_i\right)}_{f^o},$$

where the cost coefficients c_j and exponents b_j are given in Table 1. Here d_i is the depth of well i, Q_i^m is the design pumping rate, h^{min} is the minimum allowable head, h_i is the hydraulic head in well i, t_f is the total time horizon, and z_{gs} is the elevation of the ground surface. Injection wells are assumed to operate under gravity feed. In f^c, the first term denotes the cost to install all the wells, and the second term accounts for the additional cost for pumps for the extraction wells. In f^o we have a lift cost that applies to the extraction wells and a different operational cost that applies to the injection wells.

Table 1: Objective Function Data

data	value	units
c_0	5.5×10^3	$\$/m_0^b$
c_1	5.75×10^3	$\$/[m^3/s)^{b_1} \cdot m^{b_2}]$
c_2	2.90×10^{-4}	$\$/m^4$
c_3	1.45×10^{-4}	$\$/m^3$
b_0	0.3	-
b_1	0.45	-
b_2	0.64	-
z_{gs}	60 confined	m
z_{gs}	30 unconfined	m
d_i	z_{gs}	m
Q_i^m	$1.5Q_i$	m^3/s

5 Constraints

We constrain the hydraulic head and pumping rates for the objective function given in (11). The constraints are given by

$$Q_T = \sum_{i=1}^{n} Q_i \leq Q_T^{min}, \tag{12}$$

$$Q^{emax} \leq Q_i \leq Q^{imax}, \; i = 1, ..., n, \tag{13}$$

and

$$h^{min} \leq h_i \leq h^{max}, \; i = 1, ..., n, \tag{14}$$

where Q_T is the net pumping rate, Q_T^{min} is minimum allowable total extraction rate, Q^{emax} is the maximum extraction rate at any well, Q^{imax} is the maximum injection rate at any well, h^{max} is the maximum allowable head, and h^{min} is the minimum allowable head. Values for the bounds in the constraints are given in Table 2. We require that the wells be at least 200 m from the boundary on which Dirichlet boundary conditions are applied, *i. e.*

$$0 \leq x_i, y_i \leq 800. \tag{15}$$

Constraint (12) sets a minimum target for extraction, which is the purpose of the well field. For the problem considered here, the installation costs are far more that the operating costs for a single year. Therefore, once the minimum extraction target is reached, it would only make sense to drill additional wells if the long-term operating savings is significant. Since five wells extracting at the maximum level satisfy (12) with equality, one logical formulation of the problem is to find the optimal location of five wells, each extracting as much as possible.

Constraint (13) reflects physical limits on the pumps and well design.

The upper bound in constraint (14) keeps the hydraulic head below the surface elevation and the lower bound ensures that excessive drawdown will not occur. This constraint is a linear function of the pumping rates, but a highly nonlinear function of the locations of the wells.

Table 2: Constraint Data

data	value	units
Q^T	-3.2×10^{-2}	m^3/s
Q^{emax}	-6.4×10^{-3}	m^3/s
Q^{imax}	6.4×10^{-3}	m^3/s
h^{min}	40 confined	m
h^{max}	60 confined	m
h^{min}	10 unconfined	m
h^{max}	30 unconfined	m

5.1 Optimization Problem Formulation

In this section we describe how we packaged the problem for the optimization algorithm. The objective function f^T is discontinuous, and some of the constraints (13) and (15) are simple bounds on the variables. Implicit filtering, the optimization method we use in this paper, is designed to handle difficult objective functions and bound constraints.

The constraint on the heads (14) is highly nonlinear. If we set $n = 5$, then the pumping rates are all $Q_T^{min}/5$ and the linear constraint (12) on the pumping rates is satisfied automatically. If we set $n > 5$, then (12) and (14) are treated in the same way. Our implementation of implicit filtering incorporates constraints other than simple bounds into the objective function by having the function report a failure when the constraints are violated. This is a standard approach for many sampling methods [6, 19, 29]. The optimization method will assign an artificial (see § 6.2) value to the function in that case.

