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Optimal management of a regional aquifer under salinization conditions

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Abstract. Salinization of an aquifer results from the movement and dispersion of saline water bodies within it and/or from inflow of saline waters across boundaries, including through recharge. Salinity does not exceed a few thousand parts per million, so the effects of density on the flow can be neglected. The objective of management is to maximize the net benefit from the water extracted subject to constraints on the amount of salt taken out with the water. The management model presented in this paper contains simulation of flow and transport of salinity, developed for a two-dimensional essentially horizontal confined aquifer, linked to a nonsmooth optimization algorithm. The simulator is based on a finite element formulation, in which the convective term is treated by the streamline-upwind Petrov-Galerkin (SUPG) method. SUPG is shown to reduce substantially the oscillations present in conventional finite element solutions of the transport equation, especially when the advective term dominates. The derivatives of the dependent variables, heads and concentrations at points in the field, with respect to the decision variables, the pumping rates, are computed in the simulator, using analytical expressions based on sensitivity theory. These derivatives are transmitted to the optimization algorithm, which uses the bundle-trust method for nonsmooth optimization. Application to a synthetic aquifer is demonstrated and analyzed.

1. Introduction

Most of the aquifer management problems that are described in the literature deal with remediation of the polluted aquifer [*Gorelick et al*., 1984; *Ahlfeld et al*., 1988a, 1988b; *Culver and Shoemaker*, 1992, 1997; *Xiang et al*., 1995]. Common techniques of remediation are withdrawal of the polluted water by pumping and/or in situ treatment, for example, by bioremediation. The objectives in these cases are to minimize the residual mass of pollutant at the end of the remediation period and/or to minimize the total duration or cost of pumping and treatment which is required to reduce the residual contaminant in the ground to some desired level. For most remediation problems the solute concentration appears in constraints on the quality at the end of management period and/or in the objective [*Gorelick et al*., 1984; *Chang et al*., 1992; *Culver and Shoemaker*, 1992, 1997].

In all these cases, when solute concentration appears in the objective or the constraints, it is considered only at the end of period rather than over the entire management period. The work presented here focuses on long-term extraction of water from an aquifer, where the quality of the water pumped is important. It has been found that while the two problems, remediation and resource management, may seem similar and amenable to solution by similar methods, in fact, the one we address here requires a quite different approach. The proposed formulation of the objective function and the constraints is different from those which appear in the literature. The purpose of the paper is (1) to propose a novel formulation of groundwater resource management with specific consideration of its salinity and (2) to apply a method for optimization of the resulting nonsmooth nonlinear optimization model.

The goal is optimal utilization of the water pumped out of an aquifer that is subject to salinization, from existing saline regions within the aquifer and/or recharge or inflows which are saline. There are pumping and recharging wells and possibly springs whose discharge is determined by the head in the aquifer. The objectives are to maximize the total amount of water of acceptable salinity that can be extracted over the planning horizon and to minimize the total cost of pumping and treatment of the extracted water. Another objective, which can also be set as constraint, is to minimize the total amount of salt extracted with the pumped water. The rationale for this last consideration is that the water extracted is then used for irrigation, and the salt in it causes salinization of the irrigated soils.

The quality of the pumped water depends on the flow and concentration distribution over time and the resulting concentration at the pumping wells. Simulation is used to evaluate these variables. A problem similar in certain aspects to the one we address is management of a coastal aquifer with seawater

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intrusion. The goal is the same: to pump as much water as possible, subject to head, quantity constraints, and constraints on concentration level [*Das and Datta*, 1999]. Two approaches exist to describe the seawater interface: sharp or with dispersion. The rigorous approach is to consider the advective-dispersive salt transport process with density-dependent flow. This is very complicated, especially for large-scale aquifers. *Das and Datta* [1999] used this approach and could therefore apply it only for a very small hypothetical problem. A sharp interface approach to saltwater intrusion was used by *Willis and Finney* [1988] and *Emch and Yeh* [1998]. Water quality in the freshwater zone does not appear in these management problems.

A major difference between the sea intrusion problem and the one addressed here is the range of salinity considered. We deal with salinity that does not exceed a few thousand parts per million (up to 900 ppm in our case). In this range the effect of density on flow can be neglected, and the solution of the flow and transport equations can be decoupled. We develop a model for a regional, confined, two-dimensional vertically averaged heterogeneous aquifer, where the flow can be considered essentially horizontal. Application to three dimensions can be based on the same mathematical model, but the numerical scheme would have to be modified.

The field case upon which our application is based is a 600 km^2 regional aquifer located in Israel's western Galilee, where the management goal is to operate its 32 wells so as to maximize long-term pumping volume and minimize total salt extraction.

2. Formulation of the Management Model

Consider a groundwater management problem, taking into account the existence of saline water within the aquifer itself and/or in its recharge or the inflows through its boundaries. There are a number of wells spread throughout the aquifer; some of them pump freshwater, while others pump water of various salinity. The objective is to pump as much water out of the aquifer with adequate quality, subject to constraints on hydraulic heads at certain prescribed points, on concentration levels at the pumping wells, or/and on the salt mass withdrawn with the water. The length of the management period may be as long as 20–50 years. This planning horizon can be divided into time periods, each several years long, during which the pumping rates remain constant, each several years long.

Two objectives are considered for management of the groundwater resource under salinization: (1) maximizing the net benefit from the water pumped and treated for removal of salinity, where the treatment cost depends on salt concentration in all management periods, and (2) maximizing the total amount of water of acceptable quality pumped.

The formulation of two multiperiod models is as follows:

1. Maximum net value is the benefit from the water pumped minus the cost of pumping and treatment

$$\max F = \sum_{tp=1}^{N_{tp}} \sum_{ip=1}^{N_{ip}} Q_{tp,ip} \int_t [\gamma - \alpha(c_{ip}(t), Q_{tp,ip}) - \beta[Q_{tp,ip}, h_{ip}(t)]\, dt, \tag{1}$$

subject to constraints on heads at specified points

$$h_i \geq h_i^*, \tag{2}$$

on the quantities pumped from wells

$$Q_{\min,ip} \leq Q_{tp,ip} \leq Q_{\max,ip}, \tag{3}$$

and on the total amount of salt extracted with the water and/or the maximum salinity of water extracted at specified wells

$$\max_t c_{tp,ip}(t) \leq c_{ip}^*, \tag{4}$$

$$\max_t Q_{tp,ip} c_{tp,ip}(t) \leq m_{ip}^*. \tag{5}$$

2. Maximum total amount of water extracted is

$$\max F = \sum_{tp=1}^{N_{tp}} \sum_{ip=1}^{N_{ip}} Q_{tp,ip}, \tag{6}$$

subject to

$$h_i \geq h_i^*, \tag{7}$$

$$Q_{\min,ip} \leq Q_{tp,ip} \leq Q_{\max,ip}, \qquad \forall\, tp, \quad \forall\, ip \tag{8}$$

