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Locally Optimal Pumping and Treatment Rates in Uncertain Environments

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Abstract. Stochastic control theory can be applied to the problem of groundwater remediation in order to determine optimal pumping and treatment rates in an uncertain environment. The approach utilizes stochastic dynamic programming that optimizes a cost functional for treatment subject to the constraints of the contaminant transport equations via a search over the state-control space. However, this approach for even small problems requires huge amounts of memory to solve numerically and is exceptionally prohibitive even using finite elements for the state-control space and time large jumps present. The approach here is to reduce the computational complexity by casting the contaminant flow equations to be linear locally while allowing for jumps and small background fluctuations in the dynamical system. The quasi-LQGP problem can then be used to determine the local optimal rates for pumping and treating, which does not require prohibitive amounts of memory. This linearized model can then be used as the starting iterate to hopefully accelerate the solution to the true nonlinear system for the contaminant transport equations.

1. Introduction

Groundwater remediation via well pumping has long been modelled as a control problem. Shortly after the development of stochastic (Itô) calculus, random processes were added to model unknown sources and sinks, and random events. This has produced a large amount of work, as has been documented by Yakowitz [**24**] and Gorelick [**9**], among others. Many models included background noise in the form of a Wiener or Gaussian process. The addition of random jumps and later Poisson processes became possible through the original work of theorists such as Florentin [**7**], Itô [**13**], Kushner [**16**], and Gihman and Skorohod [**8**], and continued by people such as Karlin and Taylor [**14**], Ryan and Hanson [**19**], Mariton [**18**], and Westman and Hanson[**20, 22**].

One general approach is to use stochastic dynamic programming, but this requires a large amount of memory. Large random jumps can be especially troublesome, even when finite elements are used, in part due to the Curse of Dimensionality

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[**11**]. The analytical and numerical concerns have been approached in a number of different ways. Kushner and Dupuis include a numerical treatment of jump diffusion processes in [**17**]. A discrete-time problem including random shocks of a Poisson type is found in a work of Das [**6**]. Hanson and Westman [**12**] presented a computational treatment of jump-diffusions for optimal portfolio and consumption policies where the jumps can either be purely random or quasi-deterministic (scheduled jump times, but random jump amplitudes). Zhang, Yin and Boukas [**25**] elaborate on the hedging point policies for the scheduling of a continuous time marketing-production system. Westman and Hanson [**20**] solved the LQGP problem (linear dynamics, quadratic costs, and subject to Gaussian and Poisson random disturbances) in continuous time, using a manufacturing application as an example. A nonlinear dynamical state version of the LQGP problem is presented in [**22**] where a canonical formulation and numerical method is given. The LQGP problem was extended by allowing for more complicated jumps described as state dependent Poisson processes [**21**] and varying local behavior of the system, known as the quasi-LQGP problem [**23**], which is demonstrated using a manufacturing system. The last method is extended here to discrete-time analysis while looking at an application involving groundwater remediation.

The groundwater remediation problem itself has been examined as either a continuous-time or discrete-time problem; both have been examined analytically and numerically from the control standpoint such as in [**10**] and [**4**]. This formulation utilizes a Gaussian noise process to represent uncertainties in the level of contamination and allows for new discrete random sources for contamination to occur modelled as a compound Poisson process. The focus in this paper is in the remediation of the aquifer subject to a hybrid form of random disturbances for the contamination.

Discretization of the system of stochastic partial differential equations as a quasi-linear stochastic difference system should give insight into results for the continuous time system. One hope is that the result from the discrete-time control problem could be used as an initial iterate to speed the continuous time numerics.

We will start by introducing the physical model and the governing equations. Section 3 introduces the control problem, including the discretization procedure. Stochastic dynamic programming is done, and the formal solution for the groundwater remediation problem are given. The final section summarizes the results and includes comments about numerical treatment for groundwater remediation application.

2. Groundwater Model

The aquifer in our model is homogeneous and isotropic, and contains a single contaminant. The horizontal directions of the aquifer are much bigger than the vertical direction, which allows us to use Bear's (see [**3**]) essentially horizontal aquifer assumption; thus all state variables are vertically averaged. There is an unknown source that is relatively small compared to the aquifer as a whole. The entering water from this source has a known contaminant concentration, but the leakage rate into the aquifer is a stochastic process. In addition, and independently of the previous process, random jumps occur in the contaminant concentration.

