

An Algorithm and its Application of Multi-stage Identification Model of Nonlinear Dynamical System

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Abstract In view of different characters in the development period, the growth period and the stabilization period of a kind of fermentative process, this paper proposes one kind of nonlinear multi-stage dynamical system and its identification model. This model is a kind of special optimal control problem restrained by multi-level programming. Because the level set of sub-control problem is locally uniform bounded and lower semi-continuous, we obtain the controllability of the sub-control problem and nonempty compactness of its optimal solution set. Then we construct the optimization algorithm and apply it to the parameter identification in batch microbial fermentation. Numerical results show that this multi-stage model can not only characterize the practical process better than we've used before, but also increase the precision and make it more effective.

Keywords Nonlinear dynamical system; Optimal control; Microbial fermentation; Parameter Identification

1 Introduction

1,3-propanediol(1,3-PD) possesses potential applications on a large commercial scale, especially as a monomer of polyesters or polyurethanes, its microbial production is recently paid attention to in the world for its low cost, high production and no pollution, etc. It is considered to be one of the bulk chemicals, which is likely to be produced by bio-processes on large scales. These researches include the quantitative description of the cell growth kinetics of multiple-inhibitions, the metabolic overflow kinetics of substrate consumption and product formation[1-3], feeding strategy of glycerol in fed-batch culture[4] and model analysis and simulations to determine the optimal operation conditions[5], and so on. However, a comparison between experimental data and computational results of the concentration showed that most of the continuous fermentation data were lower than the calculated values in the previous works, for example, the errors of substrate's values reach 50% in [6]. This indicates that the kinetics models presented by these researchers can't formulate the actual fermentation processes very well. The improvement of these kinetics models includes studies of microbial production in a more complex bioprocess, especially for a multi-stage process, but no analysis of parameters in these models have been done. We construct a parameter identification model for the system in batch fermentations in this paper to decrease the errors.

The rest of this paper is organized as follows. In section 2, we propose a kind of nonlinear multi-stage dynamical system and its identification model. In section 3, we prove that the level set of sub-control problem is locally uniform bounded and lower semi-continuous, then obtain the controllability of the sub-control problem and nonempty compactness of its optimal solution set. section 4 is devoted to construct an optimization algorithm to find the optimal parameters. Finally, Numerical results are obtained.

2 Nonlinear Multi-Stage Dynamical System

Based on the batch culture of glycerol bioconversion to 1,3-PD, we propose the nonlinear multi-stage dynamical system. Mass balances of biomass, substrate and products in batch microbial cultures are given as follows (see [7]).

$$\dot{x}(t) = f(x, u_p), t \in I := [0, t_f], x(0) = x_0 \quad (1)$$

where $x(t) \in R^5$ is state variable, $u_p \in R^{10}$ are parameters to be identified.

$$f(x, u_p) := (\mu x_1(t), -q_2 x_1(t), q_3 x_1(t), q_4 x_1(t), q_5 x_1(t)) \quad (2)$$

$$\mu = u_p(1) \frac{x_2(t)}{x_2(t) + 0.28} \prod_{i=2}^5 \left(1 - \frac{x_i(t)}{x_i^*}\right) \quad (3)$$

$$q_2 = u_p(2) + \frac{\mu}{u_p(3)} + u_p(4) \frac{x_2(t)}{x_2(t) + 11.43} \quad (4)$$

$$q_3 = u_p(5) + \mu u_p(6) + u_p(7) \frac{x_2(t)}{x_2(t) + 15.5} \quad (5)$$

$$q_4 = u_p(8) + \mu u_p(9) + u_p(10) \frac{x_2(t)}{x_2(t) + 85.71} \quad (6)$$

$$q_5 = q_2 \left(\frac{0.0025}{0.06 + \mu x_2(t)} + \frac{5.18}{50.45 + \mu x_2(t)} \right) \quad (7)$$

$u_p(i), i = 1, 2, \dots, 10$, are parameters to be identified with initial values

$$u_p^0 := (0.67, 2.2, 0.0082, 28.58, -2.69, 67.67, 26.59, -0.97, 33.07, 5.74) \in R^{10}$$