and the total amount of salt taken out from some wells and/or from all wells:

$$\sum_{tp=1}^{N_{tp}} \int_t Q_{tp,ip} c_{tp,ip}(t)\, dt \leq M_{ip}^*, \quad \forall\, ip, \tag{9}$$

$$\sum_{ip=1}^{N_{\text{ips}}} \sum_{tp=1}^{N_{tp}} \int_t Q_{tp,ip} c_{tp,ip}(t)\, dt \leq \text{TM}_{\text{ips}}^*, \tag{10}$$

where $c_{ip}(t)$ is the salt concentration at the well of the water extracted ip in time period t; c_{cp}^* is the limit on concentration at control point cp (the control points are usually the pumping wells); m_{ip}^* is the limit on salt mass pumped by well ip per time unit (the same time unit as appears in the denominator of the pumping rate); M_{ip}^* is the limit on total salt mass pumped by well ip; TM_{ips}^* is the limit on total salt mass pumped by a selected set ips of wells; $Q_{tp,ip}$ is the pumping rate of well ip in time period tp (constant during the period); h_i/h^* is the hydraulic head/lower bound on head at control point i; $Q_{\min,ip}/Q_{\max,ip}$ are the minimum/maximum allowed pumping rate at well ip; γ is the benefit of a cubic meter of water of required quality; $\alpha(c_{ip}(t), Q_{tp,ip})$ is the cost of saline water treatment, a function of quantity and salinity; and $\beta(h_{ip}(t), Q_{tp,ip})$ is the cost of pumping, a function of quantity and head.

Constraint (5) limits the maximum value of concentrations over all times and is therefore a water quality control. This condition should be imposed only at points which are considered to be critical, to minimize the number of constraints. Constraint (4) reflects the capacity of treatment or restrictions on use of the saline water. Constraint (9) is on total salt mass extracted at a specific well, and (10) is on total salt mass pumped from the entire aquifer over the planning horizon.

Some of the constraints may be missing in a particular situation. The formulation above shows which types may be expected to appear under real conditions, as we have found in developing the model and in its application to a real field situation.

3. Formulation of the Simulation Model

A simulation model is needed to evaluate the objective function (1) and constraints (4), (5), (9), and (10). The model predicts the response of the physical system, flow and transport, to different pumping strategies. The system is described mathematically by partial differential equations expressing mass balance of water and salt. The simulation model that describes regional, vertically averaged flow and solute transport in a heterogeneous, isotropic, confined aquifer is based on the following equations:

Darcy's law

$$q = -K\nabla h, \tag{11}$$

Mass balance for the water

$$S\frac{\partial h}{\partial t} + \nabla\cdot(Kb\nabla h) = w - \sum_{j=1}^{N_p} Q_{pj}\delta(x-x_j) + \sum_{j=1}^{N_i} Q_{ij}\delta(x-x_j) - \sum_{j=1}^{k} Q_{sj}\delta(x-x_j), \tag{12}$$

Mass balance for the solute

$$R\frac{\partial(ncb)}{\partial t} + \nabla\cdot(cbq) = \nabla\cdot(Dnb\nabla c) + wc_w - \sum_{j=1}^{N_p} cQ_{pj}\delta(x-x_j) + \sum_{j=1}^{N_i} c_{sj}Q_{ij}\delta(x-x_j) - \sum_{j=1}^{N_s} cQ_{sj}\delta(x-x_j), \tag{13}$$

where h is the hydraulic head (L); b is the thickness of the aquifer (L); q is the specific discharge (L/T); Q_{ij} and Q_{pj} are the rates of the j injection/pumping well (L^3/T); N_p, N_i, and N_s are the total numbers of pumping and injecting wells and springs, respectively; w is the leakage flux (L/T); δ is the Dirac delta function at location x_j (L^{-2}); n is the porosity; S is the storativity; R is the retardation coefficient, $R = 1$ for saline water; K is the hydraulic conductivity (L/T); c is the concentration of solute averaged over the depth (M/L^3); c_{sj} is the concentration of injected water for well j (M/L^3); c_w is the solute concentration in leakage water (M/L^3); Q_{sj} is the spring flow rate (L^3/T) given by

$$Q_{sj} = \max\,[0, \chi(h - h_d)], \tag{14}$$

where h_d is the threshold level, below which $Q_{sj} = 0$, χ is the spring coefficient (L^2/T), D is the hydrodynamic dispersion tensor (L^2/T), which for isotropic media is expressed as follows:

$$D_{ij} = D_d + a_T|V|\delta_{ij} + (a_L - a_T)V_iV_j/|V|, \tag{15}$$

where a_L is the longitudinal dispersivity of the porous medium (L), a_T is the transversal dispersivity of the porous medium (L), and V_i/V_j is the velocity in the i/j direction.

The boundary conditions for mass balance of water and salt are of the Neuman or Dirichlet type. Equation (11) is incorporated into (12), which is then multiplied by c and subtracted from (12). The sink terms cancel out, resulting in the following expression:

$$R\frac{\partial(ncb)}{\partial t} + q\cdot\nabla(bc) = \nabla\cdot(Dnb\nabla c) + cS\frac{\partial h}{\partial t} + w(c_w - c) + \sum_{j=1}^{N_i}(c_{sj} - c)Q_{ij}\delta(x-x_j). \tag{16}$$

The decision variables are pumping rates. They change during the optimization search. All other aquifer parameters, including the initial and boundary conditions, are known and do not change during the optimization search procedure.

The system of differential equations (11), (12), and (16) with appropriate initial and boundary conditions is solved numerically. The groundwater flow and Darcy's law are solved by finite elements, while the salinity transport equation (16) is solved by the streamline-upwind Petrov-Galerkin (SUPG) method, as detailed in Appendix A.

4. Solution Approach and Methodology

Most groundwater management models are nonlinear, because of the presence of the concentration equations, and are solved with packages such as MINOS [*Ahlfeld et al.*, 1988a; *Emch and Yeh*, 1998; *Das and Datta*, 1999] or NLSOL [*Xiang et al.*, 1995]. These solvers use gradient methods to find a search direction and are based on the implicit assumption that the objective function and constraints are convex and smooth. It is clearly important to determine whether the objective and constraints are indeed smooth and convex, and yet relatively little effort has been devoted to the study of contaminant concentration behavior as the function of pumping rates. Those who studied this problem found nonconvex and nonsmooth behavior of the concentration distribution [*Gorelick et al.*, 1984; *Xiang et al.*, 1995; *Ahlfeld and Sprong*, 1998].

