Eigenvalue-Based Method for Automatically Adjusting the Sampling Interval

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When using a sampled data control or optimization algorithm, one of the most important decisions to be made is to select the sampling period. The faster the process dynamics are, the higher should be sampling frequency be. The most frequently used rule of thumb is to select the sampling period as one-tenth to one-twentieth of the effective process time constant (for example, Smith and Corripio, 1985). The majority of processes, however, are nonlinear and then the effective time "constant" is not constant, but a function of the variable values at the local steady state. A large set point change can result in a very large change of the effective time constant. Looking at a simple example, consider an isothermal CSTR undergoing a third-order reaction:

$$V\frac{dc_A}{dt}=\frac{F}{V}c_{Ao}-\frac{F}{V}c_A-Vkc_A^3$$

Changing the conversion from 1% to 99% increases the time constant from 0.01 to 3,320!

Conventional sampled data algorithms employ a discrete model that relates inputs and outputs obtained between equal intervals of time δt; time is the independent model variable. Harmon et al. (1990) showed that variability in the effective time constant can be considerably reduced if one considers, instead of time, the cumulative amount of a quantity generated, consumed, or fed as the independent dynamic model variable. This work shows that by replacing time with an alternate variable β related to the dominant eigenvalue(s), it is possible for a class of autonomous nonlinear dynamic systems that includes many biochemical and chemical reaction networks in CSTRs to render the real part of the dominant eigenvalue(s) constant. Sampling takes place whenever β increases by $\delta\beta$ (instead of when t increases by δt), and the discrete model relates inputs and outputs spaced by $\delta\beta$.

Proposed Method

We start with the following easily proved lemma:

Lemma 1

Consider the dynamic system:

$$\dot{\underline{x}}=\underline{f}[\underline{x}(t),\underline{u}(t)];\ \underline{x}\in X\subset\mathbb{R}^n,\ \underline{u}\in U\subset\mathbb{R}^m,\ t\in\mathbb{R}^+\qquad(1)$$

Let the eigenvalues of $(\partial\underline{f}/\partial\underline{x})$ be $\lambda_i(\underline{x},\underline{u})$, $i=1,\ldots,n$ (need not be distinct). Then, for any scalar $g(\underline{x},\underline{u})$ the eigenvalues of $(\partial/\partial\underline{x}\ [(1/g\,\underline{f}]$ at any steady state $(\underline{x}_s,\underline{u}_s)$ of Eq. 1 are:

$$\frac{\lambda_i(\underline{x}_s,\underline{u}_s)}{g(\underline{x}_s,\underline{u}_s)}$$

where $i=1,\ldots,n$.

Proof

Differentiating we obtain:

$$\frac{\partial}{\partial\underline{x}}\left(\frac{1}{g}\underline{f}\right)=\frac{1}{g}\frac{\partial\underline{f}}{\partial\underline{x}}+\underline{f}\left[\frac{\partial\left(\frac{1}{g}\right)}{\partial\underline{x}}\right]^T$$

Since at a steady state of Eq. 1 $\underline{f}(\underline{x}_s,\underline{u}_s)=\underline{0}$,

$$\frac{\partial}{\partial\underline{x}}\left(\frac{1}{g}\underline{f}\right)\Bigg|_s=\frac{1}{g}\frac{\partial\underline{f}}{\partial\underline{x}}\Bigg|_s,$$

from which the lemma directly follows. An immediate consequence of the above lemma is the following theorem.

Theorem 1

Consider the system of Eq. 1 as in Lemma 1 and the system:

$$\frac{d\beta(t)}{dt}=g[\underline{x}(t),\underline{u}(t)];\ \beta\in\mathbb{R}$$

where $g(\underline{x}_s,\underline{u}_s)=-Re[\lambda_i(\underline{x}_s,\underline{u}_s)]$. [Here $Re[\lambda_i]$ denotes the real part of λ_i.] Then the Jacobian of the system:

$$\frac{d\underline{x}(\beta)}{d\beta}=\frac{1}{g(\underline{x}(\beta),\underline{u}(\beta))}\underline{f}[\underline{x}(\beta),\underline{u}(\beta)]\qquad(2)$$

has, at any steady state $(\underline{x}_s, \underline{u}_s)$, eigenvalues with real part

$$-\frac{Re[\lambda_j]}{Re[\lambda_i]} \quad \text{for } j=1, \ldots, n.$$

Proof

Follows directly from Lemma 1.