The parameters $u_p \in R^{10}$ range in $U_{ad} \subset R^{10}$

$$U_{ad} = \prod_{i=1}^{10} [u_p^0(i) - 0.5 \mid u_p^0(i) \mid, u_p^0(i) + 0.5 \mid u_p^0(i) \mid] \quad (8)$$

where $x_1^* = 10.0, x_2^* = 2039.0, x_3^* = 939.5, x_4^* = 1026.0, x_5^* = 361.0$. The range of the state variables are as follows.

$$S_0 = [0.001, x_1^*] \times [100, x_2^*] \times [0, x_3^*] \times [0, x_4^*] \times [0, x_5^*] \subset R^5 \quad (9)$$

Property 1. For all $u_p \in U_{ad}$, $f(x, u_p)$ given by (2) is measurable in t on $I = [0, t_f]$,

(i) For all $u_p \in U_{ad}$, $f(x, u_p)$ satisfies linear growth conditions.

(ii) For all $u_p \in U_{ad}$, $f(x, u_p)$ is Lipschitz continuous in $x \in S_0$.

(iii) For all $x \in S_0$, $f(x, u_p)$ is continuous in $u_p \in U_{ad}$.

Property 2. For all $u_p \in U_{ad}$ and $x_0 \in S_0$, the system (1) has an unique solution, written as $x(t) = x(t; 0, x_0, u_p)$. $x(t; 0, x_0, u_p)$ is continuous in $u_p \in U_{ad}$.

Suppose S_1 is a solution set of the system (1) on $u_p \in U_{ad}$.

$$S_1(0, t_f) := \{x(t; 0, x_0, u_p) \in C^1(0, t_f; \mathbb{R}^5) | x(t; 0, x_0, u_p) \text{ is solution of (1)}\} \quad (10)$$

Property 3. The set $S_1(0, t_f)$ given by (10) is a nonempty compact set in $C(0, t_f; \mathbb{R}^5)$.

Definition 1. Define the development period, the growth period and the stabilization period of the fermentative process as stage I, stage II and stage III, respectively.

The intervals of each stage are written as $I_1 = [0, t_{f_1}]$, $I_2 = [t_{f_1}, t_{f_2}]$ and $I_3 = [t_{f_2}, t_f]$, where $0 < t_{f_1} < t_{f_2} < t_f$. Let $t_{f_0} = 0$, $t_{f_3} = t_f$, $x^0(t_{f_0}) = x_0$, $u_t := (t_{f_1}, t_{f_2}) \in D := [a_1, b_1] \times [a_2, b_2] \subset \mathbb{R}^2$ is time parameters to be identified. The parameters of each stage are $u_p^i \in U_{ad}$, $i = 1, 2, 3$. Let $u := [u_p^1, u_p^2, u_p^3] \in \mathbb{R}^{30}$. The state variables are $x^i(t) \in \mathbb{R}^5$, $i = 1, 2, 3$. The dynamical systems of each stage are as follows.

$$\begin{aligned} \dot{x}^i(t) &= f(x^i, u_p^i), \quad t \in I_i, \quad i = 1, 2, 3. \\ x^i(t_{f,i-1}) &= \begin{cases} x_0, & i = 1 \\ x^{i-1}(t_{f,i-1}), & i = 2, 3 \end{cases} \end{aligned} \quad (11)$$

The solution of each system is unique, written as

$$x^i(t) = x^i(t; t_{f,i-1}, x^{i-1}(t_{f,i-1}), u_p^i), \quad i = 1, 2, 3.$$

The dynamical system of each stage can compose the system (1) through the initial values. Let $u_p^i = u_p$, $i = 1, 2, 3$. For all $u_p^i \in U_{ad}$, we have

$$x^i(t; t_{f,i-1}, x^{i-1}(t_{f,i-1}), u_p^i) \in S_1(I_i), \quad i = 1, 2, 3.$$

3 The Identification Model and Its Properties of Nonlinear Multi-Stage Dynamical System

Suppose $y(t) \in C^1(0, t_f; \mathbb{R}^5)$ is obtained by experiments. In order that $x^i(t)$ approximates $y(t)$ as possible as it can, we define the objective function as

$$\begin{aligned} J_i(t_{f_i}, x^{i-1}(t_{f,i-1}), u_p^i) &:= \int_{t_{f,i-1}}^{t_{f_i}} \|x^i(t; t_{f,i-1}, x^{i-1}(t_{f,i-1}), u_p^i) - y(t)\|^2 dt \\ & \quad i = 1, 2, 3. \end{aligned} \quad (12)$$