Thus classical optimization methods based on smoothness and convexity may fail for groundwater management models that include solute concentration. One approach which has been used for nonsmooth and nonconvex function minimization is based on search methods such as genetic algorithm and simulated annealing [*McKinney and Lin*, 1994; *Dougherty and Marryott*, 1991]. An alternative approach is to use specially designed descent methods, such as subgradient and Bundle methods, which will be considered below. These methods were developed initially for nonsmooth convex minimization and then extended to minimize certain types of nonconvex functions.

The Bundle-Trust algorithm [*Schramm and Zowe*, 1992] was chosen to solve the management problems addressed in this work. Bundle methods are a modification of classical gradient methods applicable to a nondifferentiable, nonsmooth, and sometimes nonconvex function. They can deal with functions that are continuous with discontinuous finite derivatives. The idea of the Bundle method is to use the subgradients and function values stored from previous iterations (stored in a "bundle") to search for the descent direction and then to perform a line search in this direction. If there was a significant decrease of the function value at kth iteration, the algorithm makes a "serious step," and if not, the algorithm makes a "null step." In both "null" and "serious" steps the new subgradient is added to the bundle. The algorithm is presented in Appendix B.

The Bundle-Trust method solves nonlinear nonsmooth problems subject to linear and box constraints, using the *Powell* [1985] algorithm to solve the inner quadratic programming problem with such constraints. Nonlinear constraints are incorporated into the objective with a penalty parameter. The original problem min $F(Q)$ subject to

$$g_i(Q) \le G_i, \qquad \forall\, i$$
$$AQ \le b \tag{17}$$

$$l \le Q \le u$$

is converted into either modified problem as follows:

$$\min\, [F(Q) + \sum_i P_i \max\,(0,\, g_i - G_i)] \tag{18}$$

$$\min\, \{F(Q) + P \max_i\, [\max\,(0,\, g_i - G_i)]\}$$

subject to

$$AQ \le b, \qquad l \le Q \le u,$$

where $F(Q)$ is the objective, g_i/G_i are the nonlinear constraints and their upper bound, respectively, and P is a penalty parameter. The modified objective becomes nonsmooth because of the nonsmooth form of the constraints max $(0,\, g)$, even if all the original functions were smooth. The algorithm is of the subgradient type. Therefore the derivatives of the contaminant concentration (in the constraints or objective) with respect to decision variables (pumping rates) are required. *Gorelick et al.* [1984] computed these derivatives by perturbation, while *Chang et al.* [1992], *Ahlfeld et al.* [1988a], and *Xiang et al.* [1995] used sensitivity analysis for this purpose. The linear constraints may either be left as constraints or incorporated into the objective function as another penalty term. The two strategies are denoted as penalty linear constraints (PLC) and direct linear constraints (DLC). They are both tested, and one or the other is selected according to the computational efficiency observed. The box constraints on Q are treated directly in the optimization algorithm.

5. Sensitivity Theory

For many purposes, such as sensitivity of optimal solutions or other system responses to perturbations of input system parameters, derivatives of system response functions with respect to input parameters are needed. These derivatives are defined by sensitivity theory for linear and nonlinear algebraic equations, with and without constraints, which was developed for the field of radiation transport [*Oblow*, 1978; *Cacuci et al.*, 1980].

Sensitivity is used in two ways: in the "forward problem," when the optimal solution is found and the goal is to compute the sensitivity of the optimum to perturbations in system inputs, and in the "backward problem," where derivatives are required in the search for the optimal solution. This is the case for groundwater management.

The concentration is a nonlinear function of the decision variables (pumping rates and well locations), because of their nonlinear relations in the dispersive part of the mass balance equation. The derivative of the objective function (1) with respect to the pumping rate at well ip and time period tp is given by

$$\frac{\partial F}{\partial Q_{\mathrm{tpj},jp}} = \sum_t\, [\gamma - \alpha(c_{jp}(t_{\mathrm{tpj}}),\, Q_{\mathrm{tpj,jip}}) - \beta(h_{jp}(t_{\mathrm{tpj}}),\, Q_{\mathrm{tpj,jip}})]\Delta t$$
$$+ \sum_{\mathrm{tpi}=1}^{\mathrm{tpj}} \sum_{ip=1}^{N_{ip}} Q_{\mathrm{tpi},ip} \sum_t \left[\frac{\partial\alpha(c_{ip}(t_{\mathrm{tpi}}))}{\partial c_{ip}(t_{\mathrm{tpi}})} \frac{\partial c_{ip}(t_{\mathrm{tpi}})}{\partial Q_{\mathrm{tpj},jp}} \right.$$
$$\left. + \frac{\partial\beta(h_{ip}(t_{\mathrm{tpi}}))}{\partial h_{ip}(t_{\mathrm{tpi}})} \frac{\partial h_{ip}(t_{\mathrm{tpi}})}{\partial Q_{\mathrm{tpj},jp}} \right]\Delta t. \tag{19}$$

The concentration at a control point at a given time depends on the pumping rates at all wells in all the preceding periods. Thus there is a derivative of the concentration at well jp and time t of time period TP with respect to the pumping rate of well ip at time period tp:

$$\frac{\partial c(x_{jp},\, t_{TP})}{\partial Q_{tp,ip}}, \qquad \forall\ \mathrm{ip}, \quad \mathrm{tp} \le \mathrm{TP}. \tag{20}$$

These derivatives are called "state sensitivity." They can be computed by direct differentiation of the differential equations [*Chang et al.*, 1992; *Ahlfeld et al.*, 1988a; *Xiang et al.*, 1995] or by "adjoint sensitivity equations" [*Sykes et al.*, 1985].

All authors who used sensitivity theory for groundwater management problems solved the flow and contaminant transport equations by the Galerkin finite element method. *Chang et al.* [1992] and *Ahlfeld et al.* [1988a] derived the sensitivity equations in matrix form, based on the finite element discretization, while *Xiang et al.* [1995] and *Gordon* [1999] first derived the analytical differential equations of the derivatives and then performed the discretization of the new equations.

Consider the governing differential equations (11), (12), and (16) and differentiate them with respect to the pumping rate $Q_{i,tp}$ (for each well i at time period tp). This results in the following system:

$$\tilde{q} = -K\nabla\tilde{h}, \tag{21}$$

$$S\,\frac{\partial\tilde{h}}{\partial t} + \nabla\cdot(Kb\nabla\tilde{h}) = \delta(x - x_j) - \sum_{j=1}^{N_s} \chi\tilde{h}\,\delta(x - x_j)\,\vartheta_h, \tag{22}$$

$$R\,\frac{\partial(n\tilde{c}b)}{\partial t} + q\cdot\nabla(b\tilde{c}) - \nabla\cdot(Dnb\nabla\tilde{c}) - \tilde{c}S\,\frac{\partial h}{\partial t} + w\tilde{c}$$
$$+ \tilde{c}Q_{ii}\delta(x - x_i) = -\tilde{q}\cdot\nabla(bc) + \nabla\cdot(\tilde{D}nb\nabla c)$$
$$+ cS\,\frac{\partial\tilde{h}}{\partial t} + (c_s - c)\,\delta(x - x_i), \tag{23}$$

where

$$\tilde{h} = \frac{\partial h}{\partial Q_{i,tp}}, \qquad \tilde{q} = \frac{\partial q}{\partial Q_{i,tp}}, \qquad \tilde{c} = \frac{\partial c}{\partial Q_{i,tp}}. \tag{24}$$

