Filtering Approximation Using Systematic Perturbations of a Discrete-Time Stochastic Dynamical System*

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Abstract

The standard problem of groundwater pollutant remediation by well pumping is modeled as a discrete-time LQG stochastic optimal control problem. The control is approximated by using a variation of differential dynamic programming (DDP) that includes systematic perturbations. Kalman filtering is used to estimate the partially observed state variables in a tractable format. This is a filtering application of the DDP method used by the authors in an earlier perturbation paper.

1. Introduction

Well pumping is the current standard method for groundwater pollutant remediation [7]. One way it can be modeled is as a partially observed discrete-time stochastic optimal control system. The system is approximated in this paper by systematic perturbations due to small stochastic noise. The analysis of the problem is a variation on that used by Kitanidis and co-workers [6], for approximate solutions to the optimal control, utilizing differential dynamic programming (DDP) [4] to find an analytic solution for the discrete-time problem without searching the whole state space. However, calculations used here follow the systematic perturbations of the optimal control problem, with corrections, given in an earlier paper by Kern and Hanson [5], and are briefly reviewed in Section 2.

The motivation for the groundwater application is also influenced by an example of Culver and Shoemaker [1]. A key variation is that they do not consider any stochastic events in their model, while the model used here includes a Gaussian random process. There are other differences in the objective and state transition equations, as well. While the model used here has a limited number of variables, DDP lends itself to larger scale problems in applications such as reservoir management [6] and groundwater quality remediation [3, 1] that otherwise risk computational complexity due to a large number of variables [2].

A three stage stochastic optimal control problem in discrete-time example is formulated in Section 3. The regular control for each stage is found in Section 4.

The presence of white noise in both state and observations make an accurate estimation of the state more difficult. An accurate approximation for the state at a particular moment, given information up to that time step, should minimize the influence of the stochastic processes. The Kalman filtering equations do exactly this by minimizing the spread of the error-estimate probability density [8]. The state estimate filter will be examined in Section 5.

2. General Control Problem and Stochastic Perturbation

The general discrete-time stochastic optimal control problem has the expected total cost function,

$$[\mathrm{J}] = E_{\{w\}}\left[f_N(\vec{x}_N) + \sum_{k=1}^{N-1} c_k(\vec{x}_k, \vec{u}_k)\right], \qquad (1)$$

where f_N is the specified final cost function and c_k is the kth stage cost function for $k = 1, \ldots, N-1$. The expectation operator, $E_{\{w\}} = \Pi_{k=1}^{N-1} E_{w_k}$, denotes the expectation over independent discrete-time noise $\vec{w}_k$, so $E_{\{w\}}$ is separable between stages. The optimal objective is to minimize the expected total cost function (1) subject to the linear state transition equation [6],

$$\vec{x}_{k+1} = \Phi_k \vec{x}_k + \Psi_k \vec{u}_k + \vec{\mu}_k + \vec{w}_k,\ k = 1, \ldots, N-1, \qquad (2)$$

where Φ_k and Ψ_k are known state and control coefficient matrices, respectively; the state of the system $\vec{x}_k$ is a $n \times 1$ vector; the control $\vec{u}_k$ is a $m \times 1$ vector; $\vec{\mu}_k$ is a $n \times 1$ known input vector; and $\vec{w}_k$ is a normally distributed, $n \times 1$ random vector, such that

$$E_{w_k}[\vec{w}_k] = \vec{0}, \quad E_{\{w\}}[\vec{w}_k \vec{w}_l^T] = Q_k \delta_{kl}, \qquad (3)$$

for $k, l = 1, \ldots, N-1$, where δ_{kl} is the Kronecker delta. In contrast to [5], $\vec{u}_k$, rather than $\vec{u}_{k+1}$, is applied here at stage k.

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The optimal expected total cost is

$$\min\left[\mathrm{J}\right]=\min_{\{u\}}\left[E_{\{w\}}\left[f_N(\vec{x}_N)+\sum_{k=1}^{N-1}c_k(\vec{x}_k,\vec{u}_k)\right]\right],\qquad(4)$$

where $\min_{\{u\}}=\Pi_{i=1}^{N-1}\min_{u_i}$, satisfying the Principle of Optimality separability property of the minimization operator needed to apply deterministic dynamic programming, while separability of the expectation operator over the stages permits stochastic dynamic programming. The final cost condition is $\mathrm{J}_N = f_N(\vec{x}_N) = \mathrm{J}^\star_N(\vec{x}_N)$, where the "$\star$" denotes the optimal value. Using the Principle of Optimality and substituting for $\vec{x}_N$ from the state transition equation, the recursive decomposition for stage $(N-1)$ is

$$\begin{aligned}\mathrm{J}_{N-1}(\vec{x}_{N-1},\vec{u}_{N-1}) &= \mathrm{J}^\star_N(\vec{x}_N)+c_{N-1}(\vec{x}_{N-1},\vec{u}_{N-1})\\ &= \mathrm{J}^\star_N(\Phi_{N-1}\vec{x}_{N-1}+\Psi_{N-1}\vec{u}_{N-1}\\ &+\ \vec{\mu}_{N-1}+\vec{w}_{N-1}\\ &+\ c_{N-1}(\vec{x}_{N-1},\vec{u}_{N-1})).\end{aligned}\qquad(5)$$