The groundwater is to be remediated via well pumping without injection or re-injection. The main goal of this formulation is to clean-up the groundwater to

an acceptable concentration level while minimizing the costs for treatment and anticipating the effects of random events or influences. A set of observation wells is arranged above the aquifer where measurements for the hydraulic head and contamination level are taken. A set pumping wells are used to extract the contaminated groundwater, as illustrated in Figure 1. Our control variables, therefore, are the extraction or pumping rates at all of the pumping wells.

In this presentation, there are m wells that are pumping wells. An example of the type of model being used is that of Ahlfeld, et al. [**1**], variants of which have been used by Culver and Shoemaker [**5**], and Kern and Hanson [**15**].

The derivation of the transport equations for a contaminated aquifer from first principles is done in Bear and Verruijt [**3**]. The flow transport equation can be written as

$$\begin{aligned} BS\frac{\partial H}{\partial t}dt &= \left(\nabla\cdot(T\nabla H) - \sum_{i=1}^{m} q_i \overline{\delta}\left(\xi-\xi_{p(i)},\eta-\eta_{p(i)}\right)\right)dt \\ &\quad + BS\vec{H}_c^{\top}\, d\vec{w}(t), \end{aligned} \tag{2.1}$$

where $H(\xi,\eta,t)$ is the state variable representing the hydraulic (or piezometric) head, B is the averaged aquifer thickness, S is the storativity of the aquifer, T is the transmissivity, $\vec{H}_c$ is a constant background noise vector coefficient for the Gaussian process $d\vec{w}(t)$ and q_i is the control variable for the extracting pump rate of the ith pumping well located at $\left(\xi_{p(i)},\eta_{p(i)}\right)$. The pumping wells represent finite point sinks but equation 2.1 is continuous spatially; this is rectified by using

$$\overline{\delta}(\xi-\xi_{p(i)},\eta-\eta_{p(i)}) = H(\widehat{\epsilon}-\sqrt{(\xi-\xi_{p(i)})^2+(\eta-\eta_{p(i)})^2})/(\pi\widehat{\epsilon}^2),$$

with $\widehat{\epsilon}\ll 1$.

The transmissivity, T, is defined in terms of the hydraulic conductivity, K, and the averaged aquifer thickness, i.e., $T=BK$. The isotropy assumption means that the hydraulic conductivity can be replaced with the constant $K=\kappa$ and taken outside of the divergence, not changing the dimensions of any other quantities.

The contaminant discharge is modelled in part as an ambient differential Gaussian process representing low level fluctuations in the hydraulic head and contaminant concentration due to random recharge from unknown sources, $d\vec{w}(t)$, with moments given by

$$\mathrm{E}[d\vec{w}(t)] = \vec{0} \qquad \text{and} \qquad \mathrm{Cov}[d\vec{w}(t)] = I_{nw}dt, \tag{2.2}$$

i.e., zero mean and independent components. The maximum concentration from this source is the vector coefficient $\vec{C}_c$.

The contaminant transport equation is written as

$$\begin{aligned} \theta B R_d\frac{\partial C}{\partial t}dt &= \left(\nabla\cdot(BD\nabla C) - B\vec{v}\cdot\nabla C\right)dt + \theta B R_d\vec{C}_c d\vec{w}(t) \\ &\quad + \vec{A}_c^{\top}(t)d\vec{P}(\xi,\eta,t), \end{aligned} \tag{2.3}$$

where C is the state variable representing the contaminant concentration, θ is the effective porosity, R_d is the retardation coefficient, $d\vec{P}(\xi,\eta,t)$ models rare large jumps in contaminant concentration with components selected by the vector coefficient $\vec{A}_c$, $\vec{v}$ is Darcy's velocity for porous media fluid flow, and $D=D(\vec{v})$ is the hydrodynamic dispersion tensor (includes convective dispersion and molecular diffusion). The hydrodynamic dispersion matrix D is dependent on Darcy's velocity,

$\vec{v}$:

$$D(\vec{v}) = \begin{bmatrix} D_{11} & D_{12} \\ D_{21} & D_{22} \end{bmatrix} (\vec{v}). \tag{2.4}$$

Darcy's Law defines Darcy's velocity (the porous media flow rate), $\vec{v}$, in terms of the hydraulic head:

$$\vec{v} = \begin{bmatrix} v_1 \\ v_2 \end{bmatrix} = -K\nabla H. \tag{2.5}$$

This means that the governing transport equations are uni-directionally coupled.