The last term of (22) relates to springs and exists only if the hydraulic head is higher than the threshold spring level, that is,

$$\vartheta_h = \begin{cases} 1, & h \ge h_d \\ 0, & \text{otherwise.} \end{cases} \tag{25}$$

Because the initial conditions for (12) and (16) do not depend on pumping rates, they do not appear in (22) and (23). The boundary conditions for (22) and (23) can be obtained by differentiation of the boundary conditions of the original equation. Thus they are of the same type (Dirichlet or Neuman) at each point as for original (12) and (16), but the value always is zero. The left-hand side of (12) and (16) is identical to the left-hand side of (22) and (23), respectively. The differences are only in the right-hand sides.

6. Analysis and Results

6.1. Concentration Response to Pumping

Consider the synthetic homogeneous, isotropic, confined aquifer shown in Figure 1. The aquifer is bounded by imper-

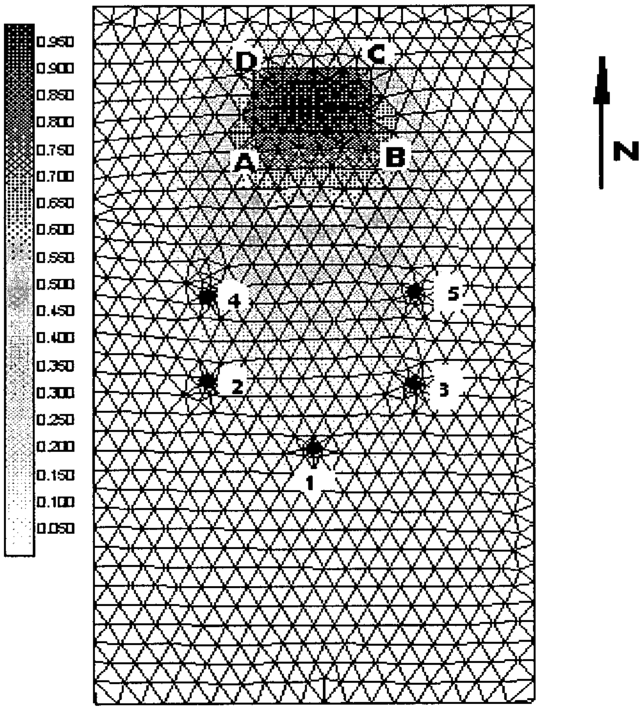

Figure 1. Synthetic aquifer with five pumping wells (numbered 1 to 5), saline accretion area ABCD, finite element grid, and the initial concentration distribution.

vious boundaries, except on the south where there is a fixed head boundary with head equal to 10 m. The data are as follows: area of 3000 × 4500 m, thickness $b = 50$ m, hydraulic conductivity $K = 10$ m/d, porosity $n = 0.2$, longitudinal dispersivity $a_L = 20$ m, transverse dispersivity $a_T = 2$ m, saline water recharge $w_s = 0.003$ m/d in rectangle ABCD, freshwater recharge throughout the rest of the aquifer $w_f = 0.0003$ m/d. Salinity enters into the aquifer with the recharge in rectangle ABCD, at a constant rate, with relative concentration $c = 1$. To facilitate the study of the management model, as described in section 6.2, the physical problem is made symmetric. However, in testing the validity of the concentration response, the salinity source was moved a little to the west. The flow field is created by superposition of the boundary condition at the river ($h = 10$ m), accretion of fresh and saline recharge, and flow to the wells. The flow is steady state. The finite element grid, which has about 800 nodes, was created by a grid-generation algorithm with an automatic numbering which was designed to minimize matrix bandwidth.

We begin by analyzing how the concentration responds to changes in the pumping strategy, similar to the analysis by *Ahlfeld and Sprong* [1998]. They studied the concentration field at the end of a remediation period and used the maximum concentration over the entire domain as a measure. They found that the response surface of this variable could be nonconvex and nonsmooth, especially when one of the wells changes from pumping to recharging or back. Our dependent variables of interest are the concentration at the pumping wells at all times, and especially their maximum values at each well, which appear in constraint (4) of the management model. The response surfaces presented in Figure 2 show maximum values over time of the relative concentration at wells (W) 3 and 5 and how they respond to pumping in a pair of wells (W2 and W4 are the first pair, and W3 and W5 are the second pair). Well 1 pumps the minimum 600 m^3/d. As shown in Figure 2, the response surfaces are nonconvex and nonsmooth.

The nonconvexity of these functions is indicated by the oscillations about a convex curve. Thus a gradient method may not work well. However, a subgradient method like bundle-trust can give good results in the optimal search by locating a "bundle" of subgradients that define the possible directions for search and choosing the best one for improving the objective function. In the case analyzed here, the pumping has a significant effect on the head and velocity fields. For example, changing of the pumping rate at a well by a factor of 3 can change the flow direction. Therefore the concentration at wells depends significantly on pumping rates. Had the influence of pumping on the velocity field been less significant, the concentration distribution would have been more homogeneous.

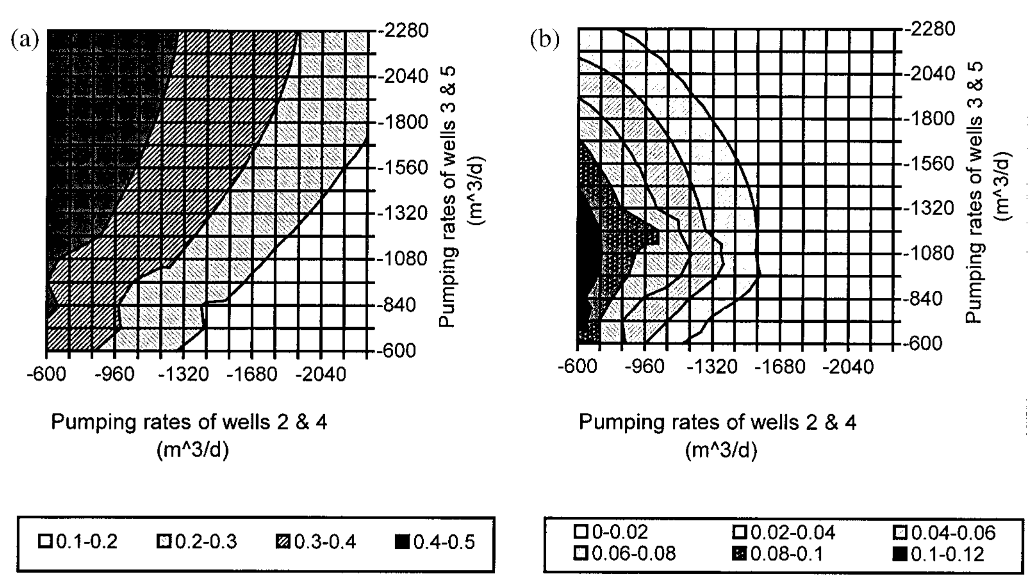

Figure 2. Relative concentration response on well pumping at (a) well 3 and (b) well 5.

