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Model Quality Assessment and Model Mismatch Detection: A Temporal Smoothness Regularization Approach

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Abstract: Most industrial controllers are designed based on process models, and hence the closed-loop performance closely depends on the model quality. Since process dynamics variations are inevitable in practical applications, plant-model quality assessment is necessary so that model mismatch can be detected in time. In this article, a novel method based on temporal smoothness regularization is presented for model quality assessment. The linear time variant (LTV) model structure is applied to approximate the process dynamics. To avoid an overfitted model, temporal smoothness regularization is imposed on the model parameter changes so that model generalization ability is guaranteed. On the basis of the LTV model structure, a data-based model quality assessment approach is proposed, and the applicability is demonstrated through representative case studies.

Keywords: Control performance assessment, model mismatch detection, temporal smoothness regularization

1. INTRODUCTION

Model-based controllers are widely applied in the process industry. Process models are built to approximate the dynamic feature of controlled processes and can guide the design of model-based controllers. In spite of the fact that industrial processes have complicated dynamic feature and significant process nonlinearity, the process dynamics can usually be well approximated by relatively simple linear models in a limited operating point range. This is the main reason why linear-model based control strategies have been successfully implemented in industrial applications, such as the model-based PID (Skogestad, 2003) and linear model predictive control (MPC) (Qin & Badgwell, 2003).

Control performance of model-based controllers is closely related to model quality. However, it must be emphasized that process dynamics variations are inevitable in practice. For a highly nonlinear process with varying operating points, the process dynamics cannot be well approximated by a linear time-invariant model, because locally linearized models at different operating points have significant divergence with each other. Another cause for dynamics variations is the time-variant nature in process characteristics, for example, the impacts of valve abrasion on process dynamics during operation. In cases of significant changes in process dynamics, model mismatch would occur and further results in performance degradation of model-based controllers. Hence, model quality assessment becomes necessary to achieve control performance maintenance.

Detection of model mismatch has gained considerable focus in the field of process engineering. A widely applied approach is to analyse statistical characteristics of the residual generated by the process model. The two-model divergence algorithm has been proposed by Huang (2001), and the model mismatch is detected by investing the divergence between the residual generated by the process model and the recently established time-series model. The local detection approach relies on a hypothetical test on the model residuals to detect model mismatch, and the major advantage is the effectiveness in detecting minor changes in model parameters (Huang, 2000). In addition, changes in the statistical feature of model residuals can be quantified by the signal entropy (Shardt & Huang, 2013). Another approach to model-mismatch detection is to evaluate the correlation between the model input and residual signals. The reasonability lies in that, in the presence of significant model mismatch the process input and residual signals would exhibit evident correlation with each other. Both partial correlation analysis (Badwe, et al., 2009) and mutual information (Chen, et al., 2013) can be applied to evaluate the correlation in process variables.

In this article, a novel approach is applied based on the temporal smoothness regularization method. The process dynamics is approached using linear time variant (LTV) model structure, which is a basis transfer function model with time-varying coefficients. By this approach, the model quality can be monitored by examining changes in the model coefficients, and model-mismatch detection becomes possible as well. For the applied LTV model structure, the overall number of model coefficients exceeds the number of collected samples, and an overfitted LTV model with poor generalization ability would be obtained. To compensate this issue, a temporal smoothness regularization term is imposed on the changes of the time-varying model coefficient. The central idea is to penalize excessively aggressive model coefficient variations and guarantee that the time-varying

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process can be approximated using relatively simple model structures. Hence, model generalization ability is preserved. The utilization of the regularization term that penalizes model parameter variations is proposed by Ohlsson, et al. (2010), and in this article the regularization term in the L_2 norm is adopted for computational efficiency. A data-driven approach to model quality assessment is proposed, which evaluates the divergence in the process dynamics during the period when the control performance is satisfactory and the monitoring period. With the model quality index in the L_2 norm defined, model mismatch is enable to be detected in time, thereby providing useful guides for further controller maintenance.