The contaminant discharge is modelled in part as an scaled, ambient differential Gaussian process $d\vec{w}(t)$ with moments given by (2.2). The contaminant concentration also has rare jumps that are modelled as a differential of a compound Poisson process, $d\vec{P}(\xi, \eta, t)$, which models a rather complex physical reality. This compound Poisson process is used to determine the location of the jump in the contaminant concentration, (ξ_{i_c}, η_{j_c}), the random state dependent size of the jump or mark, $\delta(\xi - \xi_{i_c}, \eta - \eta_{j_c})\vec{Z}(t)$, and the arrival time or rate for the jump, which can be thought of as

$$d\vec{P}(\xi, \eta, t) = \delta(\xi - \xi_{i_c}, \eta - \eta_{j_c}) d\widetilde{P}(t)\vec{Z}(t) \tag{2.6}$$

where $d\widetilde{P}(t)$ is diagonal matrix representation of the simple Poisson counting processes with moments

$$\mathrm{E}[d\widetilde{P}(t)] = [\lambda_i dt \delta_{i,j}]_{np\times np}, \mathrm{Cov}[d\widetilde{P}(t)] = [\lambda_i dt \delta_{i,j}]_{np\times np}$$

and the moments for the random jump or mark amplitude are given by

$$\mathrm{E}[\vec{Z}(t)] = \overline{Z}(t), \mathrm{Cov}[\vec{Z}(t)] = \mathrm{Diag}\left[\vec{\sigma}\vec{\sigma}^{\top}\right](t),$$

assuming that the components of $\vec{Z}(t)$ are pairwise independent, similarly the stochastic processes $d\vec{w}(t)$ and $d\vec{P}(t)$ are assumed independent of one another. The diagonalizing function is $\mathrm{Diag}[A] = [a_{i,i}\delta_{i,j}]_{n\times n}$. The compound Poisson process has the mean and covariance

$$\begin{aligned} \mathrm{E}[d\widetilde{P}(t)\vec{Z}(t)] &= \Lambda\overline{Z}dt \\ \mathrm{Cov}[d\widetilde{P}(t)\vec{Z}(t)] &= \Lambda(I_{np} + \Lambda dt)\mathrm{Diag}\left[\vec{\sigma}\vec{\sigma}^{\top} + \overline{Z}(\overline{Z})^{\top}\right](t)dt, \end{aligned}$$

where $\Lambda = [\lambda_i \delta_{i,j}]_{np\times np}$, the diagonal Poisson rate matrix.

The state variables, $H(\xi, \eta, t)$ and $C(\xi, \eta, t)$, in the governing equations (2.1) and (2.3), respectively, related by Darcy's velocity, $\vec{v}(t)$ (2.5), are vertically averaged due to the essentially two dimensional aquifer assumption, see [**3**]. The control variables are the m extraction pumping rates, $q_i(t)$.

The boundary conditions assumed can vary based on the model; here we use the same ones as Ahlfeld, et al. [**1**]. The aquifer in this case is between two rivers at $\xi = 0, \xi_r$, and idealized as being rectangular in shape. There is no flow through the boundaries in the η direction, so the boundary conditions there are

$$\frac{\partial H}{\partial \widehat{n}} = 0, \ \frac{\partial C}{\partial \widehat{n}} = 0$$

at both $\eta = 0$ and $\eta = \eta_r$, where $\widehat{n}$ is the outward pointing normal. Due to a slight gradient in the aquifer, flow generally goes in the direction of increasing ξ,

indicated by setting

$$H(0,\eta) = H_0,\ C(0,\eta) = 0,$$
$$H(\xi_r,\eta) = H_0,\ C(\xi_r,\eta) = 0.$$

The contaminant concentration is assumed to be zero since it is assumed that the rivers are not contaminated.