The identification problem can be formulated as follows.

$$\begin{aligned} OIP : \min \quad & J(u_t, u) := \sum_{i=1}^3 J_i(t_{f_i}, x^{i-1}(t_{f,i-1}), u_p^i) \\ \text{s.t.} \quad & u_t \in D \\ & u \in U_{ad}^3. \end{aligned} \quad (13)$$

The problem OIP can be divided into the following multi-level optimal control problem.

$$\begin{aligned}
 BP: \quad & \min J(u_t, u) = J(u_t, u_p^1, u_p^2, u_p^3) \\
 & \text{s.t. } u_t \in D \\
 BP1: \quad & \min J_1(t_{f_1}, x_0, u_p^1) \\
 & \text{s.t. } u_p^1 \in U_{ad} \\
 BP2: \quad & \min J_2(t_{f_2}, x^{1*}(t_{f_1}), u_p^2) \\
 & \text{s.t. } u_p^2 \in U_{ad} \\
 BP3: \quad & \min J_3(t_f, x^{2*}(t_{f_2}), u_p^3) \\
 & \text{s.t. } u_p^3 \in U_{ad}
 \end{aligned}$$

Theorem 1. The objective function $J_i(t_{f_i}, x^{i-1}(t_{f_{i-1}}), u_p^i)$ defined by (12) is continuous on $t_{f_i} \in [a_i, b_i]$ and $u_p^i \in U_{ad}$, $i=1,2,3$.

Property 4. The objective function $J(u_t, u)$ defined by (13) is continuous on $(u_t, u) \in D \times U_{ad}^3$.

Property 5. The objective function $J(u_t, u)$ of the problem OIP is locally uniform bounded on the level set of $u \in U_{ad}^3$ for $u_t \in D$.

Theorem 2. The problems OIP, BP, BP_{*i*}, $i = 1, 2, 3$, have optimal solutions.

For given $u_t \in D$, let

$$\begin{aligned}
 p(u_t) &:= \inf\{J(u_t, u) | u \in U_{ad}^3\} \\
 P(u_t) &:= \operatorname{argmin}\{J(u_t, u) | u \in U_{ad}^3\} \\
 p_i(u_t) &:= \inf\{J_i(t_{f_i}, x^{i-1}(t_{f_{i-1}}), u_p^i) | u_p^i \in U_{ad}\} \\
 P_i(u_t) &:= \operatorname{argmin}\{J_i(t_{f_i}, x^{i-1}(t_{f_{i-1}}), u_p^i) | u_p^i \in U_{ad}\}, \quad i = 1, 2, 3.
 \end{aligned}$$

Consider the problem OIP, for given $u \in U_{ad}^3$, let

$$\begin{aligned}
 q(u) &:= \inf\{J(u_t, u) | u_t \in D\} \\
 Q(u) &:= \operatorname{argmin}\{J(u_t, u) | u_t \in D\}
 \end{aligned}$$

Applying Proposition 1.35 in [8], we have

$$\begin{aligned}
 \min_{(u_t, u) \in D \times U_{ad}^3} J(u_t, u) &= \min_{u_t \in D} p(u_t) = \min_{u \in U_{ad}^3} q(u) \\
 \operatorname{argmin}_{(u_t, u) \in D \times U_{ad}^3} J(u_t, u) &= \{(u_t^*, u^*) | u^* \in \operatorname{argmin}_{u \in U_{ad}^3} q(u), u_t^* \in \operatorname{argmin}_{u_t \in D} J(u_t, u^*)\} \\
 &= \{(u_t^*, u^*) | u_t^* \in \operatorname{argmin}_{u_t \in D} p(u_t), u^* \in \operatorname{argmin}_{u \in U_{ad}^3} J(u_t^*, u)\}
 \end{aligned}$$

