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Optimal Output Selection for Control of Batch Processes

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Abstract—**Near-optimal control of batch processes can often be obtained using simple feedback structures. The maximum gain rule for selection of good outputs for feedback control is extended to nonlinear tracking problems, such as found in control of batch processes.**

I. Introduction

Optimal operation of chemical processes has been extensively studied in the last decades, but with focus on on-line optimization and continuous processes. For continuous processes, the notion of self-optimizing control has been established, and efficient methods for identification of self-optimizing variables exist [1].

Although batch processes are important in many aspects of industry, little attention has been devoted to implementation of optimal operating policies for such processes. Numerical methods for solving the open-loop optimization problem are available.

In later years it has been recognized that implementation schemes with low computational load are needed, yet guaranteeing near-optimal behavior also under disturbances. One approach that has been investigated is NCO tracking [2], but no systematic procedure to determine the appropriate outputs to control is known to the authors.

In this paper we present some results on identification of good variables to use for output feedback control in unconstrained regions for batch processes.

II. Maximum Gain Rule

Let the process be described by the following nonlinear state-space model;

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}), \tag{1}$$

$$\mathbf{y} = \mathbf{h}(\mathbf{x}), \tag{2}$$

where $\mathbf{x} \in \mathbb{R}^n$ is the state vector, $\mathbf{u} \in \mathbb{R}^m$ is the input vector and $\mathbf{y} \in \mathbb{R}^p$ is the output vector. Let the cost functional be written on Mayer form such that it only depends on the last state;

$$J = J(\mathbf{x}_f). \tag{3}$$

In a typical batch operation there are path constraints on certain outputs (states) and also on the inputs. The quality of operation is determined by the final state, and this is naturally posed as an end-point constraint. Optimal operation can then be determined by solving the following constrained optimal control problem:

$$\min_{\mathbf{u}(t), t_f} J, \tag{4}$$

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}, \mathbf{u}), \tag{5}$$

$$\mathbf{S}(\mathbf{x}, \mathbf{u}) \le \mathbf{0}, \tag{6}$$

$$\mathbf{E}(\mathbf{x}_f) \le \mathbf{0}, \tag{7}$$

where (6) describes algebraic constraints which must be satisfied for all times and (7) is the final-time constraints. For the rest of the discussion we assume that the solution to the optimization problem defined by (4)-(7) is known; the following analysis is local to the neighborhood of the optimal trajectories. A disturbance term was not included in the above model; for the following analysis it is assumed that the disturbance is fixed throughout the batch.

Assume that the active constraints are implemented. The Hamiltonian for the reduced space problem is

$$H(t) = \lambda^T \mathbf{f}\left(\mathbf{x}(t), \mathbf{u}(t)\right), \tag{8}$$

where λ is a time-varying vector of Lagrange multipliers. For problems where time does not explicitly occur in the Hamiltonian, it takes a constant value H^* along the optimal path. By a second-order Taylor polynomial in the input variation $\delta\mathbf{u}(t) = \mathbf{u}(t) - \mathbf{u}^*(t)$, we obtain

$$H = H^* + \mathbf{H}_\mathbf{u}\delta\mathbf{u} + \frac{1}{2}\delta\mathbf{u}^T\mathbf{H}_{\mathbf{uu}}\delta\mathbf{u}, \tag{9}$$

where $\mathbf{H}_\mathbf{u} = \mathbf{0}$. We define the loss as $L := H - H^*$ and rewrite (9) as

$$L = \frac{1}{2}\delta\mathbf{u}^T\mathbf{H}_{\mathbf{uu}}\delta\mathbf{u}. \tag{10}$$

In order to use (10) for selecting controlled outputs, it is necessary to pose the loss as a function of output variations instead of input variations. Equation (2) gives

$$\delta\mathbf{y} = \underbrace{\frac{\partial\mathbf{h}}{\partial\mathbf{x}^T}\frac{\partial\mathbf{x}}{\partial\mathbf{u}^T}}_{\mathbf{G}}\delta\mathbf{u}. \tag{11}$$

To obtain maximum information in the measured output, the measurements should be linearly independent. That means that the matrix $\mathbf{G}$ given by

$$\mathbf{G} = \frac{\partial\mathbf{h}}{\partial\mathbf{x}^T}\frac{\partial\mathbf{x}}{\partial\mathbf{u}^T}$$

should be nonsingular for all $t \le t_s$, where t_s denotes the switching time to the next arc. $\mathbf{G}$ can be seen as a time-varying gain measure corresponding to the gain matrix in steady-state problems. The loss may then be expressed as

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$$L = \delta \mathbf{y}^T \mathbf{G}^{-T} \mathbf{H}_{\mathbf{uu}} \mathbf{G}^{-1} \delta \mathbf{y}. \quad (12)$$

Assume that the model has been scaled such that for the expected disturbances, the maximum output deviation at any time is one. Our selection problem can then be posed as the minimization of

$$\theta(t) = \left\| \mathbf{G}_s^{-T} \mathbf{H}_{\mathbf{uu}} \mathbf{G}_s^{-1} \right\|_2 \quad (13)$$

for all $t \le t_s$, where the subscript s in $\mathbf{G}_s$ indicates that the matrix has been scaled. To find the best structure on average, the L_2-norm of $\theta(t)$ should be minimized.