We will fix the number of wells and consider the vector of design variables

$$Z = (Q_1, \ldots, Q_n, x_1, \ldots, x_n, y_1, \ldots, y_n)^T \in R^{3n}.$$

We define the feasible set for the bound constraints as

$$\mathcal{D}_0 = \{Z \mid \text{ (13) and (15) hold.}\} = \{Z \mid Z_i^{min} \le Z_i \le Z_i^{max}\}. \tag{16}$$

Our optimization problem is

$$\min_{Z \in \mathcal{D}_0} f^T(Z), \tag{17}$$

where f^T is given by (11) if (12) and (14) are satisfied and a failure is reported if either of (12) or (14) are violated.

6 Implicit Filtering

The objective function is discontinuous because of the jumps as wells are added and deleted, and noisy, because of internal iterations in the simulators. For these reasons, as we said in $\S$ 1, a conventional gradient-based optimization method may fail. A sampling method, which only evaluates the objecive function and constraints to guide the optimization, is most appropriate for this kind of problem.

In this paper we use IFFCO [7], a FORTRAN implementation of the implicit filtering algorithm [12, 13, 18]. We based this decision on our own familiarity with the optimizer and our past success with it on other problems of a similar nature [3, 6, 29]. This choice significantly influenced the decisions on handling constraints and the locations of the wells.

Implicit filtering has been described in detail and analyzed elsewhere. We refer the reader to [18] for the details of the algorithm and to [8, 13, 18] for convergence analysis. In $\S$ 6.1 we sketch the algorithm and its implementation in IFFCO only in enough detail to explain how this choice affected the formulation of the problem.

6.1 The algorithm

Implicit filtering is a projected quasi-Newton method that uses finite difference gradients. The difference increment is reduced as the optimization progresses, thereby avoiding some local minima, discontinuities, or nonsmooth regions that would trap a conventional gradient-based method. The problems considered in this paper are exactly the kind that the method was designed to solve.

Implicit filtering begins by rescaling the variables so that the feasible region is

$$\mathcal{D} = \{\xi \mid 0 \le \xi_i \le 1\}. \tag{18}$$

We will discuss the algorithm in terms of the scaled feasible region in (18) but the application in terms of the actual bounds (16).

To make the transition from f^T to the scaled form, we define ξ componentwise by

$$\xi_i = (Z_i - Z_i^{max})/(Z_i^{imax} - Z_i^{emax})$$

and let

$$f(\xi) = f^T(Z).$$

The optimization problem for f is now

$$min_{\xi \in \mathcal{D}} f(\xi).$$

For a given difference increment (called a **scale**) $\delta \in (0, 1/2]$ and $\xi \in \mathcal{D}$, we let $\nabla_\delta f(\xi)$ be the difference gradient whose components are

- the central difference gradient in the ith coordinate direction if both of $\xi \pm \delta e_i \in \mathcal{D}$, or
- the one-sided difference gradient in the i coordinate direction if only one of $x \pm \delta e_i \in \mathcal{D}$.

Since $\delta \leq 1/2$, at least one of $\xi \pm \delta e_i \in \mathcal{D}$. We let the stencil $S(\xi)$ be those points in the centered difference stencil that are in $\mathcal{D}$ and used in the computation on $\nabla_\delta f$. If

$$f(\xi) \leq \min_{\eta \in S(\xi)} f(\eta) \tag{19}$$

we say that **stencil failure** has occurred and terminate the quasi-Newton iteration at that scale.

If H is a model Hessian, a project quasi-Newton iteration from x has the general form

$$\xi(\lambda) = \mathcal{P}(\xi - \lambda H^{-1} \nabla_\delta f(\xi)),$$

where $\mathcal{P}$ is the projection onto $\mathcal{D}$

$$\mathcal{P}(\xi)_i = \begin{cases} 0 & \text{if } \xi_i \leq 0 \\ \xi_i & \text{if } 0 < \xi_i < 1 \\ 1 & \text{if } \xi_i \geq 1 \end{cases}$$

In IFFCO, the step length λ is computed with a quadratic model [7] and a step is accepted if the sufficient decrease condition

$$f(\xi(\lambda)) - f(\xi) \leq \alpha \nabla_\delta f(\xi)^T (\xi(\lambda) - \xi), \tag{20}$$

holds. In IFFCO, as is standard, $\alpha = 10^{-4}$. We say that the quasi-Newton iteration is successful if

$$\|\xi - \xi(1)\| \leq \tau\delta. \tag{21}$$

The algorithmic parameter τ can have a significant effect on the performance of the optimization. For the problems we consider here, however, we were able to successfully use the default value of $\tau = 1$.