4 Numerical Optimization Algorithm

Because for all $t \in [0, t_f]$, $y(t) \in S_0$, $x(t; t_{f_i}, x^{i-1}(t_{f, i-1}), u_p^i) \in S_0$ and $y(t) \in C^1(0, t_f, R^5)$, $S_{p^k}(t_{f_i})$ is related to $t_{f_i} \in [a_i, b_i]$ and unrelated to u_p^i . The function $J_{d_i}(t_{f_i}, x^{i-1}(t_{f, i-1}), u_p^i)$ is monotone on t_{f_i}, u_p^i . The optimal subproblem on stage I can be formulated as.

$$\begin{aligned} OP1: \quad & \min \quad p_1(t_{f_1}, u_p^{1*}) + (b_1 - t_{f_1}) \\ & s.t. \quad t_{f_1} \in [a_1, b_1] \end{aligned}$$

Where

$$\begin{aligned} p_1(t_{f_1}, u_p^{1*}) &:= \min\{J_{d1}(t_{f_1}, x_0, u_p^1) | u_p^1 \in U_{ad}\} \\ u_p^{1*} \in P_1(t_{f_1}) &:= \operatorname{argmin}\{J_{d1}(t_{f_1}, x_0, u_p^1) | u_p^1 \in U_{ad}\} \end{aligned}$$

For u_p^{1*} , the solution of (11) is $x^{1*}(t) = x^1(t; t_{f_0}, x_0, u_p^{1*})$. Let $t_{f_1}^* \in [a_1, b_1]$ be optimal solution of problem OP1,

$$p_{1, b_1}(t_{f_1}^*, u_p^{1*}) := \min\{p_1(t_{f_1}, u_p^{1*}) + (b_1 - t_{f_1}) | t_{f_1} \in [a_1, b_1]\}$$

$x^{1*}(t) = x^1(t; t_{f_0}, x_0, u_p^{1*})$. Thus the optimal subproblem on stage II can be formulated as.

$$\begin{aligned} OP2: \quad & \min \quad p_2(t_{f_2}, u_p^{2*}) + (b_2 - t_{f_2}) \\ & s.t. \quad t_{f_2} \in [a_2, b_2] \end{aligned}$$

Where

$$\begin{aligned} p_2(t_{f_2}, u_p^{2*}) &:= \min\{J_{d2}(t_{f_2}, x^{1*}(t_{f_1}^*), u_p^2) | u_p^2 \in U_{ad}\} \\ u_p^{2*} \in P_2(t_{f_2}) &:= \operatorname{argmin}\{J_{d2}(t_{f_2}, x^{1*}(t_{f_1}^*), u_p^2) | u_p^2 \in U_{ad}\} \end{aligned}$$

For u_p^{2*} , the solution of (11) is $x^{2*}(t) = x^2(t; t_{f_2}, x^{1*}(t_{f_1}^*), u_p^{2*})$, let $t_{f_2}^* \in [a_2, b_2]$ be solution of OP2,

$$p_{2, b_2}(t_{f_2}^*, u_p^{2*}) := \min\{p_2(t_{f_2}, u_p^{2*}) + (b_2 - t_{f_2}) | t_{f_2} \in [a_2, b_2]\}$$

Let $x^{2*}(t_{f_2}^*) = x^2(t_{f_2}^*; t_{f_1}^*, x^{1*}(t_{f_1}^*), u_p^{2*})$. Thus the optimal subproblem on stage III can be formulated as.

$$\begin{aligned} OP3: \quad & \min. \quad J_{d3}(t_f, x^{2*}(t_{f_2}^*), u_p^3) \\ & s.t. \quad u_p^3 \in U_{ad} \end{aligned}$$

In last problem of above, $t_f = t_{f_3}$ is fixed, the optimal variable of OP3 only includes $u_p^3 \in U_{ad}$. In order to solve OP*i*, $i = 1, 2, 3$, we need to consider the following subproblem.

$$\begin{aligned} SOPT(t_{f_i}): \quad & \min. \quad J_{di}(t_{f_i}, x_0^i, u_p^i) \\ & s.t. \quad u_p^i \in U_{ad}, \quad i = 1, 2, 3. \end{aligned} \tag{14}$$

The corresponding dynamical system is

$$x^i(t) = f(x^i, u_p^i), \quad t \in [t_{f, i-1}, t_{f_i}], \quad x^i(t_{f, i-1}) = x_0^i. \tag{15}$$

The solution set is written as

$$x^i(t) = x^i(t; t_{f,i-1}, x_0^i, u_p^i).$$

According to the monotonicity of $J_{di}(t_{f_i}, x_0^i, u_p^i)$ on u_p^i , we construct optimal algorithm $SOPT(t_{f_i})$ to solve the subproblem as follows, written as $SOPTM(t_{f_i})$.