However, the optimal cost-to-go function for the kth stage is used for the recursion:

$$\begin{aligned}f_k(\vec{x}_k) &= \mathrm{J}^\star_k(\vec{x}_k)\\ &= \min_{u_k}\left[E_{w_k}[f_{k+1}(\vec{x}_{k+1})+c_k(\vec{x}_k,\vec{u}_k)]\right]\\ &= \min_{u_k}\left[E_{w_k}[f_{k+1}(\Phi_k\vec{x}_k+\Psi_k\vec{u}_k+\vec{\mu}_k+\vec{w}_k)\right.\\ &\quad\left.+c_k(\vec{x}_k,\vec{u}_k)]\right].\end{aligned}\qquad(6)$$

Therefore, the cost-to-go at stage k is minimized given the cost-to-go at $(k+1)$st stage has been computed.

Since in (2) the control affects the state at the kth stage, both $\vec{u}_k$ and $\vec{x}_k$ are expanded to order σ^2,

$$\vec{u}_k = \vec{u}_k^{(0)}+\sigma\vec{u}_k^{(1)}+\sigma^2\vec{u}_k^{(2)}+O(\sigma^3),\qquad(7)$$

$$\vec{x}_k = \vec{x}_k^{(0)}+\sigma\vec{x}_k^{(1)}+\sigma^2\vec{x}_k^{(2)}+O(\sigma^3),\qquad(8)$$

where σ is the covariance scaling factor, $\sigma^2=\mathrm{Trace}[Q_k]$ with $0<\sigma\ll 1$ for small noise and $\vec{w}_k=\sigma\vec{w}_k^{(1)}$. Substituting into the transition equation (2),

$$\vec{x}_{k+1}^{(0)} = \Phi_k\vec{x}_k^{(0)}+\Psi_k\vec{u}_k^{(0)}+\vec{\mu}_k,\qquad(9)$$

$$\vec{x}_{k+1}^{(1)} = \Phi_k\vec{x}_k^{(1)}+\Psi_k\vec{u}_k^{(1)}+\vec{w}_k^{(1)},\qquad(10)$$

$$\vec{x}_{k+1}^{(2)} = \Phi_k\vec{x}_k^{(2)}+\Psi_k\vec{u}_k^{(2)},\qquad(11)$$

upon equating coefficients of σ^0, σ^1 and σ^2, respectively.

For the minimization in (6), the partial derivative of $f_k(\vec{x}_k)$ with respect to $\vec{u}_k$ is set equal to zero to determine the minimum:

$$\begin{aligned}\vec{0} &= E_{w_k}\Big[\Psi_k^T\nabla_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)}+\sigma\vec{x}_{k+1}^{(1)}+\sigma^2\vec{x}_{k+1}^{(2)})\\ &\quad+\nabla_{u_k}[c_k](\vec{x}_k^{(0)}+\sigma\vec{x}_k^{(1)}+\sigma^2\vec{x}_k^{(2)},\vec{u}_k^{(0)}+\sigma\vec{u}_k^{(1)}\\ &\quad+\sigma^2\vec{u}_k^{(2)})+O(\sigma^3)\Big],\end{aligned}\qquad(12)$$

using the expansions (7, 8). Note that condition (12) lacks constraints, so leads to regular optimal control $\vec{u}^{(j)}_{\mathrm{reg},k}$, for $j=1$ to N which is emphasized here for brevity, rather than more general and computationally complex optimal control. Also, since the state depends on the control from (2), $\vec{x}_k^{(j)}\to\vec{x}^{(j)}_{\mathrm{reg},k}$, but here, the state "reg" subscript is suppressed to keep the subscripts relatively simple.