The finite difference projected quasi-Newton loop in IFFCO is summarized in algorithm **fdquasi**. `fdquasi` is a naturally parallel algorithm; all the function evaluations needed to compute $\nabla_\delta f$ can be done in parallel. We exploited this simple parallelism to perform the computations reported in this paper.

Implicit filtering calls **fdquasi** repeatedly with a sequence of scales $\{\delta_k\}$. Algorithm **imfilter** is a simple sketch.

The algorithmic parameters that are important to implicit filtering are the limit $amax$ on the number of step size reductions, $pmax$ on the number of nonlinear iterations, and the parameter τ

Algorithm 1 fdquasi$(\xi, f, pmax, \tau, \delta, amax)$

```
p = 1
while p ≤ pmax and ‖ξ − P(ξ − ∇_δ f(ξ))‖ ≥ τδ do
   compute f and ∇_δ f
   if (19) holds then
      terminate and report stencil failure
   end if
   update the model Hessian H if appropriate; solve Hd = −∇_δ f(ξ)
   use a backtracking line search, with at most amax backtracks, to find a step length λ
   if amax backtracks have been taken then
      terminate and report line search failure
   end if
   x ← P(ξ + λd)
   p ← p + 1
end while
if p > pmax report iteration count failure
```

Algorithm 2 imfilter$(\xi, f, pmax, \tau, \{\delta_k\}, amax)$

```
for k = 0, . . . do
   fdquasi(ξ, f, pmax, τ, δ_k, amax)
end for
```

in the termination criterion. For the calculations reported here, we set $pmax = 100$ (the default), $\tau = 1$ (the default), and $amax = 3$ (the default). The parameters in **filter** that control the quasi-Newton loop are the sequence of scales $\{\delta_k\}$. Our choice in this work was

$$\delta_k = 2^{-k-1},\ 0 \le k \le 10.$$

The analysis of implicit filtering begins with the paradigm

$$f = f_S + \phi \tag{22}$$

where f_S is a smooth function and ϕ represents the "noise" in the problem. For the theoretical convergence results in [8, 18, 29] we assume that ϕ is an everywhere-defined function on Ω and set

$$\|\phi\|_{S(\xi)} = \max_{\eta \in S(\xi)} |\phi(\xi)|.$$

One can show that if either (19) or (21) hold, that

$$\|\mathcal{P}(\xi - \nabla f_S(\xi))\| = O(\delta + \|\phi\|_{S(\xi)}/\delta). \tag{23}$$

The convergence theory for implicit filtering [8, 13, 18] are based on (23).

IFFCO supports the SR1 [4, 10] and the BFGS [5, 11, 14, 28] quasi-Newton models of the Hessian. We used the SR1 update in this paper. In our experience the SR1 update performs better for bound-constrained problems.

Implicit filtering can be restarted after it terminates and the convergence theory [13] is stronger if one does that. In practice, restarting usually has no effect. For the problems in this paper, however, we had to restart IFFCO once to obtain consistently good results.

6.2 Failure of the function

IFFCO responds to a failure of f in two ways. If the failed function evaluation $f^T(z)$ is part of the evaluation of $\nabla_h f^T(\xi)$, then an artificial value of

$$f^* + 10^{-6}|f^*|$$

is assigned to $f(z)$. Here f^* is the largest function value in the stencil $S(\xi)$. If the function evaluation failure is part of the line search, the the value $fscale$ is assigned to f^T.

$fscale$ is an approximation to the maximum value of f^T in the feasible set $\mathcal{D}_0$ for the bound constraints (16). We set $fscale$ to 20% more than the value of f at the initial iterate in this paper.