Gain Estimation from Neighboring Optimal Control

In order to use minimization of θ to select good output variables, it is necessary to know the matrix **G**. We here present one method based on neighboring optimal control [4]. The time-varying Lagrange multipliers λ are found by solving the co-state equations

$$\dot{\lambda} = -H_{\mathbf{x}}. \quad (14)$$

backwards in time given the final condition

$$\lambda^T(t_f) = J_{\mathbf{x}}(t_f) + \nu^T \mathbf{E}_{\mathbf{x}}(t_f),$$

where ν is the Lagrange multiplier vector for the end-point constraint. Under the assumption that the end-point constraint and the objective functional do not depend explicitly on time, optimal control under sufficiently small perturbations in the state can be written as a linear time-varying feedback law that updates the originally optimal input path,

$$\mathbf{u}^*(t) - \mathbf{u}^{*,\text{old}} = -\mathbf{K}(t)\left(\mathbf{x} - \mathbf{x}^{*,\text{old}}\right), \quad (15)$$

where

$$\mathbf{K} = \mathbf{H}_{\mathbf{uu}}^{-1}\left(\mathbf{H}_{\mathbf{ux}} + \mathbf{f}_{\mathbf{u}}^T\left(\mathbf{S} - \mathbf{R}\mathbf{Q}^{-1}\mathbf{R}^T\right)\right). \quad (16)$$

The matrices **S**, **R** and **Q** are found from the Riccati equations $\dot{\mathbf{S}} = -\mathbf{S}\mathbf{A} - \mathbf{A}^T\mathbf{S} + \mathbf{S}\mathbf{B}\mathbf{S} - \mathbf{C}$, $\dot{\mathbf{R}} = -\left(\mathbf{A}^T - \mathbf{S}\mathbf{B}\right)\mathbf{R}$ and $\dot{\mathbf{Q}} = \mathbf{R}^T\mathbf{B}\mathbf{R}$ with $\mathbf{A} = \mathbf{f}_{\mathbf{x}} - \mathbf{f}_{\mathbf{u}}\mathbf{H}_{\mathbf{uu}}^{-1}\mathbf{H}_{\mathbf{ux}}$, $\mathbf{B} = \mathbf{f}_{\mathbf{u}}\mathbf{H}_{\mathbf{uu}}^{-1}\mathbf{f}_{\mathbf{u}}^T$ and $\mathbf{C} = \mathbf{H}_{\mathbf{xx}} - \mathbf{H}_{\mathbf{xu}}\mathbf{H}_{\mathbf{uu}}^{-1}\mathbf{H}_{\mathbf{ux}}$. The final conditions for the Riccati equations are $\mathbf{S}_f = J_{xx} + (\nu^T\mathbf{E}_x)_x$, $\mathbf{R}_f = \mathbf{E}^T$ and $\mathbf{Q}_f = \mathbf{0}$.

The derivative $\partial\mathbf{x}/\partial\mathbf{u}^T$ may now be approximated as the negative pseudo-inverse of **K**, and the gain measure **G** can then be computed as

$$\mathbf{G} = -\frac{\partial \mathbf{h}}{\partial \mathbf{x}^T}\mathbf{K}^{\dagger}. \quad (17)$$

III. EXAMPLE

The following example is taken from [5]. A product with concentration *P* is produced in a fed-batch bioreactor, and its growth rate depends on the biomass concentration *X*, the substrate concentration *S* as well as the reactor holdup *V*. The system is described by the following model:

$$\dot{X} = \mu(S)X - \frac{u}{V}X, \quad (18)$$

$$\dot{S} = -\frac{\mu(S)X}{Y_X} - \frac{\nu X}{Y_P} + \frac{u}{V}(S_{in} - S), \quad (19)$$

$$\dot{P} = \nu X - \frac{u}{V}P, \quad (20)$$

$$\dot{V} = u. \quad (21)$$

Parameter values and initial conditions are taken from [5]. The goal is to maximize *P* after 150 hours of operation. The open-loop solution has three arcs, whereof the first one is singular. From physical insight, [5] shows that *S* should be controlled in the singular arc.

To use the maximum gain rule, we need the Hessian from the Hamiltonian. We therefore introduce the transformation $\xi = \sqrt{u}$, and computations are made in terms of ξ.

The maximum gain rule tells us to maximize the scaled gain. We assume a maximum variation in the optimal path of 10% in each variable. The gain matrix **G** is scaled by the expected optimal variation. The comparison is shown in Table 1, and strongly suggests that *S* should be controlled in the singular arc, in agreement with [5].

State	Scaled gain
X	48055
S	62099000
P	952
V	694

TABLE 1
GAIN COMPARISON FOR STATES IN FED-BATCH REACTOR EXAMPLE

IV. CONCLUSIONS

The maximum gain rule has been extended to nonlinear systems, and the input-output map for variations has been interpreted as a notion of gain along the trajectory of the nonlinear system. The maximum gain rule correctly identifies the best output to control in a fed-batch reactor example.

The method may provide a useful approach to eliminating variables which would lead to poor control; a small scaled gain implies small gain, large optimal variation or both.

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