Next, Taylor approximations are used, assuming sufficient differentiability of f_{k+1} and c_k, about $\vec{x}_{k+1}^{(0)}$ for f_k and about $\vec{x}_k^{(0)}$ and $\vec{u}_k^{(0)}$ for c_k. Applying the expectation operator, noting that $\vec{w}_k=\sigma\vec{w}_k^{(1)}$, and collecting terms of the same order, the leading order equations are

$$\begin{aligned}\mathrm{ord}(\sigma^0):\vec{0} &= \Psi_k^T\nabla_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\\ &\quad+\nabla_{u_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)}),\end{aligned}\qquad(13)$$

$$\begin{aligned}\mathrm{ord}(\sigma^1):\vec{0} &= \Big(\Psi_k^T\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\Phi_k\\ &\quad+\nabla_{u_k}\nabla^T_{x_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)})\Big)\vec{x}_k^{(1)}\\ &\quad+\Big(\Psi_k^T\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\Psi_k\\ &\quad+\nabla_{u_k}\nabla^T_{u_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)})\Big)\vec{u}_{\mathrm{reg},k}^{(1)}.\end{aligned}\qquad(14)$$

The zeroth order equation for the regular control, i.e., $\vec{u}^{(0)}_{\mathrm{reg},k}$, is genuinely implicit and nonlinear since c_k is nonlinear in $\vec{u}_k$.

The $\mathrm{ord}(\sigma^1)$ equation is placed in operator notation:

$$\vec{0}=\mathcal{G}_{o,k}\vec{x}_k^{(1)}+\mathcal{H}_{o,k}\vec{u}_{\mathrm{reg},k}^{(1)},\qquad(15)$$

where

$$\begin{aligned}\mathcal{G}_{o,k} &\equiv \mathcal{G}_o(\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)})\\ &= \Psi_k^T\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\Phi_k\\ &\quad+\nabla_{u_k}\nabla^T_{x_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)}),\end{aligned}\qquad(16)$$

$$\begin{aligned}\mathcal{H}_{o,k} &\equiv \mathcal{H}_o(\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)})\\ &= \Psi_k^T\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\Psi_k\\ &\quad+\nabla_{u_k}\nabla^T_{u_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)}),\end{aligned}\qquad(17)$$

so that $\mathcal{H}_{o,k}$ is the Hessian matrix with respect to the control vector. This notation helps to simplify the $\mathrm{ord}(\sigma^2)$ equation:

$$\begin{aligned}\vec{0} &= \mathcal{G}_{o,k}\vec{x}_k^{(2)}+\mathcal{H}_{o,k}\vec{u}_{\mathrm{reg},k}^{(2)}\\ &\quad+\frac{\sigma^2}{2}\Psi_k^T\left((\Phi_k\vec{x}_k^{(1)})(\Phi_k\vec{x}_k^{(1)})^T:\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}\right)\\ &\quad\nabla_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\\ &\quad+\frac{\sigma^2}{2}\Psi_k^T\left((\Psi_k\vec{u}_k^{(1)})(\Psi_k\vec{u}_k^{(1)})^T:\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}\right)\\ &\quad\nabla_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\\ &\quad+\frac{\sigma^2}{2}\Psi_k^T\left(Q_k^{(2)}:\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}\right)\nabla_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\\ &\quad+\sigma^2\Psi_k^T\left((\Phi_k\vec{x}_k^{(1)})(\Psi_k\vec{u}_k^{(1)})^T:\nabla_{x_{k+1}}\nabla^T_{x_{k+1}}\right)\\ &\quad\nabla_{x_{k+1}}[f_{k+1}](\vec{x}_{k+1}^{(0)})\\ &\quad+\frac{1}{2}\left(\vec{u}_{\mathrm{reg},k}^{(1)}(\vec{u}_{\mathrm{reg},k}^{(1)})^T:\nabla_{u_k}\nabla^T_{u_k}\right)\nabla_{u_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)})\end{aligned}\qquad(18)$$

$$+\left(\vec{x}_k^{(1)}(\vec{u}_{\mathrm{reg},k}^{(1)})^T : \nabla_{x_k}\nabla_{u_k}^T\right)\nabla_{u_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg}},k^{(0)})$$
$$+\frac{1}{2}\left(\vec{x}_k^{(1)}(\vec{x}_k^{(1)})^T : \nabla_{x_k}\nabla_{x_k}^T\right)\nabla_{u_k}[c_k](\vec{x}_k^{(0)},\vec{u}_{\mathrm{reg},k}^{(0)}),$$

where "$A : B$" is the trace of the matrix product AB^T, and $Q_k^{(2)} = E_{w_k}[\vec{w}_k\vec{w}_k^T]/\sigma^2$. We can solve for the regular control$\vec{u}_{\mathrm{reg},k}$ provided $\mathcal{H}_o$ is invertible.

3. Example Control Problem Formulation

As stated previously, the motivation for this example comes from [1]. Modifying the continuous model in [3], a quadratic final cost and a small quadratic term added to the stage cost function are included here, changing the example from a singular control problem to an LQG problem (linear dynamics, quadratic costs and Gaussian noise). Here, a more concrete example for the cost functions is used than in [5]. For the moment, consider the three ($N = 3$) stage case.