3. Discretization of Transport Equation

In order to examine the equations in terms of discrete time, we will utilize the Crank-Nicolson Implicit method. In the resulting difference equation, the spatial location will be represented by the i subscript for ξ with step $\Delta\xi$ and the j transcript for η with step $\Delta\eta$. The time t will be represented by the k subscript with time step Δt.

Flow Transport Equation. Making the appropriate substitution for $d\vec{w}(t)$, the Crank-Nicolson Implicit discretization of (2.1) yields

$$\begin{aligned}\frac{H_{ijk} - H_{ijk+1}}{2} &= r_1\left(\frac{H_{i+1,j} - 2H_{i,j} + H_{i-1,j}}{(\Delta\xi)^2}\right)_{k+\frac{1}{2}} \\ &\quad + r_2\left(\frac{H_{i,j+1} - 2H_{i,j} + H_{i,j-1}}{(\Delta\eta)^2}\right)_{k+\frac{1}{2}} \\ &\quad - \frac{\Delta t}{BS}\sum_{i=1}^{m} q_i\delta\left(\xi - \xi_{i_p(i)}, \eta - \eta_{i_p(i)}\right) \\ &\quad + \vec{H}_c^{\top}\Delta\vec{w}_k,\end{aligned}$$

where $r_1 = \kappa\Delta t/(S(\Delta\xi)^2)$ and $r_2 = \kappa\Delta t/(S(\Delta\eta)^2)$. The $(k+1)/2$ subscript indicates that the average of the k and $k+1$ time steps is used. Using U_k as the control variable (pumping rates) and separating out the different time steps

$$\begin{aligned}&[(1+2r)H_{ij} - r_1\left(H_{i+1j} + H_{i-1j}\right) r_2\left(H_{ij+1} + H_{ij-1}\right)]_{k+1} \\ &= [(1-2r)H_{ij} + r_1\left(H_{i+1j} + H_{i-1j}\right) \\ &\quad + r_2\left(H_{ij+1} + H_{ij-1}\right)]_k - \frac{\Delta t}{BS}\widehat{F}U_{ijk}, + \vec{H}_c^{\top}\Delta\vec{w}_k\end{aligned} \tag{3.1}$$

where $r = r_1 + r_2$. The term $\widehat{F}$ is used to guarantee that the control U_k is added only at valid spatial locations, i.e., where a pumping well exists.

Contaminant Transport Equation. After substituting for $d\vec{w}(t)$, D from (2.4), and $d\vec{P}(\xi,\eta,t)$ from (2.6), equation (2.3) becomes

$$\begin{aligned}
\frac{\partial C}{\partial t}dt &= \frac{1}{\theta R_d}\left(\nabla\cdot(D\nabla C)+\nabla H\cdot\nabla C\right)dt+\vec{C}_c^{\top}d\vec{w}(t)+\vec{A}_c^{\top}d\vec{P}(\xi,\eta,t)\\
&= \frac{dt}{\theta R_d}\left(\left(D:\nabla(\nabla^T C)-\kappa\nabla(\nabla^T H)\nabla_v[D]\right)^T\cdot\nabla C+\left(H_{,\xi}C_{,\xi}+H_{,\eta}C_{,\eta}\right)\right)\\
&\quad+\vec{C}_c^{\top}d\vec{w}(t)+\vec{A}_c^{\top}d\vec{P}(\xi,\eta,t)\\
&= \frac{1}{\theta R_d}\left(D_{11}C_{,\xi\xi}+2D_{12}C_{,\xi\eta}+D_{22}C_{,\eta\eta}\right)dt\\
&\quad-\frac{\kappa}{\theta R_d}\left(D_{11,v_1}H_{,\xi\xi}+\left(D_{11,v_2}+D_{21,v_1}\right)H_{,\xi\eta}+D_{21,v_2}H_{,\eta\eta}\right)C_{,\xi}dt\\
&\quad-\frac{\kappa}{\theta R_d}\left(D_{12,v_1}H_{,\xi\xi}+\left(D_{12,v_2}+D_{22,v_1}\right)H_{,\xi\eta}+D_{22,v_2}H_{,\eta\eta}\right)C_{,\eta}dt\\
&\quad+\frac{1}{\theta R_d}\left(H_{,\xi}C_{,\xi}+H_{,\eta}C_{,\eta}\right)dt\\
&\quad+\vec{C}_c^{\top}d\vec{w}(t)+\vec{A}_c^{\top}d\vec{P}(\xi,\eta,t) \qquad (3.2)
\end{aligned}$$