Algorithm 1. $\langle 1 \rangle$. Input $u_p^0 \in R^{10}$, precision $\forall \varepsilon > 0$, initial value $x_0^i \in S_0$, $t_{f,i-1}, t_{f_i}$. Let $u = u_p^0$, $du = |u^0| / 100.0$.
 $\langle 2 \rangle$. Compute the numerical solution $x^i(t; t_{f,i-1}, x_0^i, u)$, $S_{jk}(t_{f_i})$, $c_{jk}(t_{f_i}, u)$ and $J_{di}(t_{f_i}, x_0^i, u)$.
 $\langle 3 \rangle$. If $J_{di}(t_{f_i}, x_0^i, u) \leq \varepsilon$, let $u^{i*} = u$, compute $x^{i*}(t_{f_i}) = x^{i*}(t_{f_i}; t_{f,i-1}, x_0^i, u)$. Let $x_0^{i+1} = x^{i*}(t_{f_i})$, stop. Else turn to $\langle 4 \rangle$.
 $\langle 4 \rangle$. If $C_{ij}(t_{f_i}, u) < S_{ij}(t_{f_i})$, $j = 1, 3, 4, 5$, and $C_{i^2}(t_{f_i}, u) > S_{i^2}(t_{f_i})$, and if $u(1) - du(1) \geq 0.5u_p^0(1)$, let $u(1) = u(1) - du(1)$ and turn to $\langle 2 \rangle$.
 $\langle 5 \rangle$. If $C_{ij}(t_{f_i}, u) > S_{ij}(t_{f_i})$, $j = 1, 3, 4, 5$, and $C_{i^2}(t_{f_i}, u) < S_{i^2}(t_{f_i})$, $u(1) + du(1) \leq 1.5u_p^0(1)$, let $u(1) = u(1) + du(1)$, then turn to $\langle 2 \rangle$.
 $\langle 6 \rangle$. If $C_{i^2}(t_{f_i}, u) > S_{i^2}(t_{f_i})$,
 If $u(j) + du(j) \leq 1.5 * u_p^0(j)$, let $u(j) = u(j) + du(j)$, $j = 2, 4$.
 If $u(3) - du(3) \geq 0.5 * u_p^0(3)$, let $u(3) = u(3) - du(3)$
 Else if $u(3) + du(3) \leq 1.5 * u_p^0(3)$, let $u(3) = u(3) + du(3)$,
 If $u(j) - du(j) \geq 0.5 * u_p^0(j)$, let $u(j) = u(j) - du(j)$, $j = 2, 4$. Turn to $\langle 2 \rangle$.
 $\langle 7 \rangle$. If $C_{ij}(t_{f_i}, u) > S_{ij}(t_{f_i})$, $j = 3, 4, 5$,
 If $u(j) - du(j) \geq 0.5 * u_p^0(j)$, let $u(j) = u(j) - du(j)$, $j = 5, 6, \dots, 10$.
 Else if $u(j) + du(j) \leq 1.5 * u_p^0(j)$, let $u(j) = u(j) + du(j)$, $j = 5, 6, \dots, 10$. Turn to $\langle 2 \rangle$.

In OP1 and OP2, the objective function $p_i(t_{f_i}, u_p^{i*})$ is increasing on $t_{f_i} \in [a_i, b_i]$. Thus we can construct the optimal algorithm as follows, written as OPT_i .

