On-line Estimation in Fed-batch Fermentation Process by Using State Space Model and Unscented Kalman Filter

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Abstract: On-line estimation of unmeasurable biological variables is important in fermentation processes, directly influencing the optimal control performance of the fermentation system as well as the quality and yield of the targeted product. In this study, a novel strategy for state estimation of fed-batch fermentation process is proposed. By combining a simple and reliable mechanistic dynamic model with the sample-based regressive measurement model, a state space model is developed. An improved algorithm, swarm energy conservation particle swarm optimization (SECPSO), is presented for the parameter identification in the mechanistic model, and the support vector machines (SVM) method is adopted to establish the nonlinear measurement model. The unscented Kalman filter (UKF) is designed for the state space model to reduce the disturbances of the noises in the fermentation process. The proposed on-line estimation method is demonstrated by the simulation experiments of a penicillin fed-batch fermentation process.

1. Introduction

A key problem in fermentation process control is how to monitor the process variables, such as biomass, substrate or product concentrations, in a reliable and cost effective manner. Fermentation processes are generically characterized as complex systems exhibiting non-linear and time-varying dynamics [1]. The optimal control for a fed-batch fermentation system presents a challenge to control engineers because it is difficult to on-line estimate the unmeasurable biological variables[2].

Although many efforts have been made in the development of new hardware sensors and chemical analyzers, commercial reliable and cost effective instruments for on-line measurement are very limited. Hence, some on-line estimation methods, which are based on the mechanistic models or data-driven models, have been proposed for fermentation processes [3].

The support vector machines (SVM) method, which has solid theoretical foundation rooted in statistical learning theory, is regarded as a state-of-the-art technique in the data-driven nonlinear modeling applications. It has been successfully introduced for the soft-sensor applications to estimate the key process variables in fed-batch fermentation processes [4].

The unscented Kalman filter (UKF) proposed by Julier and Uhlmann avoids the linearization in the EKF update formula by an unscented transformation (UT) and overcomes the drawbacks of the EKF. The performance of the UKF is better than that of the EKF in terms of robustness and speed of convergence [5].

In this paper, a state space model of a fermentation process is established, in which a simple and reliable mechanistic model is used to predict the nonlinear dynamic equations and the SVM regression is adopted as the measurement equations. The parameters in dynamic equations are identified by swarm energy conservation particle swarm optimization (SECPSO) algorithm. The key state variables are on-line estimated by UKF. The proposed method is applied to a simulated

penicillin fed-batch fermentation process.

2. Method

2.1 State Space Model of Fermentation Process.

A fed-batch fermentation process is described in a state space model as follows:

$$\begin{cases} \dfrac{dx(t)}{dt} = f(x(t), u(t)) + w(t) \\ y(t) = h(x(t)) + v(t) \end{cases} \tag{1}$$

Where x is the state vector, y is the measurement vector, w is the vector of process noise, assumed to be white Gaussian with zero mean and covariance Q, v is the vector of measurement noise, assumed to be white Gaussian with zero mean and covariance R, t is time, f and h are general functions that represent the process model and measurement model, respectively.

For using more prior knowledge, all available measured variables should be chosen to construct the SVM models. Hence, the SVM method is adopted to supplement the nonlinear measurement equations.

$$y = \mathrm{SVM}(x) \tag{2}$$

where SVM denotes the nonlinear formulation established using SVM model.

2.2 Parameter Identification Using SECPSO.

The particle swarm optimization (PSO) is an evolutionary computation technique developed by Kennedy and Eberhart based on the simulation of a simplified social model [6]. The best position in the searching history of the ith particle is represented as X_i^* and the best position of the particle among the population is represented as X^*. For the standard PSO algorithm, in the (k+1)th iteration each particle updates its velocity and position according to the following equations:

$$V_i^{k+1} = \omega_1 V_i^k + \eta_1 rand()(X_i^* - X_i^k) + \eta_2 rand()(X^* - X_i^*) \tag{3}$$

$$X_i^{k+1} = X_i^k + V_i^{k+1} \tag{4}$$

Where ω_1 is the inertia weight that determines how much a particle holds its current velocity in the next iteration, η_1 and η_2 are learning factors that control the maximum step size, and *rand*() is an independent uniformly distributed random variable in the range [0, 1].