We can now find the discretized version of each term. Applying the Crank-Nicolson Implicit Method to the above equation, equation,

$$\begin{aligned}
&\left[\left(1+2rc_{11}D_{11}+2rc_{22}D_{22}\right)C_{i,j}\right.\\
&-rc_{12}D_{12}\left(-C_{i+1,j+1}+C_{i+1,j-1}+C_{i-1,j+1}-C_{i-1,j-1}\right)\\
&-\left(rc_{11}D_{11}+rc_1\gamma_1\right)C_{i+1,j}-\frac{1}{2}\left(rc_{11}D_{11}-rc_1\gamma_1\right)C_{i-1,j}\\
&\left.-\left(rc_{22}D_{22}+rc_2\gamma_2\right)C_{i,j+1}-\left(rc_{22}D_{22}-rc_2\gamma_2\right)C_{i,j-1}\right]_{k+1}\\
&\quad=\left[\left(1-2rc_{11}D_{11}-2rc_{22}D_{22}\right)C_{i,j}\right.\\
&\quad+rc_{12}D_{12}\left(C_{i+1,j+1}-C_{i+1,j-1}-C_{i-1,j+1}+C_{i-1,j-1}\right)\\
&\quad+\left(rc_{11}D_{11}+rc_1\gamma_1\right)C_{i+1,j}+\left(rc_{11}D_{11}-rc_1\gamma_1\right)C_{i-1,j} \qquad (3.3)\\
&\quad+\left(rc_{22}D_{22}+\gamma_2 rc_2\right)C_{i,j+1}+\left(rc_{22}D_{22}-rc_2\gamma_2\right)C_{i,j-1}\\
&\quad\left.+\vec{C}_c^{\top}\Delta\vec{w}+\vec{A}_c^{\top}\Delta\vec{P}\right]_k,
\end{aligned}$$

where

$$\begin{aligned}
rc_\alpha &= \frac{\Delta t}{\theta R_d\Delta\xi_\alpha},\ \alpha=1,2,\\
rc_{11} &= \frac{\Delta t}{\theta R_d(\Delta\xi)^2},\ rc_{12}=\frac{\Delta t}{4\theta R_d\Delta\xi\Delta\eta},\ rc_{22}=\frac{\Delta t}{\theta R_d(\Delta\eta)^2},\\
\gamma_1 &= \kappa\left[H_{,1}-\left(D_{11,v_1}\cdot H_{,11}+\left(D_{11,v_2}+D_{12,v_1}\right)\cdot H_{,12}\right.\right.\\
&\quad\left.\left.+\ D_{12,v_2}\cdot H_{,22}\right)\right]_{i,j,k+\frac{1}{2}},\\
\gamma_2 &= \kappa\left[H_{,2}-\left(D_{12,v_1}\cdot H_{,11}+\left(D_{12,v_2}+D_{22,v_1}\right)\cdot H_{12}\right.\right.\\
&\quad\left.\left.+\ D_{22,v_2}\cdot H_{,22}\right)\right]_{i,j,k+\frac{1}{2}}.
\end{aligned}$$