Algorithm 2. $\langle 1 \rangle$. Choose precision $\varepsilon > 0$, step size $dt = (b_i - a_i) / 100$, let $t_{f_i} = a_i, t_l = a_i$. Applying $SOPTM(t_{f_i})$ to solve $SOPT(t_{f_i})$, we can obtain $u_p^{i*} \in U_{ad}$. And let

$$p_{li}(t_l) = J_{di}(t_{f_i}, x_0^i, u_p^{i*}) \leq J_{di}(t_{f_i}, x_0^i, u), \forall u \in U_{ad}$$

$\langle 2 \rangle$. Let $t_{f_i} = t_{f_i} + dt$, if $t_{f_i} > b_i$, $t_{f_i}^* = t_l$, stop. Else use $SOPTM(t_{f_i})$ to solve the subproblem $SOPT(t_{f_i})$ and obtain the optimal solution $u_p^{i*} \in U_{ad}$, and

$$p_i(t_{f_i}, u_p^{i*}) = J_{di}(t_{f_i}, x_0^i, u_p^{i*})$$

$\langle 3 \rangle$. If $p_i(t_{f_i}, u_p^{i*}) \leq p_{li}(t_l) + \varepsilon$, let $t_l = t_{f_i}^*$, $p_{li}(t_l) = p_i(t_{f_i}, u_p^{i*})$, turn to $\langle 2 \rangle$;
 Else $t_{f_i}^* = t_l$, stop.

With the aid of Algorithm 1 and Algorithm 2, we can construct the optimal algorithm to solve OIP1 as following.

Algorithm 3. $\langle 1 \rangle$. Input precision $\varepsilon > 0$, the initial value $u_p^0 \in R^{10}$, $du = u^0/100.0$, $x_0 \in R^5$, and $0 < a_i < b_i, i = 1, 2, \dots, t_f$. Let $i = 1$.
 $\langle 2 \rangle$. Let $dt = (b_i - a_i)/100$. $t_{f_i} = a_i$, $t_l = a_i$. Applying OPT_i to solve the subproblem OP_i , the optimal solution is $u_p^{i*} \in U_{ad}$, $t_{f_i}^* \in [a_i, b_i]$ and $x^{i*}(t_{f_i}^*)$.
 $\langle 3 \rangle$. Let $i = i + 1$, if $i \leq 2$, turn to $\langle 2 \rangle$; else turn to $\langle 4 \rangle$.
 $\langle 4 \rangle$. Applying $SOPTM(t_{f_3})$ to solve the subproblem OP_3 , its optimal solution is $u_p^{3*} \in U_{ad}$ and $x^{3*}(t_{f_3})$. Output the optimal solution $(t_{f_1}^*, t_{f_2}^*) \in D$, u_p^{1*}, u_p^{2*} , and $u_p^{3*} \in U_{ad}$, $J_{di}(t_{f_i}, x_0^i, u_p^{i*}), i = 1, 2, 3$.

5 Numerical Results

Suppose the experimental data $y(t_j) \in S_0 \subset R^5$, $j = 1, 2, \dots, l$ at $t_j \in [0, t_f]$ is given. $x(t_j, u_p) \in S_0 \subset R^5$, $j = 1, 2, \dots, l$ denote the calculated values at t_j of the system (1) The corresponding absolute error $oj^1(u_p)$ and relative error $oj^2(u_p)$ are as follows.

$$oj^1(u_p) := \sum_{j=1}^l \sum_{k=1}^5 \frac{(x_k(t_j, u_p) - y_k(t_j))^2}{5l}$$

$$oj^2(u_p) := \sum_{j=1}^l \sum_{k=1}^5 \frac{(x_k(t_j, u_p) - y_k(t_j))^2}{5l(y_k(t_j))^2}$$

The original errors of the system (1) are as follows.

$$oj^1(u_p^0) = 894.86, \quad oj^2(u_p^0) = 0.35$$

The corresponding absolute errors and relative errors for each stage are respectively as following.

$$oj^1(u_p^{1*}) := 118.656 \quad oj^2(u_p^{1*}) = 0.147$$

$$oj^1(u_p^{2*}) := 121.535 \quad oj^2(u_p^{2*}) = 0.154$$

$$oj^1(u_p^{3*}) := 67.859 \quad oj^2(u_p^{3*}) = 0.0184$$

The sum total of absolute errors and relative errors for three stages are as following.

$$oj^1(u_p^{1*}, u_p^{2*}, u_p^{3*}) = 308.05 \quad oj^2(u_p^{1*}, u_p^{2*}, u_p^{3*}) = 0.156.$$

We can find easily that the sum total of absolute errors and relative errors for three stages are less than ones for the system (1). And this multi-stage model can not only formulate the practical process better than we've used before, but also became more effective.

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