The fitness value J in the SECPSO algorithm is the root mean square error (RMSE) for the simplified mechanistic model values compared with the actual desired values. The fitness value J of the algorithm is calculated according to the following equation

$$J = \sqrt{\frac{\sum_{i=1}^{N} (\overline{x}_i - x_i)^T (\overline{x}_i - x_i)}{N}} \tag{5}$$

Where x_i is the actual value, $\overline{x}_i$ is the output of simplified model, and N is the number of samples.

We attempt to make the failure experience of the worst particle useful. The worst position in the searching history of the ith particle is represented as X_i° and the worst position of the particle among the population is represented as X°. In this way, the algorithm updates its velocity equation according to the best value and the worst value of individual and population. The particle can change its status with more information. The update of velocity vector equation with the worst particle is:

$$V_i^{k+1} = \omega_1 V_i^k + \eta_1 rand()(X_i^* - X_i^k) - \mu_1 rand()(X_i^\circ - X_i^k) + \eta_2 rand()(X^* - X_i^*) - \mu_2 rand()(X_i^\circ - X_i^k) \quad (6)$$

Where μ_1 and μ_2 are impact factors, which are used to affect the worst value of individual and population in the updating of the velocity. Other parameters are the same as those in the standard PSO.

The energy of the *i*th particle is represented as $g_i = V_i^T V_i$. The energy of the swarm is described as

$$G = \sum_{i=1}^{m} g_i = \sum_{i=1}^{m} V_i^T V_i \quad (7)$$

We set a swarming coefficient $\tau \in [0,1]$ in the SECPSO algorithm. The number of good particles is $\tau \times m$ and that of bad particles is $(1-\tau) \times m$. The particles are arranged according to the fitness value J by ascending order. The $\tau \times m$ particles in the front of the sequence are the good sub-swarm and the rest of particles are the bad sub-swarm. The good particles update their velocity and position according to Eq.(4) and Eq.(6). After the update, the energy of good sub-swarm is represented as

$$G_1 = \sum_{i=1}^{\tau x m} V_i^T V_i \quad (8)$$

The bad particles update their velocity according to Eq.(3) and their position according to the following equations

$$X_i^{k+1} = X_i^k + \delta V_i^{k+1} \quad (9)$$

$$\delta V_{i+1}^T V_{i+1} = \frac{G - G_1}{m(1-\tau)} \quad (10)$$

where δ is the penalty coefficient, representing the difference between the swarm energy G and the good sub-swarm energy G_1, which affects each bad particle uniformly.

2.3 UKF Algorithm.

Unlike the EKF, the UKF does not approximate the nonlinear process and measurement model. The UKF uses a minimal set of sample points to capture the true mean and covariance of the nonlinear process [7].

The following discrete-time state space model is considered, which is from the forward Euler discretization of Eq.(1) and with the same variable declarations.

$$\begin{cases} x(k+1) = f(x(k), u(k)) + w(k) \\ y(k) = h(x(k)) + v(k) \end{cases} \quad (11)$$

A general framework for recursive estimation of states based on the UKF technique is presented as follows.

Initialization: (k = 0)

$$\hat{x}_0 = E(x_0), \; P_0 = E[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T] \quad (12)$$

For $\tau \in \{1, 2, \ldots, \infty\}$

Step 1: Selection of sigma points. The *n*-dimensional variable x_{k-1} with mean $\hat{x}_{k-1}$ and covariance P_{k-1} is approximated by sigma points selected

$$\begin{cases} \chi_{i,k-1} = \hat{x}_{k-1}, & i = 0, \\ \chi_{i,k-1} = \hat{x}_{k-1} + (\sqrt{(n+\lambda)P_{k-1}})_i, & i = 1,\ldots,n, \\ \chi_{i,k-1} = \hat{x}_{k-1} - (\sqrt{(n+\lambda)P_{k-1}})_{i-n}, & i = n+1,\ldots,2n \end{cases} \tag{13}$$

Step 2: Prediction. Each point is instantiated through the process model to yield a set of transformed samples

$$\chi_{i,k|k-1} = f(\chi_{i,k-1}, \mu_{k-1}), \quad i = 0,1,\ldots,2n, \tag{14}$$