Combined Vector Equation. Let the vector representing the combined head and contaminant concentration state variables, arranged linearly in a vector rather

than in grid matrix notation, at time t_k or stage k be

$$\vec{X}_k = \begin{bmatrix} \vec{H}_k \\ \vec{C}_k \end{bmatrix}.$$

Note that this nx-vector includes the values of the state variables at each point at every interior grid point (ξ_i, η_j) in the domain, where $nx = 2 \cdot ng$ and ng is the total number of interior grid points in the domain. Rewriting the discretized equations 3.2 and 3.4 in vector form

$$\begin{aligned} \widetilde{\Gamma}_k \vec{H}_{k+1} &= \widetilde{\Phi}_k \vec{H}_k + \widetilde{\Psi}_k \vec{U}_k + \widetilde{\Theta}_k \Delta \vec{w}_k \\ \Gamma'_k(H) \vec{C}_{k+1} &= \widetilde{\Phi}'_k(H) \vec{C} + \Theta'_k \vec{w}_k + \Upsilon'_k \Delta \widetilde{P}_k \end{aligned}$$

Therefore, the combined vector equation is

$$\Gamma_k \vec{X}_{k+1} = \widehat{\Phi}_k \vec{X}_k + \widehat{\Psi}_k \vec{U}_k + \widehat{\Theta}_k \vec{w}_k + \widehat{\Upsilon}_k \vec{P}_k \tag{3.4}$$

or assuming Γ_k is invertible,

$$\vec{X}_{k+1} = G_k(\vec{X}_k, \vec{U}_k, \Delta \vec{w}_k, \Delta \vec{P}_k) \equiv \Phi_k \vec{X}_k + \Psi_k \vec{U}_k + \Theta_k \Delta \vec{w}_k + \Upsilon_k \Delta \vec{P}_k, \tag{3.5}$$

for $k = 1, \ldots, N-1$. The coefficient matrices Φ, Ψ and Θ are time dependent only.

4. Control Problem

It is at this point that we restate the main goal of our application: to minimize the costs of groundwater remediation to an acceptable level. Thus an appropriate cost functional is needed before performing stochastic dynamic programming to optimize the control.

The general form of the cost functional is

$$J_N[X, U] = f_N(\vec{X}_N) + \sum_{k=1}^{N-1} c_k(\vec{X}_k, \vec{U}_k),$$

with $f_N(\vec{X}_N)$ representing the final costs, $c_k(\vec{X}_k, \vec{U}_k)$ the running costs for times $k = 1$ to $N-1$, where $X = [\vec{X}_i]_{1 \times N} = [X_{i,j}]_{nx \times N}$ and $U = [\vec{U}_i]_{1 \times (N-1)} = [U_{i,j}]_{m \times (N-1)}$ are the global state and control history matrices.

One possible form for the groundwater remediation model is the quadratic cost functional:

$$\begin{aligned} J_N[X, U] &= \frac{1}{2} \vec{X}_N^\top S_N \vec{X}_N \\ &\quad + \sum_{k=1}^{N-1} \left(\vec{\alpha} - \beta \vec{X}_k \right)^\top \vec{U}_k + \frac{1}{2} \epsilon \vec{U}_k^\top \vec{U}_k \Big), \end{aligned}$$

where S_N is the symmetric, positive-definite, state final cost coefficient matrix and ϵ is the control quadratic cost coefficient per stage. The stage costs come from water extraction and treatment, with constant $(N-1)$-vector $\vec{\alpha}$ and constant $((N-1) \times nx)$-matrix β. The small quadratic term, known as the cheap control model, helps to make the problem more robust, i.e., a quasi-LQGP problem (quasi-linear dynamics, quadratic costs with Gaussian and Poisson processes) and ensures that a unique unconstrained interior minimum exists. The final costs may come from the maximum allowable contaminant concentration in combination with any fixed costs. The next step is to apply discrete-time stochastic dynamic programming and find the control values.

The required optimal, expected total costs are

$$J_1^*(\vec{x}_1) = \min_{\{u\}} \left[\mathrm{E}_{\{w,P\}} \left[J_N[X,U] | \vec{X}_1 = \vec{x}_1, U = u \right] \right], \tag{4.1}$$

subject to discrete dynamical constraints in (3.2,3.4). Bellman's Principle of Optimality states that an optimal policy has the property that whatever the initial state and initial decisions for the control are, the remaining decisions must constitute an optimal policy with regard to the state resulting from the first decision [**2**]. The control values are found via a backwards sweep through time.