Table 1. Formulation of the Optimization Problems

Run	T1	T2	T3	T4	T5	T6	T7
Objective (equation)	(1)	(1)	(6)	(6)	(6)	(6)	(6)
Constraints							
Head and pumping (equations)	(2) and (3)	(2) and (3)	(2) and (3)	(2) and (3)	(2) and (3)	(2) and (3)	(2) and (3)
$Q_{\min}/Q_{\max}$, m^3/d	2400/600	2400/600	2400/600	2400/600	2400/600	2400/600	2400/600
Equation (2) h^*, m	104	10	10	10	10	10	10
Equation (4) c^* (4) at Wells 1, 2, and 3	0.1	···	···	···	···	···	···
Equation (4) c^* (4) at Wells 4 and 5	0.4	···	···	···	···	···	···
Equation (5) m^* (5) at Wells 1, 2, and 3	···	240	240	···	···	240	···
Equation (5) m^* (5) at Wells 4 and 5	···	960	960	···	···	720 and 480	···
Equation (9) M^* (9) at Wells 1, 2, and 3	···	···	···	24,000	···	···	24,000
Equation (9) M^* (9) at Wells 4 and 5	···	···	···	48,000	···	···	72,000 and 48,000
Equation (10) TM* (10)	···	···	···	···	16	···	···
Initial value of pumping, m^3/d	600	600	600	600	600	600	600

The saline front first reaches wells 4 and 5, and they capture most of salt mass. The concentration rises at a well with increasing pumping rate at the same well as more water reaches the well, pulling the saline front toward it. The concentration decreases with the increase of pumping in the other wells because of a change in the direction of saline water motion. The concentration at the second row of wells (W2 and W3) initially behaves identically to the first row; that is, it rises with increase of pumping rate at the same well and decreases when the pumping at opposite wells increases; the explanation is the same as for the first row. Further increase of pumping leads to decrease of concentration, because the first row traps most of the salt mass and essentially all of the saline water is pumped by it.

This analysis indicates that if lowering the concentration in the water pumped by the wells is the only criterion, then pumping as much as possible is the optimal strategy. Thus, with objective function (1), head and pumping constraints (2) and (3), and the only quality constraints of the form (4), the optimal strategy is to pump as much as allowed by the well capacities, and constraint on concentration level (4) is not always active. The resulting model is a linear program. The optimization tests justify this statement.

6.2. Formulation of the Water Resource Management Model

Seven management problems (runs T1–T7) are presented in Table 1. Table 1 contains the following input data: the equations included in the test problem and the bounds for the corresponding constraints. Table 2 gives the results: optimal pumping from each well and the wells at which the constraints are binding. The solution strategy that gave the best results is specified: PLC, equal to the linear constraints are added to the objective function as a penalty term, or DLC, equal to the linear constraints are retained and introduced directly into the optimization model. The cost function α and benefit function γ in (1) are shown in Figure 3.

All tests have a symmetric structure (limits on head and concentration values are symmetric for wells located symmetrically), except runs T6 and T7. In runs T6 and T7 the limits for constraints (5) and (8) are not the same at wells 4 and 5 that

Table 2. Formulation of the Optimal Solutions

Run	Wells Where Head Constraints Are Met	Wells Where Concentration Constraints Are Met	Optimal Pumping Rate, m^3/d					Type of Problem Giving Best Solution[a]
			Well 1	Well 2	Well 3	Well 4	Well 5	
T1	1, 4, and 5	2 and 3	885.5	879.0	918.7	1651	1615	PLC
T2	1[b]	···	1178[c]	1225[c]	1238[c]	1008[c]	1008[c]	multiperiod and PLC
			1224[d]	1251[d]	1267[d]	936[d]	933[d]	
			1231[e]	1134[e]	1164[e]	1017[e]	1057[e]	
			851[f]	831[f]	881[f]	1248[f]	1029[f]	
T3	All	···	803.1	998.9	998.3	1589.6	1590.5	PLC and DLC
T4	None	1, 4, and 5	605.6	670.5	663.5	742.8	741	PLC
T5	None	(10)[g]	600	1031.5	1152.7	600	600	PLC
T6	1–4	5	762.9	1058.5	1116.7	1666.3	1329.2	DLC
T7	None	1 and 5	680	810.1	780.3	956.4	771.5	PLC

[a]PLC stands for penalty linear constraints; DLC stands for direct linear constraints.
[b]Head constraints are met for first three periods.
[c]Value for first management period.
[d]Value for second management period.
[e]Value for third management period.
[f]Value for fourth management period.
[g]Constraint (10), on the total salt mass extracted, is met.

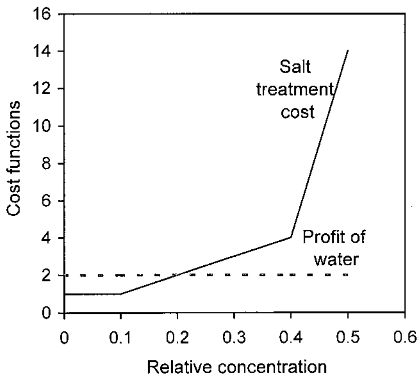

Figure 3. Benefit from water pumped (γ in equation (1)) and salt treatment cost (α in equation (1)).

are located symmetrically in the flow field, so as to test a nonsymmetric case.

The nonlinear constraints are incorporated into the objective function as a penalty term, in the following form: max $[F(Q) - \Sigma_{ip} P \max(0, g_{ip} - G_{ip})]$, where g_{ip} and G_{ip} are the constraints that depend on concentration and their upper bound, respectively. The box constraints are treated in the model directly. All tests were run for a single time period ($N_{tp} = 1$ in (1)–(10)) and multiperiod ($N_{tp} = 4$). In the latter case the time horizon of 50 years was divided into four equal subperiods. The role of all periods in the optimization model is equal, that is, the model is identical with respect to all periods. It should be recalled, however, that pumping at early times has an influence on later concentrations, while later decisions do not affect early concentrations, and hence the solution can have different pumping rates in different periods. Each test was run 4 times: once with the constraints (2) included as a penalty term in the objective, once with constraints kept separate, once with a single period, and once with a multiperiod. The best results for each test are shown in Table 2. Figure 4 presents the concentration distributions at the end of the management period for minimum and maximum extraction from the aquifer and one of the optimal solutions (test T3). Only in test T2 did the multiperiod give a better solution than the single period. This results from difficulties in reaching the optimal solution, because of the complexity of the problem.