This approach to handling constraints is natural and essential if the failure of the objective function is a consequence of, for example, an internal iteration's failure to converge. In the case of the problem considered here, while the constraints are directly specified by (14), the evaluation of h_i requires a call to the simulator which, as a function of the well locations, is highly nonlinear even for the continuous problem. For the discrete problem considered here, where the well locations are not rounded to grid points before the call to the simulator, the constraint function is discontinuous.

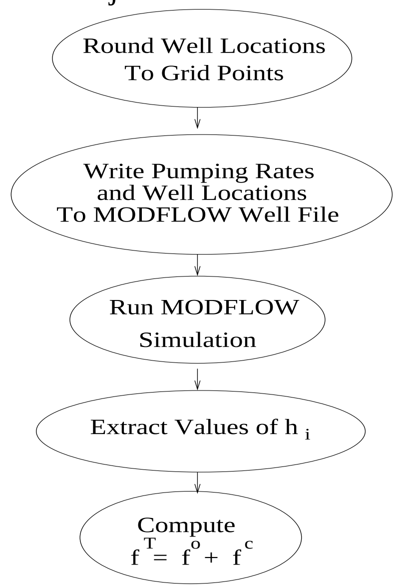
7 Evaluation of the Objective Function

IFFCO requires an external subroutine to evaluate the objective function f^T. To do this we must compute the hydraulic head values, $\{h_i\}$, at the well locations $\{(x_i, y_i)\}$ for a given set of pumping rates $\{Q_i\}$. Computation of $\{h_i\}$ uses a groundwater flow simulator to solve (1). For this work we use the U.S. Geological Survey code MODFLOW 96 [23]. MODFLOW is a block-centered finite difference code that simulates saturated groundwater flow and allows for a variety of boundary conditions and irregular physical domains. MODFLOW is widely used and well supported.

A MODFLOW simulation requires an input file containing the location and pumping rates of the wells in the model. Note that each function evaluation requires a new set of pumping rates and thus the MODFLOW well file must be created each time the objective function is evaluated. Moreover, once the MODFLOW simulation is complete, the values of h_i must be extracted from the MODFLOW output file. A typical function evaluation is shown in Figure 1.

To generate the necessary data files to run MODFLOW we use the **G**roundwater **M**odeling **S**ystem (GMS), version 3.1. GMS is a modular interface to a variety of flow and transport codes, including MODFLOW. GMS has a graphical environment that allows the user to generate grids, define characteristics of the porous media, and visualize solutions. GMS was used to generate the starting heads for (7), to create the necessary data files for MODFLOW, to determine an appropriate initial iterate for the optimization, and then again to test the results of the optimizer.

Figure 1: Objective Function Evaluation



8 Numerical Results

8.1 Spatial Discretization

For the confined aquifer we discretize the domain $\Omega = [0, 1000] \times [0, 1000] \times [0, 30]$ (m) on an equally spaced $50 \times 50 \times 10$ grid. For the unconfined aquifer, we used MODFLOW to determine the saturated domain $\Omega_{unc} = [0, 1000] \times [0, 1000] \times [0, 27] \subset \Omega$ and then discretized Ω_{unc} on an equally spaced $50 \times 50 \times 10$ grid.

8.2 Initial Iterate

IFFCO requires a feasible initial iterate. Figure 2 shows the steady state flow field for the confined aquifer. Since the head value is high in the lower left corner we initially placed one well there. After the wells are activated, the constraint on the drawdown is violated if the wells are too close together. We looked at several different initial iterates until we found one that satisfied the drawdown constraint for both the confined and unconfined aquifer. We found that placing the remaining four wells close to the specified head boundaries and significantly apart from each other was feasible for both physical domains. Figure 3 shows the relative location of the wells and the pressure head field for confined aquifer with the wells pumping at the initial iterate. Note the same initial well locations were used for both aquifers.