The discrete-time stochastic optimal control problem has the cost objective

$$[\mathrm{J}] = E_{\{w\}}\left[f_3(\vec{x}_3) + \sum_{k=1}^{2} c_k(\vec{x}_k,\vec{u}_k)\right], \tag{19}$$

where $f_3(\vec{x}_3) = \frac{1}{2}\vec{x}_3^T S_3 \vec{x}_3$ is the specified quadratic final cost, with $S_3^T = S_3$ and $S_3 > 0$, and

$$c_k(\vec{x}_k,\vec{u}_k) = \left(\vec{\alpha} - H_k\vec{\beta}\right)^T \vec{u}_k + \frac{1}{2}\epsilon\vec{u}_k^T\vec{u}_k,$$

is the kth stage quadratic cost for $k = 1, 2$, with small parameter ϵ, where $\alpha_i = 1.1\times 10^{-3}$ is the treatment cost coefficient, and $\beta_i = 10^{-5}$ is the pumping cost coefficient, for $i = 1$ to 2.

The objective will be minimized subject to the linear state transition equation (2) with $N = 3$, and Φ_k, Ψ_k, μ_k are defined from the groundwater equations. The state $\vec{x}_k$ is a 2×1 vector defined as:

$$\vec{x}_k = \begin{bmatrix} H_k \\ C_k \end{bmatrix}, \tag{20}$$

where H_k is the hydraulic head and C_k the pollutant concentration at the observation wells for stage k. A single observation well is assumed to be located at the same site as one of two pumping wells. The control is assumed to be the pumping rate in liters per second at each pumping well, so the control is a 2×1 vector. The control constraint for the kth stage is $0 \le u_{k,i} \le 25.3$, for $i, k = 1$ to 2. The value 25.3 was chosen based on values from Table 2 in Culver and Shoemaker [1], p.828.

The example optimal expected total cost is

$$\min[\mathrm{J}] = \min_{\{\vec{u}\}}\left[E_{\{w\}}\left[\frac{1}{2}\vec{x}_3^T S_3\vec{x}_3 \right.\right. \tag{21}$$
$$\left.\left. + \sum_{k=1}^{2}\left(\left(\vec{\alpha} - H_k\vec{\beta}\right)^T\vec{u}_k + \frac{1}{2}\epsilon\vec{u}_k^T\vec{u}_k\right)\right]\right].$$

The final cost condition is denoted by $\mathrm{J}_3 = f_3(\vec{x}_3) = \mathrm{J}_3^*(\vec{x}_3)$.

4. Finding the Control

The equations from Section 2 will be used to find the regular control for this problem. The results follow those of the general feedback control for the LQG problem.

Stage 2 Control. Recall the cost-to-go from (6) is

$$\begin{aligned} f_2(\vec{x}_2) &= \min_{u_2}[E_{w_2}[f_3(\Phi_2\vec{x}_2 + \Psi_2\vec{u}_2 + \vec{\mu}_2 + \vec{w}_2) \\ &\quad + c_2(\vec{x}_2,\vec{u}_2)]]. \end{aligned} \tag{22}$$

Making the appropriate substitutions into (13) gives

$$0 = \Psi_2^T S_3(\Phi_2\vec{x}_2^{(0)} + \Psi_2\vec{u}_2^{(0)} + \vec{\mu}_2) + \vec{\alpha} - H_2^{(0)}\vec{\beta} + \epsilon\vec{u}_2^{(0)} \tag{23}$$

so that $\vec{u}_{reg,2}^{(0)} = L_2\vec{x}_2^{(0)} + \vec{\mathcal{K}}_2$, where

$$\begin{aligned} L_2 &\equiv -\mathcal{H}_{o,2}^{-1}\mathcal{G}_{o,2}, & \vec{\mathcal{K}}_2 &\equiv -\mathcal{H}_{o,2}^{-1}(\Psi_2^T S_3\vec{\mu}_2 + \vec{\alpha}), \\ \mathcal{H}_{o,2} &\equiv \Psi_2^T S_3\Psi_2 + \epsilon I_2, & \mathcal{G}_{o,2} &\equiv (\Psi_2^T S_3\Phi_2 - \widehat{\beta}), \end{aligned}$$
$$\widehat{\beta} \equiv \begin{bmatrix} \beta_1 & 0 \\ \beta_2 & 0 \end{bmatrix} = \begin{bmatrix} \vec{\beta} & \vec{0} \end{bmatrix},$$

and I_2 is the 2×2 identity matrix, assuming $\mathcal{H}_{o,2}$ is invertible. The ord(σ^1) equation (15) and ord(σ^2) equation (19) have the same form:

$$0 = \mathcal{G}_{o,2}\vec{x}_2^{(j)} + \mathcal{H}_{o,2}\vec{u}_2^{(j)} \;\Rightarrow \vec{u}_{\mathrm{reg},2}^{(j)} = L_2\vec{x}_2^{(j)}, \tag{24}$$

for $j = 1$ to 2, noting that third derivatives are zero here. Note that all three orders for the regular control have the same affine form with the same linear coefficient L_2. Thus, the optimal value for this stage from (6) is

$$\begin{aligned} f_2(\vec{x}_2) &= \frac{1}{2}\vec{x}_{\mathrm{reg},3}^{(0)T}S_3\vec{x}_{\mathrm{reg},3}^{(0)} + \sigma\vec{x}_{\mathrm{reg},3}^{(0)T}S_3 \\ &\quad \left(\Phi_2\vec{x}_2^{(1)} + \Psi_2\vec{u}_{\mathrm{reg},2}^{(1)} + \sigma\left(\Phi_2\vec{x}_2^{(2)} + \Psi_2\vec{u}_{\mathrm{reg},2}^{(2)}\right)\right) \\ &\quad + \frac{\sigma^2}{2}S_3 : \left(\left(\Phi_2\vec{x}_2^{(1)} + \Psi_2\vec{u}_{\mathrm{reg},2}^{(1)}\right)\right. \\ &\quad \left.\left(\Phi_2\vec{x}_2^{(1)} + \Psi_2\vec{u}_{\mathrm{reg},2}^{(1)}\right)^T + Q_2^{(0)}\right) \\ &\quad + \left(\vec{\alpha} - \widehat{\beta}\vec{x}_2^{(0)}\right)^T\vec{u}_{\mathrm{reg},2}^{(0)} + \frac{1}{2}\epsilon\vec{u}_{\mathrm{reg},2}^{(0)T}\vec{u}_{\mathrm{reg},2}^{(0)} \\ &\quad + \sigma\left(-\vec{u}_{\mathrm{reg},2}^{(0)T}\widehat{\beta}\left(\vec{x}_2^{(1)} + \sigma\vec{x}_2^{(2)}\right)\right. \\ &\quad \left. + \left(\vec{\alpha} - \widehat{\beta}\vec{x}_2^{(0)} + \epsilon\vec{u}_{\mathrm{reg},2}^{(0)}\right)^T\left(\vec{u}_{\mathrm{reg},2}^{(1)} + \sigma\vec{u}_{\mathrm{reg},2}^{(2)}\right)\right) \\ &\quad + \frac{\sigma^2}{2}\left(\epsilon\vec{u}_{\mathrm{reg},2}^{(1)T}\vec{u}_{\mathrm{reg},2}^{(1)} - 2\widehat{\beta}^T : \vec{x}_2^{(1)}\vec{u}_{\mathrm{reg},2}^{(1)T}\right) + O(\sigma^3), \end{aligned} \tag{25}$$

where $\vec{x}_{\mathrm{reg},3}^{(0)} \equiv \Phi_2\vec{x}_2^{(0)} + \Psi_2\vec{u}_{\mathrm{reg},2}^{(0)} + \vec{\mu}_2$, and the control is given by the regular optimal control,

$$\begin{aligned} \vec{u}_{\mathrm{reg},2} &= \vec{u}_{\mathrm{reg},2}(\vec{x}_2) = \vec{\mathcal{K}}_2 + \sum_{j=0}^{2}\sigma^j L_2\vec{x}_2^{(j)} + O(\sigma^3) \\ &= \vec{\mathcal{K}}_2 + L_2\vec{x}_2 + O(\sigma^3), \end{aligned} \tag{26}$$

consistent with the linear (affine) feedback control form for the LQG problem.

Stage 1 Control. The expectation, expansion and optimization of the O(σ^0) equation, using (6), (26) and (26), yields

$$\begin{aligned}\vec{0} &= \Psi_1^T\widehat{\Phi}_2^T S_3\left(\widehat{\Phi}_2\vec{x}_2^{(0)}+\widehat{\mu}_2\right)-\Psi_1^T\widehat{\beta}^T\left(L_2\vec{x}_2^{(0)}+\vec{\mathcal{K}}_2\right)\\ &+\Psi_1^T L_2^T\left(\vec{\alpha}-\widehat{\beta}\vec{x}_2^{(0)}\right)+\epsilon\Psi_1^T L_2^T\left(L_2\vec{x}_2^{(0)}+\vec{\mathcal{K}}_2\right)\\ &+\vec{\alpha}-\widehat{\beta}\vec{x}_1^{(0)}+\epsilon\vec{u}_1^{(0)}, \qquad (27)\end{aligned}$$