From Theorem 1 follows that if

a) There exists a positive function $g(\underline{x}, \underline{u})$ such that $-g(\underline{x}_s, \underline{u}_s)$ is equal to the real part of the dominant eigenvalue(s) at each steady state

b) $\beta(t) = \int_0^t g[\underline{x}(r), \underline{u}(r)]dr$ can be measured on-line

then, instead of relying on the model of Eq. 1 for sampled data controller design, one can use the equivalent model of Eq. 2. For example, using the Euler method, an approximate discretization of Eq. 2 is:

$$\underline{x}(\beta+\delta\beta) = \underline{x}(\beta) + \delta\beta\frac{f(\beta)}{g(\beta)} \tag{3}$$

Since the real part of the dominant eigenvalue of Eq. 2 is equal to -1 or, equivalently, the dominant time constant is 1 (units of β), an appropriate sampling "period" $\delta\beta$ can be easily selected.

Assumption a requires open-loop stability. Assumption b is needed so that the time instants to sample can be calculated. To satisfy this one may be able to use a steady-state model to obtain a $g(\underline{x}, \underline{u})$ that both satisfies Assumption a and is a function of variables that can be measured continuously in time. (An example of this is given at the end of this section.)

Processes on which $\delta\beta$ sampling can be easily used include many chemical and biochemical reaction networks in isothermal constant-volume CSTRs that are subject to variations in the feed composition. For these systems, the dominant eigenvalue is flow rate/volume at all steady states. Thus, β can be chosen as the cumulative volume fed, and sampling would take place at instants when a prespecified volume has been delivered. For example, consider the reaction network:

$$2A \underset{k_{-1}}{\overset{k_1}{\rightleftharpoons}} B$$

with reaction rate $r = k_1c_A^2 - k_{-1}c_B$. If the reaction takes place in a constant-volume isothermal CSTR, the process can be modeled as:

$$\frac{dc_A}{dt} = \frac{F}{V}c_{Ao} - \frac{F}{V}c_A - 2(k_1c_A^2 - k_{-1}c_B)$$
$$\frac{dc_B}{dt} = \frac{F}{V}c_{Bo} - \frac{F}{V}c_B + k_1c_A^2 - k_{-1}c_B$$

and the eigenvalues are $-(F_s/V)$ and $-[(F_s/V) + k_{-1} + 4k_1c_{As}]$. Clearly, $-(F_s/V)$ is the dominant eigenvalue at all steady states. Thus, one can choose $\beta(t) = \int_0^t[F(r)/V]dr$ (provided that the lower bound of F is positive). If the above reaction is irreversible $(k_{-1}=0)$ and c_B is not measured, then the mode of eigenvalue $-(F_s/V)$ is not observable. The observable eigenvalue is $-[(F_s/V) + 4k_1c_{As}]$. If c_A is not measured continuously on-line, then $g = (F/V) + 4k_1c_A$ cannot be used. However, we can use the steady-state version of the model to obtain:

$$c_{As} = \frac{F_s}{4k_1V}\left(-1+\sqrt{1+\frac{8k_1Vc_{Ao}}{F_s}}\right).$$

Thus, the observable eigenvalue can be expressed as:

$$-\frac{F_s}{V}\sqrt{1+\frac{8k_1Vc_{Aos}}{F_s}}$$

and if c_{Ao} is constant, we can select:

$$\beta(t) = \int_0^t \frac{F(r)}{V}\sqrt{1+\frac{8k_1Vc_{Ao}}{F(r)}}\,dr.$$

Then discretization can be based on the model:

$$\frac{dc_A}{d\beta} = \frac{\frac{F}{V}C_{Ao} - \frac{F}{V}c_A - 2k_1c_A^2}{\frac{F}{V}\sqrt{1+\frac{8k_1Vc_{Ao}}{F}}}$$

which has the "time constant" equal to 1 at all steady states.

To demonstrate the concept of basing sampled data controller design on Eq. 2 instead of Eq. 1, the next section presents an adaptive controller that uses $\delta\beta$ as the sampling period to control a fermentor's biomass concentration by manipulating the dilution rate.

