A variational framework for groundwater remediation

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Abstract: We present certain variants of dynamic programming and allied variational methods that arise in problems of groundwater remediation and related identification problems.

Key-Words: Groundwater remediation, identification, forward dynamic programming, hybrid systems, parabolic control problems.

1 Introduction and general statement of the problems

It is well known that problems of groundwater remediation require the development and application of optimal control methods; this is due to the great practical importance of groundwater remediation, and to the large costs associated with remediation procedures. A number of algorithms have been developed on the basis of dynamic programming; as representatives of a large amount of published work, we mention [4,7].

In the present paper, we present a number of new aspects of dynamic programming and allied variational calculus that are relevant to groundwater remediation. The main aspects of our contribution are: formulation of the problems as variable endtime optimal control, the use of forward dynamic programming (cf. [2]), hybrid systems approach to control and identification, and the derivation of necessary conditions (necessary conditions for different types of partial differential equations may be found in [6]).

The relevant system dynamics consists of 3 sets of equations: the evolution of piezometric head, Darcy's law for the velocity field, and equations of transport (advection and diffusion) for the contaminants and remediating agents. The related fluid mechanics background may be found in [5,8]. Control (extraction and injection) is applied at discrete locations of the spatial domain.

In this work, we wish to emphasise the control theoretic aspects, and for this reason we shall formulate the appropriate dynamics in a general form, without details about the physical aspects of the model. Our goal is to explore the variational methods that can be useful for optimising the cost of remediation.

2 A class of parabolic control problems

We describe a relatively general class of parabolic control problems that includes many of the problems arising in groundwater remediation and associated identification (site characterization) problems. The dynamics of the controlled system is given by

$$\frac{\partial y^{\alpha}(t,x)}{\partial t} =$$
$$= \nabla \bullet (A^{\alpha}(t,x,h(t,x),\nabla h(t,x))\nabla y^{\alpha}(t,x)) +$$
$$+\nabla \bullet (B^{\alpha}(t,x,h(t,x),\nabla h(t,x))y^{\alpha}(t,x)) +$$

$$+c^{\alpha}(t,x,y(t,x)) + \sum_{\mu\in M}[g_{\mu}^{0\alpha}(t) + g_{\mu}^{1\alpha}(t)\cdot$$

$$\cdot y^{\alpha}(t,x_{\mu})]u^{\mu}(t)\delta(x-x_{\mu}) \text{ for } (t,x)\in(0,T)\times\Omega;$$
$$y^{\alpha}(0^{+},x) = y_{0}^{\alpha}(x) \quad \text{for } x\in\Omega;$$
$$\gamma^{\alpha}(t,x)y^{\alpha}(t,x) = \varphi^{\alpha}(t,x) \text{ for } (t,x)\in(0,T)\times\partial\Omega$$

(1)

The function h(t,x) solves

$$\frac{\partial h(t,x)}{\partial t} = \nabla \bullet (A^0(t,x)\nabla h(t,x)) +$$

$$+\nabla \bullet (B^0(t,x)h(t,x)) + \sum_{\mu \in M} [g_\mu^{00}(t) +$$

$$+g_\mu^{10}(t)h(t,x_\mu)]u_\mu(t)\delta(x-x_\mu)$$

$$\text{for } (t,x) \in (0,T)\times\Omega;$$

$$h(0^+,x) = h_0(t,x) \text{ for } x \in \Omega;$$

$$\gamma^0(t,x)h(t,x) = \psi(t,x) \text{ for } (t,x) \in (0,T)\times\partial\Omega$$

(2)

The controls are the functions $u_\mu(t)$ and the set M of control locations $\{x_\mu\}$ is divided into two sets M^+ and M^- with corresponding control constraints

$$0 \le U_\mu^{1+} \le u_\mu \le U_\mu^{2+} \text{ for } \mu \in M^+;$$

$$U_\mu^{1-} \le u_\mu \le U_\mu^{2-} \le 0 \text{ for } \mu \in M^-;$$

$$\sum_{\mu \in M^\pm} a_\mu^\pm u_\mu(t) \le U_0^\pm \qquad (3)$$

The functions $g_\mu^{i\alpha}$ satisfy

$$g_\mu^{0\alpha}(t) > 0,\ g_\mu^{1\alpha}(t) = 0 \text{ for } \mu \in M^+;$$
$$g_\mu^{0\alpha}(t) = 0,\ g_\mu^{1\alpha}(t) > 0 \text{ for } \mu \in M^- \qquad (4)$$