The value of the objective function of the single and multiperiod problems is the same if the pumping rates remain the same over all time periods. The solution of the multiperiod problem should be at least as good as that of the single period, since the extra flexibility of changing pumping rates between periods affords an added opportunity to improve the solution, for example, by pumping more water in the first period, before the saline front has reached the wells.

6.3. Discussion

Table 2 summarizes the best solutions for these tests which show the following:

1. All solutions reached by the optimization procedure are feasible.

2. For the symmetric model with symmetric constraints we expect to obtain a symmetric solution. In tests T3 and T4 the pumping rates of wells 2 and 3 and 4 and 5 are essentially identical, but for tests T1, T2, and T5 there are differences between the values for pairs of opposite wells. They are due to the numerical aspects of the search procedure in the optimization. The grid used is not absolutely symmetric. Although the heads, velocities, and concentration fields are practically symmetric (they are identical to the second or third significant digit), the derivatives of the concentration with respect to pumping rates can become nonsymmetric, since they are quite small and therefore more sensitive to numerical accuracy. Hence the optimization search process can lead to a nonsymmetric optimal solution. For tests with symmetric constraints defined at each pair of wells, the nonsymmetry does not exceed 3%, except in the multiperiod case T2, for which the search

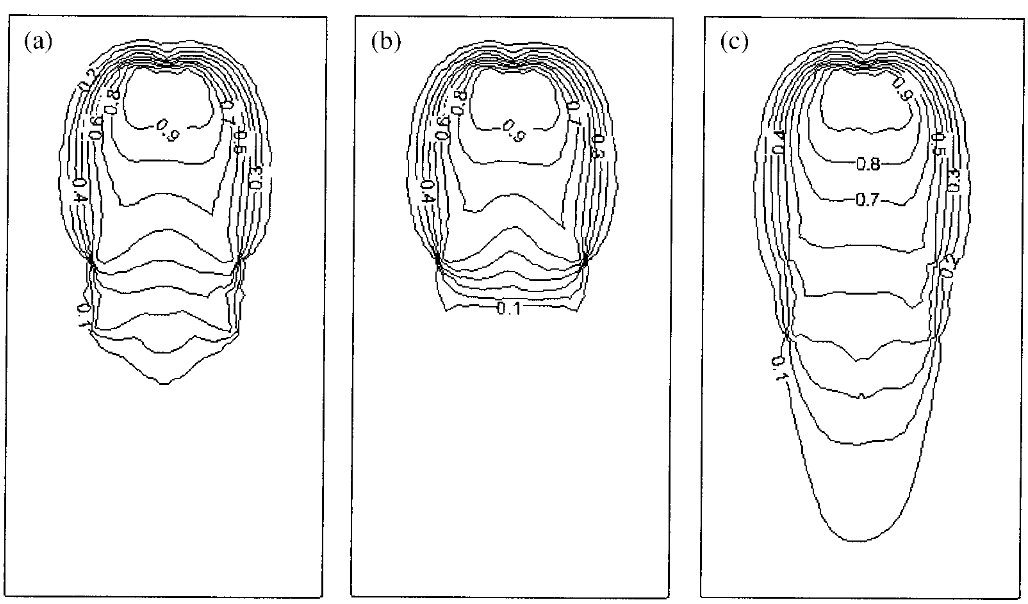

Figure 4. Concentration distribution at the end of the management period (a) with minimum pumping, (b) with maximum pumping, and (c) at optimal solution for test T3.

was terminated at a local optimum. The nonsymmetry reaches 10% for test T5, where the total salt mass is bounded.

3. Asymmetry in constraint limits leads to significant nonsymmetry of the optimal solution. For example, compare tests T4 and T7 (Table 1). All data for the two tests are identical except the limit on saline water pumping at well 4, that is 48,000 1/d for T4 and 72,000 1/d for T7. Owing to the possibility of pumping more water at well 4, one of the wells capturing the main part of the saline water, the salinization of the other wells decreases, and hence the pumping rates of all wells increase. The pumping rates at optimal point for test T7 are different at symmetric physical locations.

4. There is at least one binding constraint at the optimal solution for each test. For tests T1, T3, and T6 the solution reached is the global optimum, since the pumping is bounded by constraints on head or concentration at all wells, and consequently the pumping at all wells reaches their best feasible value. In the remaining tests the global optimum may not have been reached due to nonconvexity of the problem, and the optimal search was terminated at a local optimum.

5. For all tests, four combinations were considered: single-period and multiperiod models and the two methods for dealing with the linear constraints, direct and incorporation into an augmented objective function. As a rule, the best solutions were obtained for single-period management with the head constraint incorporated into the objective (PLC), as is shown in Table 2.

6. The inner quadratic programming problem is solved by the code QL0001 of Schittkowski's method (C-version (A. Nemirovski, personal communication, 1998)) based on the algorithm of *Powell* [1985] that starts from a feasible point. Thus keeping the linear constraints separate (DLC) reduces significantly the number of initial points for optimization search. The advantage of DLC is that points generated during the search remain within the feasible domain of box and linear constraints and the algorithm converges faster. However, because of the nonlinear, nonsmooth, and nonconvex behavior of the objective function, the requirement to remain always within the feasible domain may prevent reaching the optimal solution. As a result, the algorithm interrupts the search and does not find the best solution. Only for two tests T3 and T6 does the direct incorporation of the linear constraints give a better solution for cases where the linear constraints turn out to be binding.

7. The multiple period formulation gives the best solution only for the test T2. For the remaining tests the search of the optimal solution of the multiple-period model terminates at a point at which the objective function value is larger then objective value for the single-period model.

6.4. Computational Aspects

The optimization and simulation models, except the solution of the inner quadratic programming problem in the optimization, were written in Visual C++ and run on a Pentium II 350. The simulation and optimization models were tested separately on standard problems published in the literature. The detailed description is given by *Gordon* [1999]. The optimization runs took between 10 and 120 iterations. Each requires a simulation run. For the small problem presented here, about 800 grid nodes and 200 time steps, the optimal search takes from several minutes up to 2 hours.

The suite of simulation and optimization programs was also tested on two additional problems: the remediation problem published by *Xiang et al*. [1995] and a two-dimensional confined aquifer, resembling in shape, properties, and well locations the Na'aman in Israel's western Galilee. Only a few general details of the latter example are provided here, since space is limited. More about these examples will be published at a later date.