where $\widehat{\Phi}_2\equiv\Phi_2+\Psi_2 L_2$ and $\widehat{\mu}_2\equiv\vec{\mu}_2+\Psi_2\vec{\mathcal{K}}_2$. Assuming invertibility of $\mathcal{H}_{o,1}$, the coefficient of $\vec{x}_1^{(0)}$ in (27), then

$$\vec{u}_{\text{reg},1}^{(0)}=L_1\vec{x}_1^{(0)}+\vec{\mathcal{K}}_1, \qquad (28)$$

where

$$\begin{aligned}\mathcal{H}_{o,1} &\equiv \Psi_1^T\widehat{\Phi}_2^T S_3\widehat{\Phi}_2\Psi_1-\Psi_1^T\left(\widehat{\beta}^T L_2+L_2^T\widehat{\beta}\right)\Psi_1\\ &+\epsilon\left(I_2+\Psi_1^T L_2^T L_2\Psi_1\right),\\ L_1 &\equiv -\mathcal{H}_{o,1}^{-1}\left(\Psi_1^T\widehat{\Phi}_2^T S_3\widehat{\Phi}_2\Phi_1-\Psi_1^T\left(\widehat{\beta}^T L_2+L_2^T\widehat{\beta}\right)\Phi_1\right.\\ &\left.+\epsilon\Psi_1^T L_2^T L_2\Phi_1-\widehat{\beta}\right),\\ \vec{\mathcal{K}}_1 &\equiv -\mathcal{H}_{o,1}^{-1}\left(\Psi_1^T\widehat{\Phi}_2^T S_3\left(\widehat{\Phi}_2\vec{\mu}_1+\widehat{\mu}_2\right)\right. \qquad (29)\\ &-\Psi_1^T\left(\widehat{\beta}^T L_2+L_2^T\widehat{\beta}\right)\vec{\mu}_1+\Psi_1^T L_2^T\vec{\alpha}\\ &\left.-\Psi_1^T\widehat{\beta}^T\vec{\mathcal{K}}_2+\epsilon\Psi_1^T L_2^T\left(L_2\vec{\mu}_1+\vec{\mathcal{K}}_2\right)+\vec{\alpha}\right).\end{aligned}$$

Similarly, $\vec{u}_{\text{reg},1}^{(1)}=L_1\vec{x}_1^{(1)}$ and $\vec{u}_{\text{reg},1}^{(2)}=L_1\vec{x}_1^{(2)}$, so

$$\vec{u}_{\text{reg},1}=\vec{\mathcal{K}}_1+L_1\vec{x}_1+O(\sigma^3), \qquad (30)$$

assuming $\vec{x}_1=\vec{x}_1^{(0)}+\sigma\vec{x}_1^{(1)}+\sigma^2\vec{x}_1^{(2)}+O(\sigma^3)$. Note that if $\vec{x}_1=\vec{x}_1^{(0)}$ is specified, then $\vec{u}_{\text{reg},1}^{(1)}=\vec{u}_{\text{reg},1}^{(2)}=\vec{0}$.

5. Filtering: Finding the State Variables

The hydraulic head and pollutant concentration, i.e., the state variables, at a given stage are found during the final part of dynamic programming, the forward sweep. However, the stochastic processes present in the state transition equation (2) mean that substitution during the forward sweep could lead to inadequate results. This problem lends itself to filtering, which minimizes the spread of the error-estimate probability density, thus limiting the effect of the random process on the state estimate (Stengel [8], p. 342).

The state transition and observation equations are

$$\begin{aligned}\vec{x}_{k+1} &= \Phi_k\vec{x}_k+\Psi_k u_k+\vec{\mu}_k+\vec{w}_k, \qquad (31)\\ \vec{z}_k &= M_k\vec{x}_k+\vec{v}_k, \qquad (32)\end{aligned}$$

where $\vec{z}_k$ is the observation vector, M_k is the information matrix, and $\vec{v}_k$ is a discrete-time Gaussian noise, assumed independent, such that

$$\begin{aligned}E_{v_k}[\vec{v}_k] &= \vec{0},\\ E_{\{v\}}[\vec{v}_k\vec{v}_l^T] &= R_k\delta_{kl}=\sigma^2 R_k^{(2)}\delta_{kl},\\ E_{\{w_k,v_l\}}[\vec{w}_k\vec{v}_l^T] &= 0 \text{ for } k,l=1,2 \text{ and } k\neq l.\end{aligned}$$

Stengel [8], p.343 points out that the Kalman filtering equations only work for a control vector known without error. Hence, we will use the earlier dynamic programming results that gave an affine feedback optimal control $\vec{u}_k=L_k\vec{x}_k+\vec{\mathcal{K}}_k$, neglecting the $O(\sigma^3)$ perturbations.