The terms $c^\alpha(t,x,y(t,x))$ represent chemical or biochemical reactions. In order to describe those terms, we need to introduce some notation. We denote by I^α the set of reactions that contain y^α on the right-hand side, and by O^α the set of reactions that contain y^α on the left-hand side; the reactions in each of the sets I^α and O^α are labelled by an index i, and the set of constituents y^β on the side that does not contain y^α, for each reaction in I^α or O^α, is denoted by I_i^α or O_i^α, respectively; the rates and orders of reactions in I^α or O^α are $k_{i\alpha\beta}^\pm$, $\lambda_{i\alpha\beta}^\pm$ (with the + superscript for reactions in I^α and the - superscript for reactions in O^α). Also, we have decay coefficients $\sigma^\alpha(t,x)$, and the reaction terms are

$$c^\alpha(t,x,y(t,x)) := -\sigma^\alpha(t,x)y^\alpha(t,x) +$$

$$+\sum_{i\in I^\alpha}\prod_{\beta\in I_i^\alpha} k_{i\alpha\beta}^+(y^\beta(t,x))^{\lambda_{i\alpha\beta}^+} - \sum_{i\in O^\alpha}\prod_{\beta\in O_i^\alpha} k_{i\alpha\beta}^-(y^\beta(t,x))^{\lambda_{i\alpha\beta}^-} \qquad (5)$$

The variable h will also be denoted, whenever it is convenient, by y^0.

Let

$$G := \{\tilde{y}: \tilde{y}_\mu^\alpha(t) \ge A_\mu^\alpha \text{ for at least one } \alpha \text{ and at least one } \mu\} \qquad (6)$$

where $\tilde{y}(t) := \{y(t,x_\mu): \mu \in M\}$ and $\{A_\mu^\alpha\}$ is the set of maximum acceptable values for $y^\alpha(t,x_\mu)$. For each admissible control policy $u(t) \equiv \{u_\mu(t): \mu \in M\}$, we denote by τ the exit time of $\tilde{y}(t)$ from G, i.e.,

$$\tau := \inf\{t: \tilde{y}(t) \notin G\} \qquad (7)$$

The functional to be minimised is given by

$$J := \int_\Omega F_0(x, y(T\wedge\tau, x))dx +$$
$$+\int_\Omega \int_0^{T\wedge\tau} F_1(t,x,y(t,x))dxdt + \qquad (8)$$
$$+\int_0^{T\wedge\tau} F_2(t,\tilde{y}(t),u(t))dt$$

3 Dynamic programming

We assume that we have an approximate model for the situation described in section 2, with discretisation in the space variable only; this model has the form

$$\frac{dY(t)}{dt} = f(t,Y(t),u(t)); Y(0) = Y_0 \qquad (9)$$

The functional J of (8) is also discretised as

$$K = \Phi_0(Y(T) + \int_0^{T\wedge\tau} \Phi(t,Y(t),u(t))dt \qquad (10)$$

The dynamic programming equations for the problem (9-10) are

$$\frac{\partial V(t,Y)}{\partial t} + \inf_a \{\nabla_y V(t,Y) \bullet f(t,Y,a) + \\ +\Phi(t,Y,a)\} = 0 \quad \text{for } Y \in G,\ t \in (0,T); \qquad (11)$$
$$V(T,Y) = \Phi_0(Y)$$

The actual solution of (11) requires a second discretisation; let G_t denote the phase-space at time t; we use a discrete grid G_t, and for $\varphi \in G_t \setminus \mathsf{G}_t$, we denote by $\omega_t(\varphi)$ the set of nearest neighbours of φ. Then φ can be expressed as

$$\varphi = \sum_{\psi_j \in \omega_t(\varphi)} \lambda_j \psi_j \quad (\lambda_j \geq 1, \sum_j \lambda_j = 1) \qquad (12)$$