Application

Consider the following fermentor model (Wang and Stephanopoulos, 1985):

$$\frac{dx}{dt} = \mu x - Dx$$
$$\frac{ds}{dt} = -\frac{1}{Y}\mu x + D(s_o - s)$$
$$\frac{d\mu}{dt} = \alpha\left(\frac{\mu_m s}{K+s} - \mu\right)$$

where x is the biomass concentration, s the substrate concentration, μ the specific growth rate, D the dilution rate $(=F/V)$, and s_o the feed substrate concentration. Let the parameters be:

$Y = 0.7$ (g cell/g substrate)
$\mu_m = 0.25\ (\mathrm{h}^{-1})$
$K = 20\ (\mathrm{g \cdot m^{-3}})$
$\alpha = 0.5\ (\mathrm{h}^{-1})$

and let the inputs be constrained as follows:

$$90 \leq s_0 \leq 110$$
$$0.01 \leq D \leq 0.15$$

Then, the dominant eigenvalue at all steady states is $-D$ and we can consider $\beta(t) = \int_0^t D(r)dr$ as the independent process

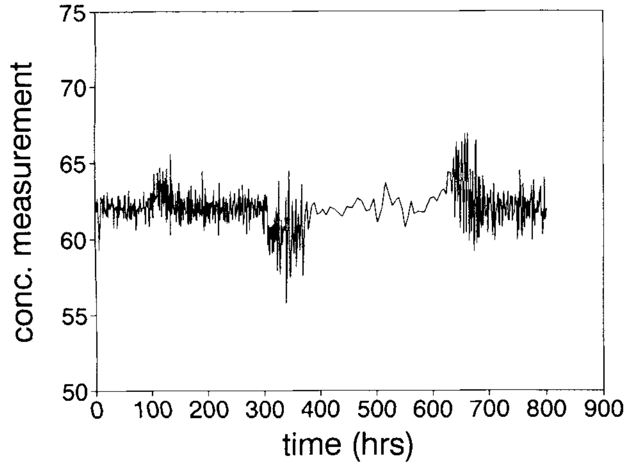

Figure 1a. Biomass concentration measurement (g·m^{-3}) vs. time (h) in response to changes in s_0.

100 for $t \in [0, 100]$; 110 for $t \in [100, 300]$; 90 for $t \in [300, 600]$; and 100 for $t \in [600, 800]$).

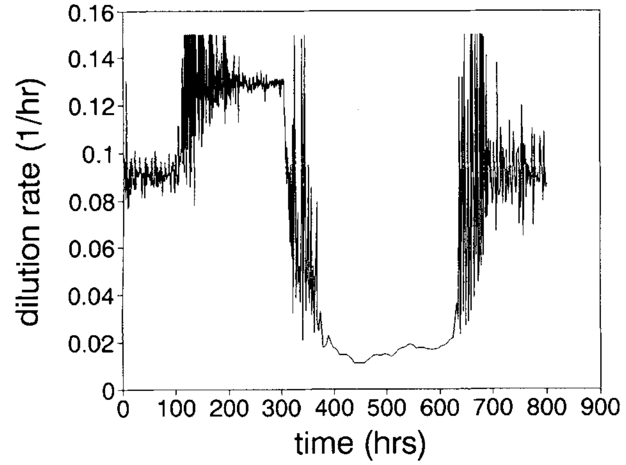

Figure 1b. Dilution rate (1/h) vs. time (h)

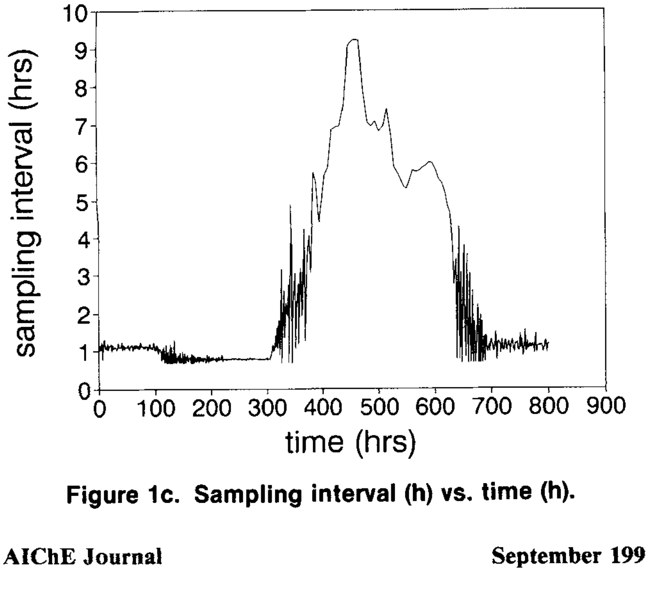

Figure 1c. Sampling interval (h) vs. time (h).