Figure 2: Steady state head, confined aquifer

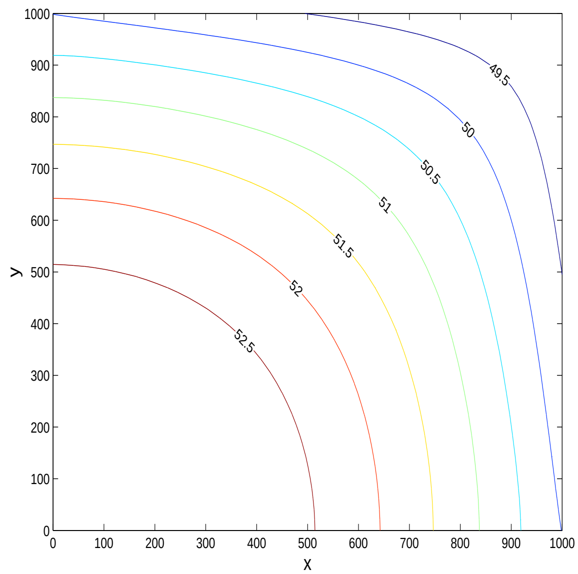
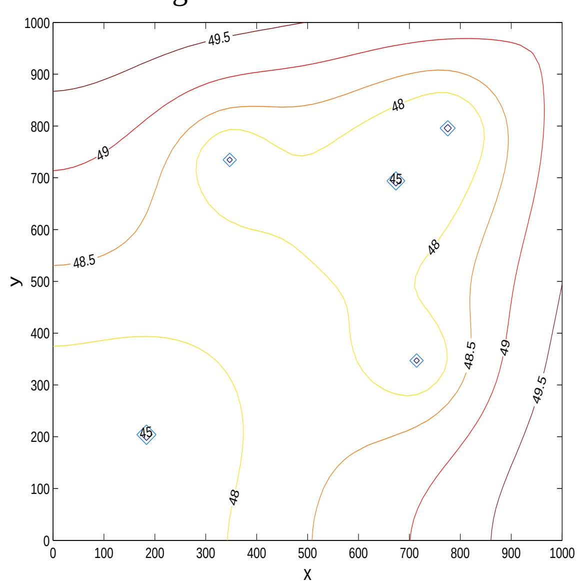


Figure 3: Initial Iterate



8.3 Results

We refer to the confined aquifer as CON and unconfined aquifer as UNC. Table 3 shows the function value obtained at the initial iterate, the minimum function value,the percent decrease in the objective function, the number of function evaluations needed for each aquifer. Table 4 shows the initial x-y coordinates for the 5 wells and the optimal locations for each aquifer.

Table 3: Decrease in Cost

Problem	f(init_co)	min f	% decrease	No. f'evals
CON	\$2.3204e+04	\$2.1830e+04	6%	275
UNC	\$2.6958e+04	\$2.3930e+04	11%	302

Table 4: Optimal Locations

X/Y	Init_Co (m)	CON (m)	UNC (m)
X(1)	350.0	401.7	464.2
Y(1)	725.0	800.0	800.0
X(2)	775.0	800.0	800.0
Y(2)	775.0	800.0	800.0
X(3)	675.0	776.9	800.0
Y(3)	675.0	481.1	445.4
X(4)	200.0	138.2	138.2
Y(4)	200.0	800.0	800.0
X(5)	725.0	798.4	800.0
Y(5)	350.0	168.9	144.8

Figure 4 shows the decrease in the objective function value over the course of the optimization.

Figures 5 and 6 show the head contours in the layers containing the wells with the wells at the optimal locations.

8.4 Optimization Landscapes

To get a better understanding of the objective function, we fixed wells 2-5 and let the x and y coordinates for well 1 vary between 20 and 800 meters. Figure 8.4 shows the landscape near the initial iterate for the confined aquifer. Note that only a subset of Ω is feasible. The infeasibility was due to violation of the head constraint (14) or because the well 1 cannot be located at the same point as wells 2-5.

Figure 8 is the surface obtained when wells 2-5 are set at the optimal locations.