As an example, consider the case of a rectangular 2-D grid, with axes φ^1, φ^2, and a point M in the interior of a rectangle PQRS; then we can set

$$M = \mu\lambda P + \mu(1-\lambda)Q + (1-\mu)\lambda R + \\ +(1-\mu)(1-\lambda)S; \qquad (13)$$
$$\lambda := \frac{\varphi^1_M - \varphi^1_P}{\varphi^1_Q - \varphi^1_P},\ \mu := \frac{\varphi^2_M - \varphi^2_P}{\varphi^2_S - \varphi^2_P}$$

The set-valued function ω_t can be extended to a function ϖ_t defined for all $\varphi \in G_t$ by

$$\varpi_t(\varphi) = \omega_t(\varphi), \text{ if } \varphi \in G_t \setminus \mathsf{G}_t; \\ \varpi_t(\varphi) = \varphi, \text{ if } \varphi \in \mathsf{G}_t \qquad (14)$$

Further, we discretise the time-interval [0,T] (note that this discretisation applies only to the dynamic programming equation, not to the state-dynamics equation):

$$\mathsf{P}(0,t) := \{0 \equiv t_0 < t_1 < t_2 < \ldots < t_N \equiv T\}$$

(15)

We also set $\delta t_k := t_k - t_{k-1}$.

The discretised equation for V with discretisation in time only would be

$$V(t_k,\varphi) = \\ = \inf_a \{V(t_{k+1}, f(t_k,\varphi,a) + \Phi(t_k,\varphi,a)\}; \\ V(t_k,\varphi) = 0 \text{ for } \varphi \in \partial(G_{t_k}); \qquad (16) \\ V(T,\varphi) = \Phi_0(\varphi)$$

For the discrete grid G_t, there is no natural concept of topological boundary, and we substitute the concept of the *pseudo-boundary*, defined as the set of points of G_t that do not have a full set of nearest neighbours; this pseudo-boundary will be denoted by $\psi bd(\mathsf{G}_t)$. Eq. (16) is not directly useful for calculations; it is necessary to have an equation over the grid G_t, and we can use the equations

$$W(t_k,\varphi) = \\ = \inf_a \{ \sum_{\psi_j \in \varpi_{t_k}(f(t_k,\varphi,a))} \lambda_j W(t_{k+1},\psi_j) + \\ +\Phi(t_k,\varphi,a)\} \text{ for } \varphi \in \mathsf{G}_{t_k} \setminus \psi bd(\mathsf{G}_{t_k}); \qquad (17) \\ W(t_k,\varphi) = 0 \text{ for } \varphi \in \psi bd(\mathsf{G}_{t_k}); \\ W(t_N,\varphi) = \Phi_0(\varphi)$$

The system (17) defines a recursive scheme for the evaluation of the value function over the discrete set $\mathsf{P} \times \mathsf{G}_t$, and thus is suited for machine calculations.

4 The case of fully implicit time-discretisation

The design of numerical schemes for the dynamic programming equations must be sufficiently flexible to be appended to many different kinds of discretisation of the original state dynamics, i.e. the system of parabolic controlled partial differential equations described in section 2. Many existing codes for the numerical solution of the state dynamics utilise a finite-difference or finite-element discretisation in the spatial variables and a fully implicit scheme in time; the application of ordinary dynamic programming for such discretisations naturally leads to the problem of calculating the transition coefficients $\partial\varphi(t_{k+1}) / \partial\varphi(t_k)$. This is a difficult task that involves the inversions of large Jacobians. We have proposed in [2] a method of forward dynamic programming that avoids these difficulties (however, there is a tradeoff: our method introduces new complexities, but not of the type of matrix inversion). Here, we shall summarise our approach.

Suppose we have a fully implicit time discretisation for the controlled dynamical system, say

$$\varphi(t_{k-1}) = g(t_k, \varphi(t_k), u(t_k)); \\ \varphi(0) = \varphi_0 \qquad (18)$$

The forward dynamic programming recursion for (18) is given by

$$V(t_{k+1},\varphi) =$$
$$= \inf_a \{V(t_k, g(t_{k+1},\varphi,a)) + \Phi(t_{k+1},\varphi,a)\},$$
$$\text{for } k = 0,1,2,\ldots,N-1;$$
$$V(t_N,\varphi) =$$
$$= \inf_a \{V(t_{N-1}, g(t_N,\varphi,a)) + \Phi_0(\varphi)\}$$

(19)

Because the time direction is now the opposite of the usual dynamic programming, we need a penalty term to enforce the initial condition for (18), for example

$$V(0,\varphi) = \frac{1}{\varepsilon}(\varphi - \varphi_0)^2 \qquad (20)$$

The actual numerical solution of (19-20) requires a second discretisation over the grid G_t, as in the case of section 3.