The predicted mean and covariance are computed as

$$\hat{x}_{k|k-1} = \sum_{i=1}^{2n} W_i^{(m)} \chi_{i,k|k-1} \tag{15}$$

$$P_{k|k-1} = \sum_{i=0}^{2n} W_i^{(c)} [\chi_{i,k|k-1} - \hat{x}_{k|k-1}] \times [\chi_{i,k|k-1} - \hat{x}_{k|k-1}]^T + Q \tag{16}$$

Step 3: Update. As the measurement equation is nonlinear, the measurement update is performed as

$$y_{i,k|k-1} = h(\chi_{i,k-1}), \quad i = 0,1,\ldots,2n, \tag{17}$$

$$\hat{y}_{k|k-1} = \sum_{i=0}^{2n} W_i^{(m)} y_{i,k|k-1} \tag{18}$$

$$P_{y_k y_k} = \sum_{i=0}^{2n} W_i^{(c)} [y_{i,k|k-1} - \hat{y}_{k|k-1}] \times [y_{i,k|k-1} - \hat{y}_{k|k-1}]^T + R \tag{19}$$

$$P_{x_k y_k} = \sum_{i=0}^{2n} W_i^{(c)} [\chi_{i,k|k-1} - \hat{x}_{k|k-1}] \times [y_{i,k|k-1} - \hat{y}_{k|k-1}]^T \tag{20}$$

$$K = P_{x_k y_k} P_{y_k y_k}^{-1} \tag{21}$$

$$\hat{x}_k = \hat{x}_{k|k-1} + K(y_k - \hat{y}_{k|k-1}) \tag{22}$$

$$P_k = P_{k|k-1} - K P_{y_k yk} K^T \tag{23}$$

Step 4: Repeat of Steps 1 to 3 for the next sample. In the UKF implementation, the following variable definitions are used

$$\begin{cases} W_0^{(m)} = \lambda / (n+\lambda), & i = 0, \\ W_0^{(c)} = \lambda / (n+\lambda) + (1 - \alpha^2 + \beta), & i = 0, \\ W_i^{(m)} = W_i^{(c)} = 1/(2(n+\lambda)), & i = n+1,\ldots,2n \end{cases} \tag{24}$$

Where β is used to incorporate prior knowledge of the distribution of x. For Gaussian distributions, $\beta = 2$ is the optimal [8].

Clearly, the implementation of the UKF is convenient, because it does not need to calculate the Jacobian matrices, while it is necessary in the EKF.That is the advantage of using UKF for the state space model with SVM measurement equations.

3. Case Study and Results

3.1 Application in Fed-batch Penicillin Fermentation.

The complicated fermentation model for penicillin production in a fed-batch fermentor is used as the simulator of the process. A state space model for the process is established using the proposed modeling method. The dynamic equations are as follows[9]:

$$\begin{cases} \dfrac{dV_l}{dt} = F - F_{loss} \\ \dfrac{dC_x}{dt} = \mu C_x - \dfrac{C_x}{V_l}\dfrac{dV_l}{dt} \\ \dfrac{dC_p}{dt} = \mu_p C_x - K_d C_p - \dfrac{C_p}{V_l}\dfrac{dV_l}{dt} \\ \dfrac{dC_s}{dt} = -(\dfrac{\mu}{Y_{x/s}} + \dfrac{\mu_p}{Y_{p/s}} + Q_m)C_x + \dfrac{FS_0}{V_l} - \dfrac{C_s}{V_l}\dfrac{dV_l}{dt} \\ F_{loss} = V_l \lambda_{loss}(e^{5[(T-T_0)/(T_e-T_0)]} - 1) \\ \mu = \mu_{\max}\dfrac{C_s}{K_s C_x + C_s} \\ \mu_p = \mu_{p\max}\dfrac{C_s}{K_i + C_s + C_s^2 / K_p} \end{cases} \tag{25}$$

The measurement equations are

$$\begin{cases} C_0 = SVM_0(C_x, C_s, C_p, V_l) \\ C_c = SVM_c(C_x, C_s, C_p, V_l) \\ Q_{heat} = SVM_{heat}(C_x, C_s, C_p, V_l) \\ V_l = V_l \end{cases} \tag{26}$$

Where the measurement vector is $y = [C_0, C_c, Q_{heat}, V_l]^T$ .The values of the parameters obtained using the SECPSO algorithm for the penicillin state space model are listed in Table 1.