variable. One disadvantage that the switch to β has is that the process ceases to be linear with respect to the manipulated variable D. However, this is easily overcome by considering $1/D$ as the manipulated variable. An adaptive controller can then be based on the on-line identification of a linear discrete model such as:

$$x_m(\beta+\delta\beta) = \theta_1 x_m(\beta) + \theta_2 \frac{1}{D}(\beta) + \theta_3 \tag{4}$$

with $\delta\beta = 0.1$ (10% of the "time" constant). A simple algorithm, a self-tuning regulator of the Åström and Wittenmark (1973) type, is obtained by coupling a recursive least-squares estimator of the parameters θ_i (see, for example, Papadoulis et al., 1987 for a UDU factorization of a least-squares estimator with variable forgetting) with a deadbeat control law. The results of this algorithm for large disturbance changes are presented in Figure 1. The biomass concentration set point was 62 g·m^{-3}, its measurement was corrupted with white noise of standard deviation 0.6 g·m^{-3}, and s_0 changed from 100 g·m^{-3} at time 0 h to 110 g·m^{-3} at 100 h to 90 g·m^{-3} at 300 h and back to 100 g·m^{-3} at 600 h. It can be seen from Figure 1a that when a change in s_0 caused D to drop, the algorithm increased the sampling interval without deterioration of performance. Figure 1b shows how D changes and demonstrates an advantage of the ability of the algorithm to decrease the sampling frequency: less wear on the control valves. Figure 1c depicts the changes in sampling interval.

Discussion

The proposed $\delta\beta$-based discretization is not necessarily advantageous over the conventional δt discretization. It may change a process from being linear in the manipulated variable(s) to being nonlinear. However, as was demonstrated earlier, this can often be overcome by redefining the manipulated variable. A more serious drawback arises for processes subject to significant constant dead times. If the independent variable is switched to β, these dead times become variable. On the other hand, the most frequently encountered dead times are transportation lags, which vary inversely to the associated flow rate. If the dominant eigenvalue is proportional to this flow rate, then in a $\delta\beta$ discretization the varying dead time becomes approximately constant.

Acknowledgment

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Notation

c_A = concentration of A
c_{A_0} = feed concentration of A
c_B = concentration of B
c_{B_0} = feed concentration of B
D = dilution rate
F = flow rate
k_1 = reaction rate constant
k_{-1} = reaction rate constant
K = half-saturation constant
s = substrate concentration
s_0 = feed substrate concentration

t = time
x = biomass concentration
x_m = biomass concentration measurement
$\underline{x}$ = state variables vector
$\underline{u}$ = input (manipulated variables and disturbances) vector
V = volume
Y = yield

Greek letters

α = specific growth rate adaptability constant
β = alternate dynamic model independent variable
μ = specific growth rate
μ_m = maximum specific growth rate
θ_i = parameter estimated on-line

Subscript

s = steady state

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Errata

In the article titled "Continuous Olefin Copolymerization with Soluble Ziegler-Natta Catalysts," by Kee Jeong Kim and Kyu Yong Choi (August 1991, Vol. 37, p. 1255), incorrect numerical values of some parameters in Table 2 were inadvertently published. The following are the correct numerical values. The correct values of these parameters were used to obtain the results presented in the article.

Table 2. Numerical Values of Kinetic and Physical Parameters

Kinetic parameters

$k_{11} = 1.60 \times 10^{10} \exp(-4{,}900/RT)$ l/mol·h
$k_{12} = 7.36 \times 10^{8} \exp(-4{,}900/RT)$ l/mol·h
$k_{21} = 4.80 \times 10^{10} \exp(-6{,}200/RT)$ l/mol·h
$k_{22} = 1.06 \times 10^{9} \exp(-6{,}200/RT)$ l/mol·h
$k_d = 4.74 \times 10^{4} \exp(-6{,}000/RT)$ h^{-1}
$k_{f11} = 5.85 \times 10^{4} \exp(-3{,}475/RT)$ l/mol·h
$k_{f12} = 1.7 \times 10^{-2} k_{f11}$ l/mol·h
$k_{f21} = 2.71 \times 10^{4} \exp(-4{,}777/RT)$ l/mol·h
$k_{f22} = 3.0 \times 10^{-2} k_{f21}$ l/mol·h
$k_{f1Al} = 5.85 \times 10^{5} \exp(-3{,}475/RT)$ (mol/l)$^{1/2}$/h
$k_{f2Al} = 1.7 \times 10^{-2} k_{f1Al}$ (mol/l)$^{1/2}$/h
$k_{f1} = 5.04 \times 10^{10} \exp(-11{,}095/RT)$ h^{-1}
$k_{f2} = 1.37 \times 10^{12} \exp(-12{,}395/RT)$ h^{-1}

Physical and Reactor Design Parameters

$T_r = 300°\text{C}$

$\Theta = T(°\text{C})/T_r(°\text{C}) \quad \Theta_f = T_f(°\text{C})/T_r(°\text{C}) \quad \Theta_c = T_c(°\text{C})/T_r(°\text{C})$