The aquifer has an area of about 600 km^2, 32 pumping wells, no recharge wells, and one large spring. The current total extraction from the wells is about 30 Mm^3 per year. There are 12 regions whose properties vary by orders of magnitude. Saline water intrudes into the freshwater through various cracks, and salinization of wells is increasing. The finite element grid has about 2000 nodes. The management model covers 20 years, divided into 80 time steps. It was formulated and run with two competing objectives: maximum amount of water pumped (equation (6)) and minimum amount of salt extracted with the water (constraint 10 becomes the second objective). This example was solved and yielded a trade-off curve between the two objectives.

7. Conclusions

A model for optimal management of a regional aquifer with areas and sources of saline water, whose objective is to extract the maximum possible amount of water from the aquifer under constraints on quantity and quality of water extracted, has been developed, implemented, and tested. It includes the following components:

1. A simulator of flow using a finite element method and of transport by a streamline-upwind Galerkin-Petrov (SUPG) method is used. The SUPG method for solving transport in the aquifer gives stable and accurate solutions and is suitable for incorporation into a simulator, which provides information, including partial derivatives, for the optimization.

2. Calculation of the partial derivatives of heads and concentrations on well pumping is performed within the simulator, and the results at points, which are relevant to the management problem, are transferred to the optimization algorithm.

3. A bundle-trust optimization algorithm that uses the results of the simulator in an iterative process is used to find an optimal solution.

The combined simulation-optimization model was applied to a number of groundwater management problems. The results are presented and analyzed here.

Appendix A: Numerical Solution of the Groundwater Flow and Solute Transport and Their Sensitivities

A common numerical method for solution of groundwater flow and solute transport is finite elements. However, because of the advective term, which arises in modeling of transport, spurious oscillations appear in the numerical solution using the traditional finite element method. This happens especially for advective-dominated flow, with a high Peclet number ($Pe = UL/D$); U is flow velocity; L is a characteristic length; and D is the dispersivity.

Several methods have been developed to prevent the oscillations in the solution of advective-dominated flow problems: Lagrangian methods [*Zheng*, 1990], random walk method, and stream-upwind Petrov-Galerkin (SUPG) method [*Brooks and Hughes*, 1982]. We use the latter. The basic idea of the SUPG method is to add artificial diffusion only in the flow direction.

The standard Galerkin weighting functions are modified by adding a term, which acts only in the flow direction.

$$\bar{\psi} = \psi + \alpha U \cdot \nabla \psi, \tag{A1}$$

where ψ is the standard Galerkin weighting function, $\bar{\psi}$ is the modified weighting function, and α is intrinsic time, a coefficient which depends on the Peclet number (its calculation is given by *Hughes et al*. [1986] and *Codina et al*. [1992]). As a result of making this change, the flow and its sensitivity equations are solved by finite elements, while the transport and its sensitivity equations are solved by the SUPG method. Thus (12) and (22) take the following forms after finite element operations over space coordinates and finite differences over time:

$$(3AS/2\Delta t + H)h^{t+1} = AS(4h^t - h^{t-1})/2\Delta t + F, \tag{A2}$$

$$(3AS/2\Delta t + H)\tilde{h}^{t+1} = AS(4\tilde{h}^t - \tilde{h}^{t-1})/2\Delta t + \tilde{F}, \tag{A3}$$

$$A^e_{ij} = \int_\Omega \psi_i \psi_j \, d\Omega$$
$$\tag{A4}$$
$$H^e_{ij} = \int_\Omega bK\left[\frac{\partial \psi_i}{\partial x}\frac{\partial \psi_j}{\partial x} + \frac{\partial \psi_i}{\partial y}\frac{\partial \psi_j}{\partial y}\right] d\Omega$$

$$F^e = \int_\Gamma \psi_i bK \nabla h \cdot \vec{n} \, d\Gamma + \int_\Omega \left[-\sum_{j=1}^{N_p} Q_{pj}\delta(x - x_j) \right.$$
$$\left. + \sum_{j=1}^{N_i} Q_{ij}\delta(x - x_j) - \sum_{j=1}^{N_s} Q_{sj}\delta(x - x_j) + w \right] d\Omega \tag{A5}$$

$$\tilde{F}_i = \delta_{ij} \tag{A6}$$

$$A = \sum_e A^e, \qquad H = \sum_e H^e, \qquad F = \sum_e F^e, \tag{A7}$$

where $\vec{n}$ is the outward normal vector to the boundary, ψ_i is the ith shape function for an element e, Ω is the element area, ψ_{ij} is the Kronecker delta presenting the presence or absence of a well at that point, and the tilde signifies derivatives with respect to the pumping rate.

Application of the SUPG to the transport equation (16) and derivatives of the concentration with respect to pumping rates (23) yields the following:

$$(3A/2\Delta t + B)c^{t+1} = A(4c^t - c^{t-1})/2\Delta t + R, \tag{A8}$$

$$(3A/2\Delta t + B)\tilde{c}^{t+1} = A(4\tilde{c}^t - \tilde{c}^{t-1})/2\Delta t + \tilde{R}, \tag{A9}$$

$$B^e_{ij} = \int_\Omega b\left[D_{xx}\frac{\partial \psi_i}{\partial x}\frac{\partial \psi_j}{\partial x} + D_{yy}\frac{\partial \psi_i}{\partial y}\frac{\partial \psi_j}{\partial y} \right.$$
$$+ D_{xy}\left(\frac{\partial \psi_j}{\partial x}\frac{\partial \psi_i}{\partial y} + \frac{\partial \psi_i}{\partial x}\frac{\partial \psi_j}{\partial y}\right) + \frac{q_x}{n}\frac{\partial \psi_j}{\partial x}\psi_i + \frac{q_y}{n}\frac{\partial \psi_j}{\partial y}\psi_i$$
$$+ \left(\frac{w}{n} - \frac{S}{n}\frac{\partial h}{\partial t}\right)\psi_i\psi_j + \alpha\left(\frac{q_x}{n}\frac{\partial \psi_i}{\partial x} + \frac{q_y}{n}\frac{\partial \psi_i}{\partial y}\right)$$
$$\left. \cdot \left(\frac{q_x}{n}\frac{\partial \psi_j}{\partial x} + \frac{q_y}{n}\frac{\partial \psi_j}{\partial y}\right)\right] d\Omega + \delta_{\mathrm{ijk}} Q_{ik}/n, \tag{A10}$$

$$R^e_i = Q_{ii}c_f/n + \int_\Omega \frac{w}{n} c_w \psi_i \psi_j \, d\Omega + \int_\Gamma \psi_i b \nabla c \cdot \mathbf{n} \, d\Gamma \tag{A11}$$

$$\tilde{R}^e_i = (c_f - c_i)\delta_{ik}/n - \sum_{j=1}^{ne} c_j \int_\Omega b\left[\tilde{D}_{xx}\frac{\partial \psi_i}{\partial x}\frac{\partial \psi_j}{\partial x} + \tilde{D}_{yy}\frac{\partial \psi_i}{\partial y}\frac{\partial \psi_j}{\partial y} \right.$$
$$+ \tilde{D}_{xy}\left(\frac{\partial \psi_j}{\partial x}\frac{\partial \psi_i}{\partial y} + \frac{\partial \psi_i}{\partial x}\frac{\partial \psi_j}{\partial y}\right)$$
$$+ \frac{\tilde{q}_x}{n}\frac{\partial \psi_j}{\partial x}\psi_i + \frac{\tilde{q}_y}{n}\frac{\partial \psi_j}{\partial y}\psi_i - \frac{S}{n}\frac{\partial \tilde{h}}{\partial t}\psi_i\psi_j$$
$$\left. + \alpha\left(\frac{q_x}{n}\frac{\partial \psi_i}{\partial x} + \frac{q_y}{n}\frac{\partial \psi_y}{\partial y}\right)\left(\frac{\tilde{q}_x}{n}\frac{\partial \psi_j}{\partial x} + \frac{\tilde{q}_y}{n}\frac{\partial \psi_j}{\partial y}\right)\right] d\Omega. \tag{A12}$$