The Kalman filter equations [8] are

$$\begin{aligned}\widehat{x}_k^- &= \left(\Phi_{k-1}+\Psi_{k-1}L_{k-1}\right)\widehat{x}_{k-1}^+ +\widehat{\mu}_{k-1}\\ &\equiv \widehat{\Phi}_{k-1}\widehat{x}_{k-1}^+ +\widehat{\mu}_{k-1}, \qquad (33)\\ P_k^- &= \widehat{\Phi}_{k-1}P_{k-1}^+\widehat{\Phi}_{k-1}^T+Q_{k-1}, \qquad (34)\\ K_k &= P_k^- M_k^T\left(M_k P_k^- M_k^T+R_k\right)^{-1}, \qquad (35)\\ \widehat{x}_k^+ &= \widehat{x}_k^- +K_k\left(\vec{z}_k-M_k\widehat{x}_k^-\right), \qquad (36)\\ P_k^+ &= \left(I-K_k M_k\right)P_k^-, \qquad (37)\end{aligned}$$

where $\widehat{x}_{k-1}$ is the estimated state variable. The plus or minus indicates pre-update or post-update for that time stage, respectively, such that the state estimate error is given by $\widetilde{x}_k^\pm=\vec{x}_k-\widehat{x}_k^\pm$. The state error-estimate covariance, P_k, is defined as $P_k^\pm=E[\widetilde{x}_k^\pm\widetilde{x}_k^{\pm T}]$.

Stage 2 State Estimate. This stage is crucial in any multi-stage Kalman filter because it involves calculations with the initial state. It is reasonable to assume that there is a stochastic part to the initial condition. In order that the problem be workable numerically, an initial guess is needed: $\widehat{x}_1^\pm=E[\vec{x}_1]=\vec{x}_1^{(0)}=\widehat{x}_1^{(0)\pm}$. Note that there are no higher order terms. The error on this estimate is precisely $\widetilde{x}_1=\vec{x}_1-\widehat{x}_1=\sigma\widetilde{x}_1^{(1)}$. The error estimate covariance for the initial stage is by assumption

$$\begin{aligned}P_1^\pm &= E\left[\widetilde{x}_1^\pm\widetilde{x}_1^{\pm T}\right]=\sigma^2 P_1^{(2)\pm}=\sigma^2\Lambda_1^{(2)}\neq 0\\ \Rightarrow P_1^{(0)} &= 0;\ P_1^{(1)\pm}=0;\ P_1^{(3)\pm}=0;\ \ldots, \qquad (38)\end{aligned}$$

given $\Lambda_1^{(2)}$, assuming consistency with the small noise transition and observation equation models.

Using the asymptotically expanded state (8), each order will be found separately. Putting the initial estimate into the state estimate extrapolation (33) gives

$$\widehat{x}_2^-=\widehat{\Phi}_1\widehat{x}_1^+ +\widehat{\mu}_1. \qquad (39)$$

The pre-update state estimates (noting that $\widehat{\mu}_1^{(0)}=\widehat{\mu}_1$ above) are

$$\widehat{x}_2^{(0)-}=\widehat{\Phi}_1\widehat{x}_1^{(0)+}+\widehat{\mu}_1,\ \ \widehat{x}_2^{(1)-}=\vec{0}=\widehat{x}_2^{(2)-}. \qquad (40)$$

Since the initial covariance matrices for the state error and state noise are both O(σ^2), the state error covariance extrapolation (34) becomes $P_2^{(2)-}=\widehat{\Phi}_1\Lambda_1^{(2)}\widehat{\Phi}_1^T+Q_1^{(2)}$, and all other higher order coefficients are zero. Another result of equation (38) is that the Kalman gain matrix also has only one term that is non-zero,

$$K_2^{(0)}=P_2^{(2)-}M_2^T\left(M_2 P_2^{(2)-}M_2^T+R_2^{(2)}\right)^{-1}=K_2. \qquad (41)$$

Also, the covariance update term is

$$\begin{aligned} P_2^{(2)+} &= (I - K_2 M_2)\, P_2^{(2)-} \\ &= (I - K_2 M_2)\left(\widehat{\Phi}_1 \Lambda_1^{(2)} \widehat{\Phi}_1^T + Q_1^{(2)}\right), \end{aligned} \qquad (42)$$

and all other higher order coefficients are zero.