A modification of this approach can be used when the original dynamics is discretised by using a semi-implicit scheme, for example a Crank-Nicolson scheme.

5 Hybrid control

In many cases, the time interval used for the discretisation of the state dynamics is different (smaller) than the time interval used for making decisions (i.e., the control function has to remain constant over several steps of the time-discretisation scheme for the system of parabolic partial differential equations that describe the physical situation). Because of the discrepancy in the two time scales, it is reasonable to treat the time scale of evolution of the physical system as continuous but the time scale for control decisions as discrete; thus we are led to hybrid control. We shall use some ideas from [3]. We refer to the system (9) with cost functional (10). Let τ_k, $k = 0,1,2,\ldots$ be the discrete times of control decisions. The dynamic programming equation now contains a function $V(t,Y,a)$ parametrised by initial time, initial state, and value of the control up to time t^-; we have

$$\frac{\partial V(t,Y,a)}{\partial t} + \nabla_y V(t,Y,a) \bullet f(t,Y,a) +$$
$$+\Phi(t,Y,a) = 0 \text{ for } \tau_k < t < \tau_{k+1},\ Y \in G_t;$$
$$V(\tau_k^-, Y, a) = \inf_b V(\tau_k^+, Y, b);\ V = 0 \text{ on } \partial G_t$$

(21)

The system (20) is valid when the decision times τ_k, $k = 0,1,2,\ldots$ are fixed. In certain applications, it is necessary to allow also variable decision times, i.e. decision times that depend on certain events; this is modelled by using certain ideas from the theory of impulsive differential equations, developed by D. Bainov and his school [1]. Thus the impulse times can be functions of Y that satisfy certain conditions, say $\tau_k = \tau_k(Y)$, and then (21) is modified to include these variable impulse times. When discrete costs k(a,b) are associated with the decision to change the control value from a at time τ_k^- to b at time τ_k^+, then the impulsive condition in (21) is altered to

$$V(\tau_k^-, Y, a) = \inf_b \{k(a,b) + V(\tau_k^+, Y, b)\}$$

(22)

The ideas of hybrid control systems can be also applied to the problem of identification. Suppose the system dynamics contains an unknown function q(t), i.e. we have

$$\frac{dY}{dt} = f(t, Y(t), q(t))$$

(23)

and discrete observations z_k of the state $Y(\tau_k)$ are made at times τ_k. Our goal is to find a q(t) that minimises

$$K := \sum_k \varepsilon(Y(\tau_k), z_k) + \int_0^T \Psi(q(t))dt$$

(24)

The dynamic programming equations for this problem are

$$\frac{\partial V(t,Y)}{\partial t} + \inf_a \{\nabla_y V(t,Y) \bullet f(t,Y,a) + \Psi(a)\} = 0,$$
$$\text{for } t \neq \tau_k;$$
$$V(\tau_k^-, Y) = V(\tau_k^+, Y) + \varepsilon(Y, z_k)$$

(25)

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6 Necessary conditions

A set of necessary conditions for the problem (9-10) can be useful for checking the accuracy of numerical methods for the solution of the optimal control problem, and also they can lead to new numerical schemes (in the same way that, for example, the first order necessary conditions for optimality in static optimisation lead to a variety of numerical schemes, such as steepest decent search, conjugate gradients, variable metric methods, etc.). Let $v_\mu(t)$ denote an admissible variation of the controls $u_\mu(t)$, and let $\eta^\alpha(t)$ be the corresponding variations of the state $y^\alpha(t)$; then $\eta^\alpha(t)$ solves

$$\frac{\partial \eta^\alpha(t,x)}{\partial t} = \sum_i \sum_j \frac{\partial}{\partial x^i}(A_{ij}^\alpha(t,x)\frac{\partial \eta^\alpha(t,x)}{\partial x^j} +$$