Figure 9 shows the landscape when wells 2-5 are set pumping at the initial locations for the unconfined aquifer. Note that most of the region is infeasible for the unconfined case and this

Figure 4: Decrease in Function Values

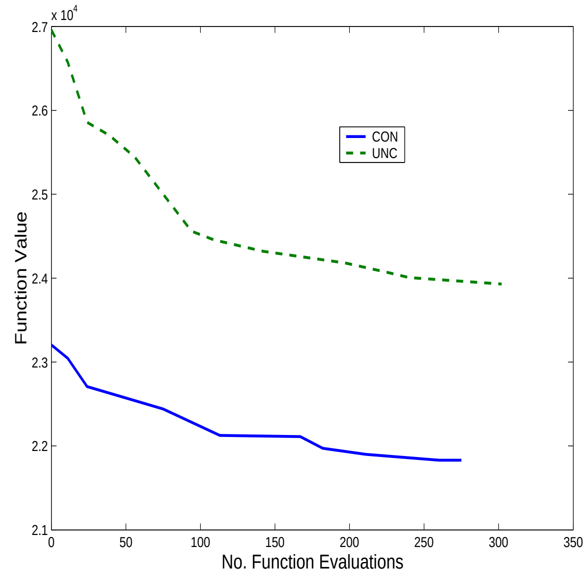
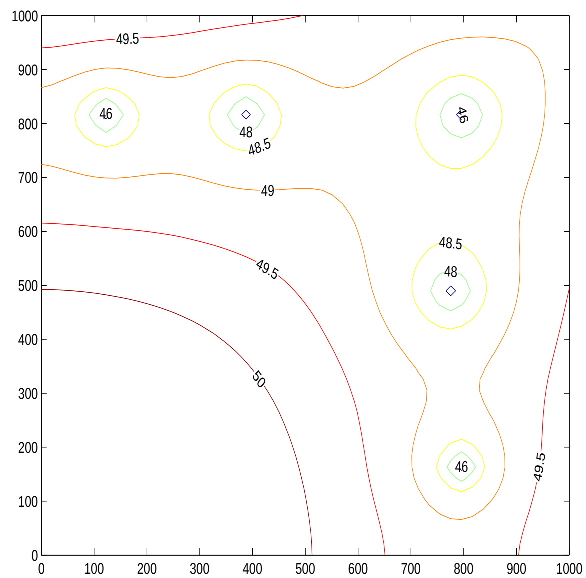


Figure 5: Confined Aquifer



choice of initial well locations due to violation of head constraint. Figure 10 is the surface obtained when wells 2-5 are set at the optimal locations.

8.5 Six well formulation

The results above are based on the heuristic that, because the installation cost (roughly \$20,000) of an extraction well is so high relative to the annual operating cost (roughly \$1,000), installing the

Figure 6: Unconfined Aquifer

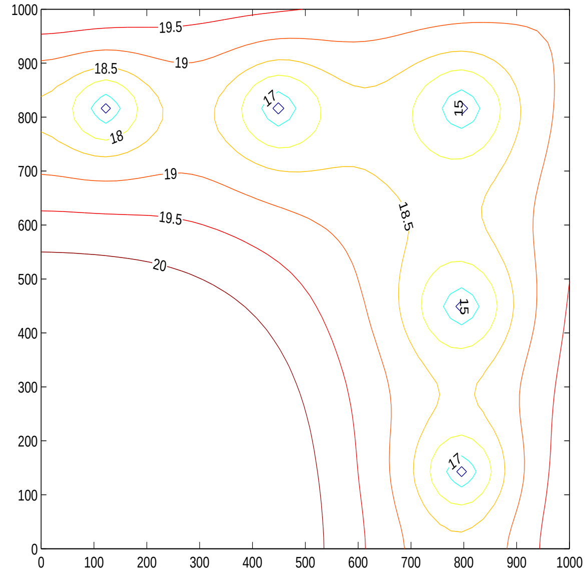
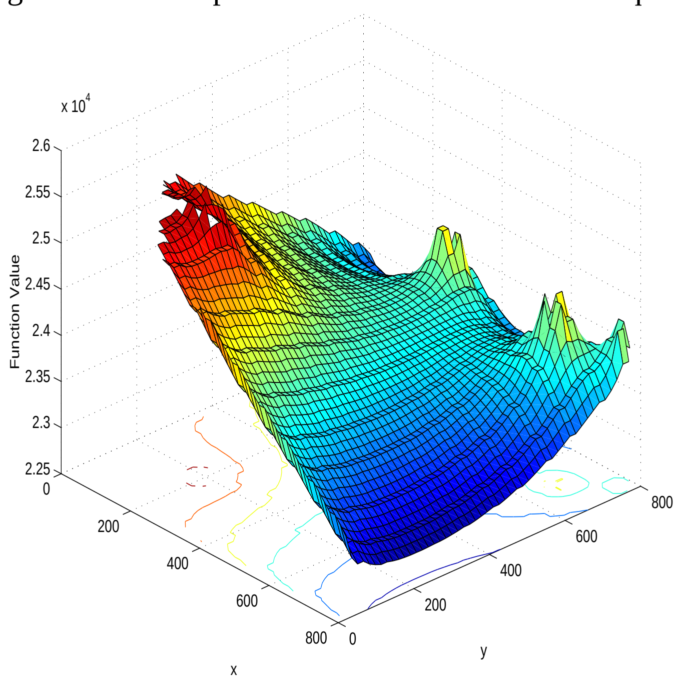