Formal Solution. Applying a discrete version of the Principle of Optimality (see [**11**] or [**15**] for instance), decomposing the optimization of the global, initial objective $J_1^*(\vec{x}_1)$ into the optimization of local objectives $J_k(\vec{x}_k)$ local objectives to the optimal expected costs gives the corresponding backward recurrence, discrete Hamilton-Jacobi-Bellman equation:

$$\begin{aligned} J_k^*(\vec{x}_k) &= \min_{\vec{u}_k} \left[\left((\vec{\alpha} - \beta \vec{x}_k)^\top \vec{u}_k + \frac{1}{2} \epsilon \vec{u}_k^\top \vec{u}_k \right) \right. \\ &\left. + \mathrm{E}_{\Delta \vec{w}_k, \Delta \vec{P}_k} \left[J_{k+1}^* \left(\Phi_k \vec{x}_k + \Psi_k \vec{u}_k + \Theta_k \vec{w}_k + \Upsilon_k \vec{P}_k \right) \right] \right], \end{aligned} \tag{4.2}$$

for $k = N-1$ to 1 in backward steps of 1, starting from the final condition

$$J_N^*(\vec{x}_N) = \frac{1}{2} \vec{x}_N^\top S_N \vec{x}_N.$$

Consequently, the kth backward iterate minimum argument inherits the quadratic properties of the final costs $f_n(\vec{x}_n)$ and the running costs $c_k(\vec{x}_n, \vec{u}_n)$,

$$J_k^*(\vec{x}_k) = \min_{\vec{u}_k} \left[\left[\frac{1}{2} \vec{u}^\top \mathcal{A} \vec{u} + \vec{u}^\top (\mathcal{B} \vec{x} + \vec{\mathcal{C}}) + \frac{1}{2} \vec{x}^\top \mathcal{D} \vec{x} + \vec{\mathcal{E}}^\top \vec{x} + \mathcal{F} \right]_k \right],$$

where $\mathcal{A}, \cdots \mathcal{F}$ are constant entities. For instance when $k = N-1$,

$$\begin{aligned} J_{N-1}^*(\vec{x}_{N-1}) = \min_{\vec{u}_{N-1}} \left[\left[\right. \right. & (\vec{\alpha} - \beta \vec{X})^\top \vec{u} + \frac{1}{2} \epsilon \vec{u}^\top \vec{u} + \frac{1}{2} (\Phi \vec{x} + \Phi \vec{u})^\top S_N (\Phi \vec{x} + \Phi \vec{u}) \\ & + (\Phi \vec{x} + \Phi \vec{u})^\top S_N \Lambda \overline{Z} \Delta t + \frac{1}{2} \Theta^\top S_N \Theta \\ & + \frac{1}{2} \mathrm{Trace} \left[\Lambda (I_q + \Lambda \Delta t) + \overline{Z} (\overline{Z})^\top \right] \mathrm{Diag} \left[\vec{\sigma} \vec{\sigma}^\top \right. \\ & \left. \left. \left. \mathrm{Diag} \left[\Upsilon^\top S_N \Upsilon \right] \right] \right]_{N-1} \right]. \end{aligned}$$

Solving the minimization problem results in an affine form of the kth regular (unconstrained) optimal control:

$$\vec{u}_{reg,k}^* = \mathcal{L}_k \vec{x}_k + \vec{\mathcal{K}}_k.$$

The resulting costs for the quasi-LQGP problem then has the quadratic form in the state only

$$J_k^*(\vec{x}_k) = \min_{\vec{u}_k} \left[\frac{1}{2} \vec{x}_k^\top \mathcal{S}_k \vec{x}_k + \vec{\mathcal{T}}_k^\top \vec{x}_k + \mathcal{R}_k \right],$$

for $k = N$ to 1 in unit backward steps, with $\mathcal{S}_N \equiv S_N$, $\vec{\mathcal{T}}_N \equiv \vec{0}$ and $\mathcal{R}_N \equiv 0$. If there are constraints on the optimal control, the final answer for both the optimized control and costs take on a more complicated form. For example, the pumping rates must be non-negative if no water is reinjected into the aquifer, and the combined

pumping rates should have a maximum, resulting in the constraints $u^*_{k,l} \geq 0,\ l = 1$ to q and $\sum_l\ u^*_{k,l} \leq U_O$, respectively.