$$+\sum_i \frac{\partial}{\partial x^i}(B_i^\alpha(t,x)\eta^\alpha(t,x)) +$$

$$+\sum_\beta \frac{\partial c^\alpha(t,x,y(t,x))}{\partial y^\beta}\eta^\beta(t,x) +$$

$$+\sum_\mu [g_\mu^{0\alpha}(t) + g_\mu^{1\alpha}(t)y^\alpha(t,x_\mu)]v_\mu(t)\cdot$$

$$\cdot\delta(x - x_\mu) +$$

$$+\sum_\mu [g_\mu^{1\alpha}(t)\eta^\alpha(t,x_\mu)u_\mu(t)\delta(x - x_\mu);$$

$$\gamma^\alpha(t,x)\eta^\alpha(t,x) = 0 \text{ on } \partial\Omega;\ \eta^\alpha(0^+,x) = 0$$

(26)

The corresponding variation of the functional J is

$$\delta J = \int_\Omega \sum_\alpha \frac{\partial F_0(y(T,x))}{\partial y^\alpha}\eta^\alpha(T,x)dx +$$

$$+\int_0^T \int_\Omega \sum_\alpha \frac{\partial F_1(t,x,y(t,x))}{\partial y^\alpha}\eta^a(t,x)dxdt +$$

$$+\int_0^T \{\sum_\alpha \sum_\mu \frac{\partial F_2(t,\tilde{y}(t),u(t))}{\partial \tilde{y}_\mu^\alpha}\tilde{\eta}_\mu^\alpha(t) +$$

$$+\sum_\mu \frac{\partial F_2(t,\tilde{y}(t),u(t))}{\partial u_\mu}v_\mu(t)\}dt$$

(27)

The necessary condition for a minimum is

$$\delta J \le 0 \ \forall \text{ admissible } v \qquad (28)$$

By using a Green's function representation of the solution of (27), we have

$$\eta^\alpha(t,x) = \sum_{\beta,\lambda}\int_0^t G_\beta^\alpha(t,x;\sigma,x_\lambda)\cdot$$
$$\cdot[g_\lambda^{0\beta}(\sigma) + g_\lambda^{1\beta}(\sigma)y^\beta(\sigma,x_\lambda)]v_\lambda(\sigma)d\sigma \qquad (29)$$

At this stage, we do not deal with the variation of τ. The variation of J becomes (after some manipulations)

$$\delta J = \sum_\mu \int_0^{T\wedge\tau} D_\mu(t;y,u)v_\mu(t)dt \qquad (30)$$

where $D_\mu(t;y,u)$ is a *function* of t but a *functional* of y and u, and it is given by

$$D_\mu(t;y,u) := \int_\Omega \sum_{\alpha,\beta} \frac{\partial F_0(y(T\wedge\tau,x))}{\partial y^\alpha}\cdot$$

$$\cdot G_\beta^\alpha(T\wedge\tau,x;t,x_\mu)[g_\mu^{0\beta}(t) + g_\mu^{1\beta}(t)y^\beta(t,x_\mu)]dx +$$

$$+\int_\Omega \int_t^{T\wedge\tau} \sum_{\alpha,\beta} \frac{\partial F_1(\sigma,x,y(\sigma,x))}{\partial y^\alpha}G_\beta^\alpha(\sigma,x;t,x_\mu)\cdot$$

$$\cdot[g_\mu^{0\beta}(t) + g_\mu^{1\beta}(t)y^\beta(t,x_\mu)]dxd\sigma +$$

$$+\int_t^{T\wedge\tau} \sum_{\alpha,\beta,\lambda} \frac{\partial F_2(\sigma,\tilde{y}(\sigma),u(\sigma))}{\partial \tilde{y}_\mu^\alpha}G_\beta^\alpha(\sigma,x_\mu;t,x_\lambda)\cdot$$

$$\cdot[g_\lambda^{0\beta}(t) + g_\lambda^{1\alpha}(t)\tilde{y}_\lambda^\beta]d\sigma + + \frac{\partial F_2(t,\tilde{y}(t),u(t))}{\partial u_\mu}$$

(31)

These equations can be further augmented by taking into account the variation of τ and by including into the calculations the adjoint equations associated (in the variables t and x) with the Green's functions $G_{\beta}^{\alpha}(\sigma, \xi; t, x)$.

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