Table 1. Values of the parameters obtained using SECPSO

K_i	K_s	K_p	K_d	λ_{loss}	$Y_{x/s}$	$Y_{p/s}$	μ_{max}	μ_{pmax}	Q_m
1.838x10^{-1}	0.2027	0.485	0.014	0.000	0.471	0.8318	0.1051	0.0017	0.0171
1		5	6	1	2				

3.2 Experiments and Results.

We set $\kappa = 0$ and $\beta = 2$. The constant α is sensitive to the filter results and its value can be decided by simulation results. The initial values of $\hat{x}_0$ are set to [0.001, 14.7, 0.1, 102]^T, which are close to the true initial values [0.1, 15, 0, 100]^T. The initialization tuning parameters, the process noise covariance Q and measurement noise covariance R for the UKF are as follows:

$$P_0 = E[(x_0 - \hat{x}_0)(x_0 - \hat{x}_0)^T] = diag([10^{-7}, 10^{-7}, 10^{-7}, 10^{-6}]) \tag{27}$$

$$Q = diag([10^{-7}, 10^{-7}, 10^{-7}, 10^{-6}]) \tag{28}$$

$$R = diag([10^{-3}, 10^{-4}, 10^{-6}, 10^{-6}]) \tag{29}$$

The measurement equation is

$$y = V_l \tag{30}$$

We set $\alpha = 1$ and $R = diag([10^{-6}])$ for the state space model without the SVM equations. The part result of the on-line estimation using different state space model is shown in Fig.1.

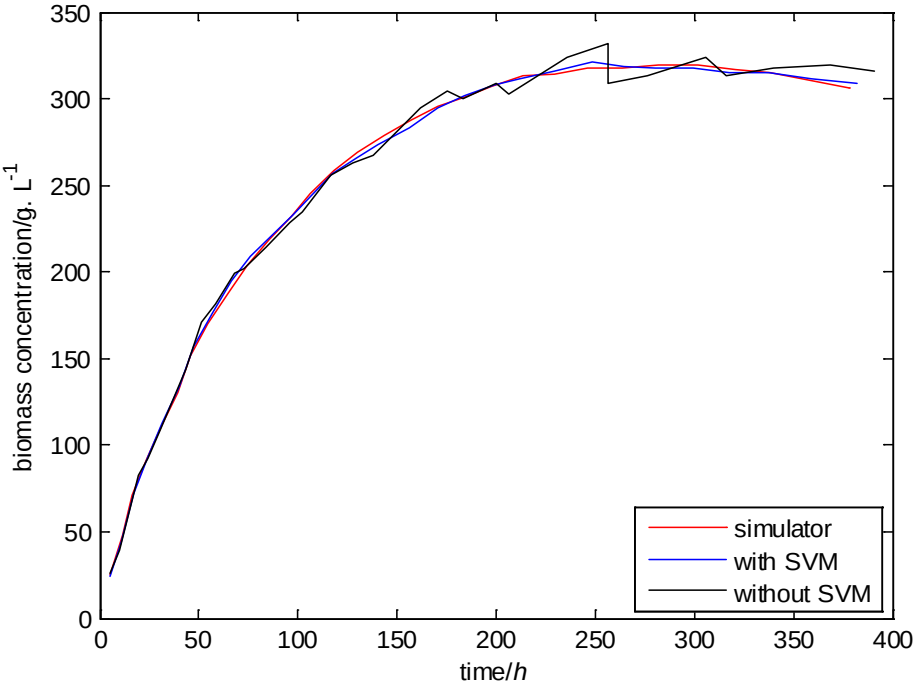

Fig.1 Comparison of biomass concentration for different models

The RMSE values for the state variables of the state space model with and without SVM equations compared with the simulator true values are listed in Table 2.

Table 2. RMSE values for different state space models compared with the simulator true values

Modeling formalism	RMSE(C_x)	RMSE(C_s)	RMSE(C_p)	RMSE(V_l)
Without SVM equations	2.8180	6.9591	0.2072	0.1381
With SVM equations	0.2308	0.0958	0.0413	0.1351

4. Conclusions

The proposed estimation method improves the accuracy of on-line estimation in a fed-batch fermentation process. The experiments, carried out using the data from the simulated penicillin fermentation, have validated the main characteristics of the proposed approach. The tracking and estimation performance of the UKF for the state space model with SVM measurement equations is compared with that using the mechanistic state model only. The results indicate that the proposed method is an effective approach to address the difficult on-line estimation of fed-batch fermentation processes.

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