The innovation process in the state update equation (36) can also be reduced by appropriate substitutions yielding

$$\vec{z}_2 - M_2 \widehat{x}_2 = M_2 \vec{x}_2 + \sigma \vec{v}_2^{(1)} - M_2 \widehat{x}_2 = M_2 \widetilde{x}_2 + \sigma \vec{v}_2^{(1)}. \qquad (43)$$

The state error for stage two, unlike the previous stage, has additional higher order terms: $\widetilde{x}_2 = \sigma \widetilde{x}_2^{(1)} + \sigma^2 \widetilde{x}_2^{(2)} + O(\sigma^3)$, there being no term of O(σ^0), since by equation (39),

$$\widetilde{x}_2^{(0)+} = \vec{x}_2^{(0)} - \widehat{x}_2^{(0)+} = \vec{x}_2^{(0)} - \left(\widehat{\Phi}_1 \widehat{x}_1^{(0)+} + \widehat{\mu}_1\right) = \vec{0}. \qquad (44)$$

Therefore, the innovation process does not effect the largest order equation and the deterministic term of the state estimate $\widehat{x}_2^{(0)+} = \widehat{x}_2^{(0)-}$ is unchanged by filtering. The state update for the next two order terms, using (40), are

$$\widehat{x}_2^{(j)+} = \widehat{x}_2^{(j)-} + K_2 \left(\vec{z}_2^{(j)} - M_2 \widehat{x}_2^{(j)-}\right) = K_2 \vec{z}_2^{(j)}, \qquad (45)$$

for $j = 1$ and 2, depending only on the second stage observations amplified by the second stage gain.

Stage 3 State Estimate. The state error covariance for the third stage, $P_3^- = \widehat{\Phi}_2 P_2^{(2)+} \widehat{\Phi}_2^T + Q_2$, is once again a single term of order σ^2, since $P_2^+ = \sigma^2 P_2^{(2)+}$ and $Q_2 = \sigma^2 Q_2^{(2)}$. Therefore, the Kalman gain matrix once again consists of a single term:

$$K_3^{(0)} = P_3^{(2)-} M_3^T \left(M_3 P_3^{(2)-} M_3^T + R_3^{(2)}\right)^{-1} = K_3. \qquad (46)$$

The pre-update state estimate is $\widehat{x}_3^- = \widehat{\Phi}_2 \widehat{x}_2^+ + \widehat{\mu}_2$, where $\widehat{\mu}_2^{(0)} = \widehat{\mu}_2$, so

$$\widehat{x}_3^{(0)-} = \widehat{\Phi}_2 \widehat{x}_2^{(0)+} + \widehat{\mu}_2, \quad \widehat{x}_3^{(j)-} = \widehat{\Phi}_2 \widehat{x}_2^{(j)+} = \widehat{\Phi}_2 K_2 \vec{z}_2^{(j)},$$

for $j = 1$ and 2. The error on this estimate is at most O(σ) since by equation (44),

$$\widetilde{x}_3^{(0)-} = \vec{x}_3^{(0)} - \left(\widehat{\Phi}_2 \widehat{x}_2^{(0)+} + \widehat{\mu}_2\right) = \widehat{\Phi}_2 \widetilde{x}_2^{(0)+} = \vec{0}. \qquad (47)$$

Therefore, the innovation process is zero for this order is

$$K_3 \left(\vec{z}_3^{(0)} - M_3 \widehat{x}_3^{(0)-}\right) = K_3 M_3 \widetilde{x}_3^{(0)-} = \vec{0},$$

and hence the largest order term of the estimate for stage three is uneffected by filtering, $\widehat{x}_3^{(0)+} = \widehat{x}_3^{(0)-} = \widehat{\Phi}_2 \widehat{x}_2^{(0)+} + \widehat{\mu}_2$. The remaining terms of the stage three state estimate are

$$\begin{aligned} \widehat{x}_3^{(j)+} &= \widehat{x}_3^{(j)-} + K_3 \left(\vec{z}_3^{(j)} - M_3 \widehat{x}_3^{(j)-}\right) \\ &= K_3 \vec{z}_3^{(j)} + (I - K_3 M_3)\, \widehat{\Phi}_2 K_2 \vec{z}_2^{(j)}, \end{aligned} \qquad (48)$$

for$j = 1$ and 2, dependent on both the second and third stage observations, given gains and model coefficients, with the only updated covariance term being $P_3^{(2)+} = (I - K_3 M_3)\, P_3^{(2)-}$.

6. Conclusions

The addition of a Gaussian stochastic process with systematic noise perturbations to a variant on an example of Culver and Shoemaker [1] suggests the use of filtering to obtain a reasonable state estimate. The Kalman filter used here gives a more tractable estimate for the state than simply using the state transition equation. When combined with the DDP approximation for the regular control, a good approximation for the optimal control policy and the minimum costs can be found. The regular control has the form of that for a general LQG feedback control policy. As expected, filtering does not effect the largest order term of the state estimate, which is deterministic. Future directions involve the development of efficient computational procedures.

7. References

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