2021 DSTA dys-ta.com
16th INTERNATIONAL CONFERENCE
Dynamical Systems – Theory and Applications
December 6-9, 2021, On-line

On minimax parameter estimation of nonlinear dynamic Brown's model for enzyme-substrate interaction with distributed delay

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Abstract: The work offers Brown's model for enzyme-substrate interaction with distributed delay. The method of minimax parameter estimation is developed. The guaranteed mean-square a posteriori error is presented in terms of minimal eigenvalue of the linear operator. An example of experimental data on electrochemical biosensor design is considered.

Keywords: delayed differential equations, parameter estimation, minimax, enzyme-substrate interaction, Brown's model, Michaelis-Menten model

1. Introduction

In this paper, we offer the algorithm for finding minimax parameter estimation of Brown's model. In [1] such a minimax method was followed for finding parameter estimation of nonstationary differential equations. Similar approaches were used for the building of prediction estimations of the Gompertzian model's dynamics by Nakonechnyi O. et al [2], [3], recurrent neural networks [4], differential equations in Hilbert space [5]. We consider the Brown's model

$$\begin{cases} \dot{n}_S(t) = -k_d n_E(t) n_S(t), \\ \dot{n}_E(t) = -k_d n_E(t) n_S(t) + k_d \int_{-\tau_{\min}}^{0} f(\tau) n_E(t+\tau) n_S(t+\tau) d\tau, \quad t \in (0, \overline{T}), \\ \dot{n}_P(t) = k_d \int_{-\tau_{\min}}^{0} f(\tau) n_E(t+\tau) n_S(t+\tau) d\tau, \end{cases} \tag{1}$$

with initial conditions $n_S(t) = n_S^0, n_E(t) = n_E^0, n_P(t) = 0, \quad t \in [-\tau_{\min}, 0]$.

Here k_d is unknown value; $f(\tau)$, $\tau \in [-\tau_{\min}, 0]$ is unknown function and this function is a quadratically integrable function; $\tau_{\min} > 0$ and $f(s) = 0,\ s < -\tau_{\min}$.

Consider that there are numbers k_0, q_1 and functions $q_2(\tau)$ and $f_0(\tau)$, $\tau \in [-\tau_{\min}, 0]$ such that the unknown parameters k_d and $f(\tau)$, $\tau \in [-\tau_{\min}, 0]$ belong to the set

$$G_1 = \left\{ (k_d, f) : |k_d - k_0| \le q_1^2, \int_{-\tau_{\min}}^{0} q_2^2(\tau) (f(\tau) - f_0(\tau))^2 d\tau \le 1 \right\} \tag{2}$$

Suppose that y_k, $k = \overline{1, N}$ are the known observations of the function $n_P(t)$, $t \in (0, \overline{T})$ with the certain k_d and $f(\tau)$, $\tau \in [-\tau_{\min}, 0]$, namely, $y_k = n_P(t_k) + \eta_k, t_k \in (0, \overline{T}), k = \overline{1, N}$.

Here η_k, $k=\overline{1,N}$ are unknown observation errors and $\sum_{k=1}^{N}\eta_k^2\sigma_k^2 \le \gamma_N^2$, where σ_k, $k=\overline{1,N}$ and γ_N are known values. Denote $I(k_d, f) = \sum_{k=1}^{N}\sigma_k^2\left(y_k - n_P(t_k)\right)^2$.

Definition 1. The a posteriori set is $G_y = \left\{(k_d, f) : I(k_d, f) \le \gamma_N^2\right\} \cap G_1$.

Definition 2. The value $\hat{k}_d$ and the function $\hat{f}(\tau)$, $\tau \in [-\tau_{\min}, 0]$ are a posteriori estimations of k_d and $f(\tau)$, $\tau \in [-\tau_{\min}, 0]$ if the following condition is fulfilled: $(\hat{k}_d, \hat{f}) \in Arg \min_{(k_d, f)\in G_1} I(k_d, f)$.

Definition 3. The guaranteed mean-square a posteriori error δ of the estimations $\hat{k}_d$ and $\hat{f}(\tau)$, $\tau \in [-\tau_{\min}, 0]$ is called the special value $\delta = \sup_{(k_d, f)\in G_y}\left(\left|k_d - \hat{k}_d\right|^2 + \int_{-\tau_{\min}}^{0}(f(\tau) - \hat{f}(\tau))^2 d\tau\right)^{1/2}$.

Theorem 1. We assume that exist value β_N^2 and the positive-definite quadratically integrable function γ_N^2, $\tau, s \in [-\tau_{\min}, 0]$ such that satisfying $G_y \subset \overline{G}_y$, where $\overline{G}_y = \left\{(k_d, f) : \bar{I}(k_d, f) \le 1\right\}$,

$$\bar{I}(k_d, f) = \beta_N^2(k_d - \hat{k}_d)^2 + \int_{-\tau_{\min}}^{0}\int_{-\tau_{\min}}^{0} K_N(\tau, s)(f(\tau) - \hat{f}(\tau))(f(s) - \hat{f}(s))d\tau ds.$$

Then the following condition for the guaranteed mean-square a posteriori error is satisfied

$$\delta \le \left(\beta_N^2 + \lambda_{\min}(K_N)\right)^{-\frac{1}{2}}. \tag{3}$$

Here $\lambda_{\min}(K_N)$ is the smallest eigenvalue of the operator $(K_N f)(\tau) = \int_{-\tau_{\min}}^{0} K_N(\tau, s) f(s) ds, \tau \in [-\tau_{\min}, 0]$.

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