The local matrices are assembled over all elements to obtain a set of systems of linear equations. It is solved by decomposition, followed by forward and backward substitution with N different right-hand sides (N is number of decision variables $+1$). All coefficient matrices have a band form. The coefficient matrices for the flow equation and Darcy's law are symmetric and positive definite. They are solved by Choleski decomposition, assembled, and stored in half bandwidth. Moreover, if the time steps and types of boundary conditions do not change (even though the values on the boundary may change with time), these matrices also do not change in time. So it is sufficient to assemble and decompose them only once and then to solve with different right-hand sides, which change in time and/or from simulation to simulation in the search of optimal management policy.

Significant saving of computation time at each simulation can be achieved by taking advantage of the difference in speed of the flow and transport processes. In many cases the flow is steady state or reaches steady state in a relatively short time. If the time steps and type of boundary conditions do not change, the matrix of coefficients does not change, under the assumption that the flow is steady or quasi steady. Under these conditions the LU decomposed matrix remains valid until the next changes of flow.

Appendix B: Bundle-Trust Algorithm

The bundle-trust method [*Schramm and Zowe*, 1992] was developed to solve nonsmooth convex and nonconvex locally Lipschitz problems, unconstrained and subjected to linear constraints. It was tested thoroughly and gives fast convergence in comparison with other descent methods developed for nonsmooth optimization. Several definitions are required for explaining the approach and method.

B1. Definition 1 [*Kiwiel*, 1985]

A function $f: R^n \to R$ is said to be locally Lipschitzian if for each bounded subset B of R^n there exists a Lipschitz constant $L = L(B) < \infty$ such that

$$|f(x_1) - f(x_2)| \le L|x_1 - x_2| \qquad \forall\, x_1, x_2 \in B.$$

The local Lipschitz property guarantees that the function is continuous and differentiable at each point of the domain.

B2. Definition 2 [*Kiwiel*, 1985]

A function f: $R^n \rightarrow R$ is called convex if

$$f(\lambda x_1 + (1-\lambda)x_2) \leq \lambda f(x_1) + (1-\lambda) f(x_2),$$

$$\forall\, \lambda \in [0, 1],\, x_1, x_2 \in R.$$

Some additional notation is needed before presenting the algorithm:

1. At each point $x \in R^n$ the subgradient $g(x)$ can be computed; for a convex function

$$f(y) \geq f(x) + \langle g(x_i), y - x \rangle \qquad \forall\, x, y \in R^n,$$

where $\langle a, b \rangle$ is a scalar product of two vectors a and b.

2. Cutting plane model f_M built on subgradients stored in bundle gives

$$f_M(x_k; x - x_k) = \max_{1 \leq i \leq j} [f(x_i) + \langle g(x_i), x - x_i \rangle] \quad \text{(B1)}$$

$$x \in R^n.$$

3. Linearization error α for a convex function gives

$$\alpha_i^k = \alpha(x_k; y_i) = f(x_k) - [f(y_i) + \langle g(y_i), x_k - y_i \rangle], \quad \text{(B2)}$$

$$\forall\, x_k, y_i \in R^n.$$

The algorithm is as follows [*Kiwiel*, 1990; *Schramm and Zowe*, 1992]:

The initial step is to choose a starting point $x_1 \in R^n$, $0 < m_1 < 1$, the step parameter t_1, maximal number of elements in bundle $J_{\max}$; compute $f(x_1)$ and $g(x_1)$; and set $y = x_1$, $k = 1$, and $J_1 = \{1\}$. For the kth iteration, compute the solution of the following quadratic programming problem:

$$(v^k, d^k) = \arg\min \left\{ v^k + \frac{1}{2t^k} \|d^k\|^2 \,\middle|\, v^k \geq g_i^T d^k - \alpha_i^k, \quad \forall\, i \in J_k \right\}. \quad \text{(B3)}$$

To find (v^k, d^k) and its Lagrange multipliers λ_i^k, where $d^k = x - x_k$ (v^k is parameter indicating the convergence), check the stopping condition, set $y = x_k + d$, compute $f(y)$, $g(y)$, and check for a serious or null step criterion. If condition $f(y) \leq f(x_k) + m_1 v^k$ is satisfied, make a serious step: $x_{k+1} = y$ and update t^{k+1}. If it is not satisfied, make a null step: $x_{k+1} = x_k$, and update (decrease) t^{k+1}. To update, select set

$$J_k^s = \{J_k^i | \lambda_k^i > 0, J_k^s < J \max\},$$

$$J_{k+1} = J_k^s \cup \{k+1\}$$

(set J_k responds on data stored in bundle)

$$g_{k+1} = g(y), \qquad f_{k+1} = f(x_{k+1}).$$

If it was a serious step:

$$\alpha_{k+1}^i = \alpha_k^i + f(x_{k+1}) - f(x_k) - g_i^T d_k, \qquad \forall\, i \in J_k^s,$$

then $\alpha_{k+1}^{k+1} = 0$. If it was a null step:

$$\alpha_{k+1}^i = \alpha_k^i, \qquad \forall\, i \in J_k^s,$$

then $\alpha_{k+1}^{k+1} = \alpha(x_k, y)$.

B3. Remarks

1. The detailed description of updating t_k and using subgradient aggregation to store data is given by *Kiwiel* [1985, 1990] and *Schramm and Zowe* [1992].

2. For a nonconvex function under assumption of its weakly semismoothness, α_k^i is replaced by $\beta_k^i = \max[\alpha_k^i, \gamma\|x_k - y\|^2]$ (γ is a parameter), and the remainder of the basic algorithm is essentially the same.

3. For a linearly constrained problem the set of linear constraints is added to the constraints in (B3), and thus the linear constraints are satisfied at each iteration.

4. The authors show that the method has linear convergence. The detailed analysis of convergence is given by *Schramm and Zowe* [1992] and *Kiwiel* [1990].

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