Figure 7: Landscape near initial iterate: confined aquifer



minimum number of wells (5) that meet the extraction target is the best approach.

To test this, we compared the five well configuration with all wells pumping at the maximum extraction rate to a six well configuration with both locations and pumping rates as decision variables. We included the installation cost (f^c in (11)) in the objective function for these runs. If the six well problem is initialized with all wells pumping at the maximum extraction rate, then one

Figure 8: Landscape near solution: confined aquifer

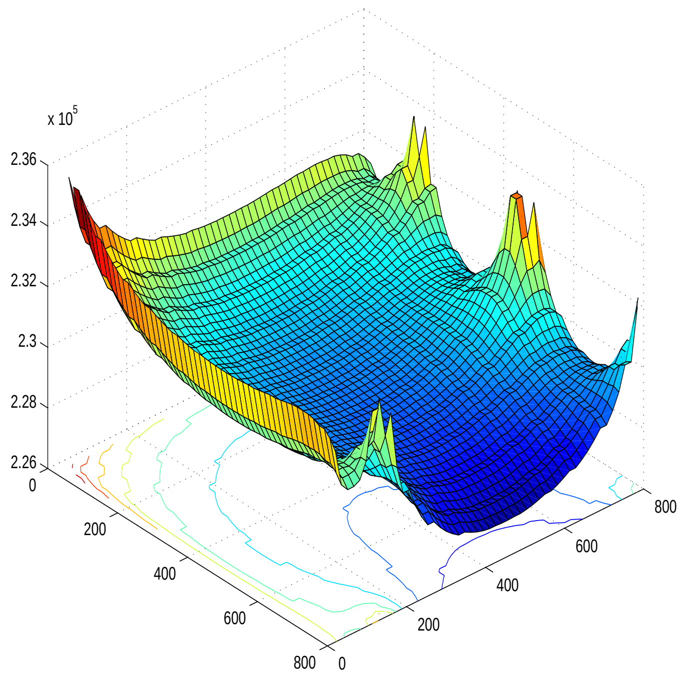
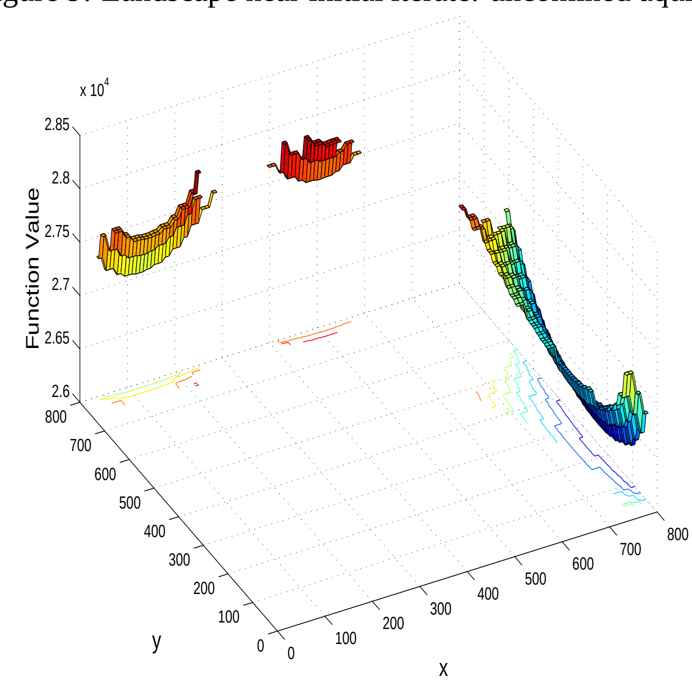
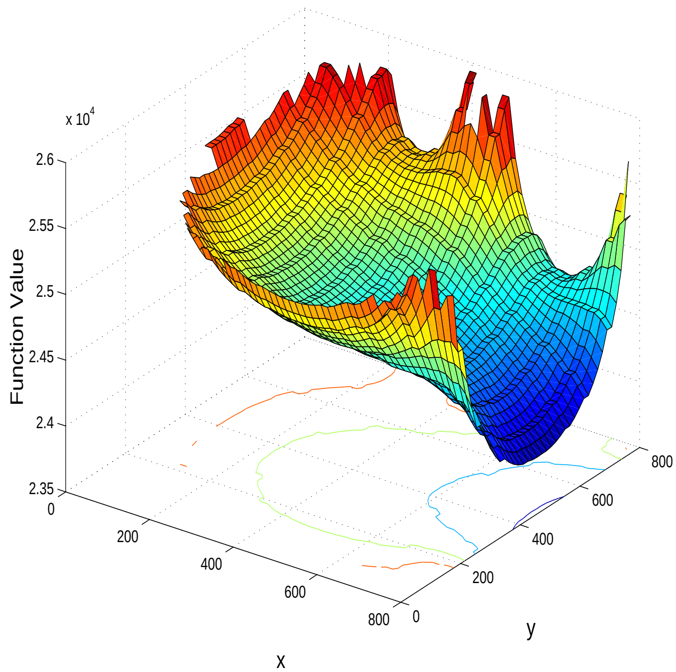


Figure 9: Landscape near initial iterate: unconfined aquifer



well shuts off in the course of the optimization and the minimum function value is within 0.2% of

Figure 10: Landscape near solution: unconfined aquifer



that found with the original five well configuration. If the six wells are initialized with

$$Q_i = Q_T^{min}/6, i = 1 \ldots 6,$$

which is a feasible and sensible initial iterate, then a suboptimal point is found. All wells remain pumping close to the initial pumping rates, although the locations align with the specified head boundary conditions.

We also considered the possibility that, over a longer time period, the six well model with the suboptimal initial iterate may be superior to the five well model. We ran both the confined and unconfined problems for one year to determine the annual operational cost. A hand calculation shows that for a time horizon of greater than 130 years for the confined aquifer and 90 years for the unconfined aquifer result in lower function values using the six well model. We ran both problems again with the longer time horizons to confirm that the six well model would outperform the five well model.

9 Downloading and Running the Test Problems

The problems can be obtained from

`http://www4.ncsu.edu/~ctk/community.html`

The test problems are packaged as compress UNIX tar files. The serial codes are for the g77 compiler and have been tested on SUN SparcStations running Solaris, various Intel platforms running Red Hat Linux 7.3 and 8.0, and an Apple Macintosh G4 running OSX 10.2. The MPI version of the codes has been tested on an IBM-SP3. IFFCO is included in the packages. The README files in the main directory explain how to assemble the files and interpret the results.

MODFLOW can be obtained directly from the USGS at the URL

`http://water.usgs.gov/software/modflow-96.html`

The USGS provides complied executables for SUN, SGI, and DOS systems, as well as UNIX source. Our packages provide makefiles for some other UNIX environments.

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