The state variables can be found by performing a forward sweep through time of the system dynamics, given the optimal control and initial conditions for the state, e.g. the initial contaminant plume and hydraulic head observations. Since our original pair of difference equations is uni-directionally coupled, it is necessary to solve for the hydraulic head at stage k before finding the contaminant concentration at the same stage.

5. Conclusions and Remarks

Improvements in well-pumping problem solution The clean-up or remediation of contaminated environments is a relevant issue for a wide spectrum of people and professionals. The results for the general model of a contaminated aquifer discussed here has a form that is useful for giving a relatively quick result numerically, despite the inclusion of multiple types of random processes in the model. The addition of a Poisson term in the discrete-time formulation makes certain types of models possible; for example, a slightly different formulation could take into account random rainfall, or additional contaminant seepage from an unknown source or sink. From a more theoretical viewpoint, the solution of a quasi-LQGP problem is extended to a discrete time dynamical system. The advantage of the explicit canonical state-space form of the quasi-LQGP solution is that it significantly reduces the large state-space dimensional computational complexity. The resulting formal solutions for the state and control variables can be used to examine the numerics for a variety of problems.

Since we are left with recursive difference equations for the state variables, and the control variables are linear in terms of the state, the number of operations for a specific groundwater remediation problem should not be excessive. It is necessary for there to be a reasonable initial guess as to the control values so that the forward sweeps for the state and backward sweeps for the control converges in a small number of iterations.

While discretizing the system before further analysis does create a lesser memory demand, the nonlinear aspects of the initial stochastic differential equations are absent, in part because of the choice of discretization procedure. While the Crank-Nicholson method is fairly robust numerically, it blurs some of the quantitative aspects of the initial system, especially with regards to the contaminant transport equation. Thus the formal solution found here should be a good solution choice, in lieu of an exact final answer for the well pumping rates.

However, if we think of this as a locally linearized solution to the problem, it could be useful as an initial choice for the numerics of the nonlinear problem. Greater accuracy to start with should lead to faster convergence to the optimized numerical answer, something useful both mathematically and practically.

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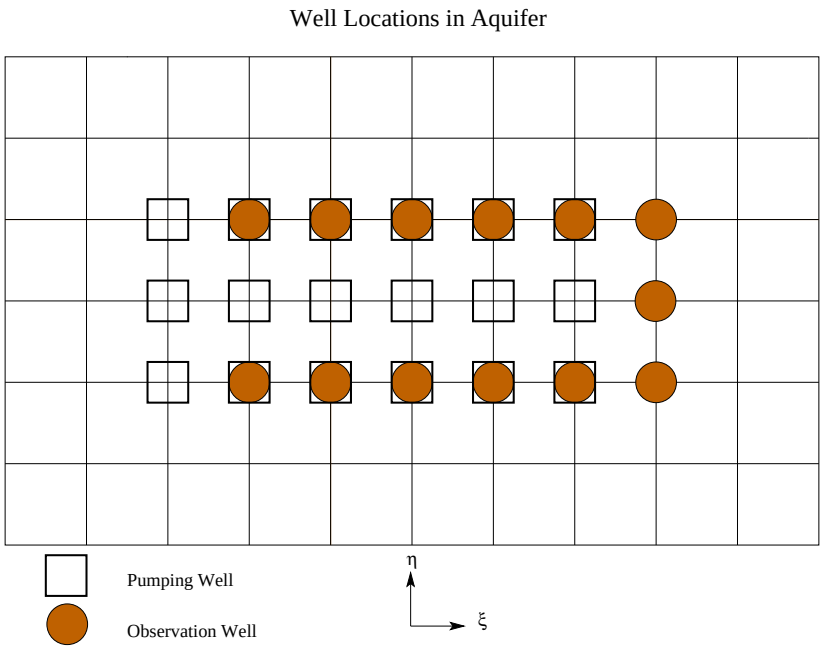

FIGURE 1. Locations of pumping and observation wells in the model aquifer.

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