The remainder of this article is organized as follows. In Section 2, the preliminary of the identification method based on the basis transfer function model is provided. In Section 3, the LTV model structure is given, which is the basis function model with temporal smoothness regularization of model coefficient variations. Furthermore, an iterative numerical method with low computational cost is presented to calculate the model coefficient. In Section 4 the data-driven model quality assessment scheme is provided. In Section 5, the effectiveness of the proposed method is demonstrated through a simulation study of a binary distillation process. Relevant conclusions are given in Section 6.

2. PRELIMINARY OF THE BASIS MODEL APPROACH

In this section, the preliminary of the process identification method based on basis models is reviewed. Since an MIMO process can be viewed as the combination of several separated MISO processes, in this article only the MISO case would be discussed, and the MIMO case is omitted for brevity. Consider the following continuous MISO process:

$$Y(s) = \sum_{i=1}^{m} G_i(s) U_i(s) \tag{1}$$

Each channel $G_i(s)$ can be approximated by a truncated basis transfer function series (Van den Hof & Ninness, 2005) :

$$\begin{aligned} G_i(s) &\doteq \sum_{k=1}^{n} c_{i,k} F_k(s) = \boldsymbol{\theta}_i^T \boldsymbol{F}(s) \\ \boldsymbol{F}(s) &= \begin{bmatrix} F_1(s) & F_2(s) & \cdots & F_n(s) \end{bmatrix}^T \end{aligned} \tag{2}$$

where $\{F_k(s)\}$ is the basis function model series and $\boldsymbol{\theta}_i$ is the model coefficient vector of the i-th channel:

$$\boldsymbol{\theta}_i = \begin{bmatrix} c_{i,1} & c_{i,2} & \cdots & c_{i,n} \end{bmatrix}^T \tag{3}$$

Commonly applied basis models include the Laguerre model series (Wahlberg, 1991):

$$F_k(s) = \frac{\sqrt{2\gamma}}{s+\gamma} \left(\frac{s-\gamma}{s+\gamma} \right)^{k-1} \tag{4}$$

and the FOPTD (first-order plus time delay) model series (Helbig, et al., 2000):

$$F_k(s) = \frac{1}{T_k s + 1} e^{-Ls} \tag{5}$$

Let $z_{i,k}(t)$ denote the filtered output of $F_k(s)$ with the input being $u_{\mathrm{i}}(t)$:

$$Z_{i,k}(s) = F_k(s) U_{\mathrm{i}}(s) \tag{6}$$

To calculate the model coefficient, the data matrix $\mathbf{Z}_i$ is formulated as follows using the samples of $\{z_{i,k}(t)\}_{k=1,\ldots,n}$:

$$\mathbf{Z}_i = \begin{bmatrix} z_{i,1}(1) & z_{i,2}(1) & \cdots & z_{i,k}(1) \\ z_{i,1}(2) & z_{i,2}(2) & \cdots & z_{i,k}(2) \\ \cdots & \cdots & \cdots & \cdots \\ z_{i,1}(N) & z_{i,2}(2) & \cdots & z_{i,k}(N) \end{bmatrix} \tag{7}$$

The model coefficient vectors $\{\boldsymbol{\theta}_i\}_{i=1,\cdots m}$ of different channels are piled as follows:

$$\boldsymbol{\varphi} = \begin{bmatrix} \boldsymbol{\theta}_1^T & \boldsymbol{\theta}_2^T & \cdots & \boldsymbol{\theta}_m^T \end{bmatrix}^T \in R^{mn} \tag{8}$$

Consequently, $\boldsymbol{\varphi}$ can be determined based on the following criterion:

$$\min_{\boldsymbol{\varphi}} \| \mathbf{Y} - \mathbf{Z}\boldsymbol{\varphi} \|_2^2 \tag{9}$$

where

$$\mathbf{Z} = \begin{bmatrix} \mathbf{Z}_1 & \mathbf{Z}_2 & \cdots & \mathbf{Z}_m \end{bmatrix} \in R^{N \times mn} \tag{10}$$

and $\mathbf{Y}$ is the process output vector defined as follows:

$$\mathbf{Y} = \begin{bmatrix} y(1) & y(2) & \cdots & y(N) \end{bmatrix}^T \in R^N \tag{11}$$

Obviously, $\boldsymbol{\varphi}$ can be calculated based on the least-squares regression:

$$\boldsymbol{\varphi} = \left(\mathbf{Z}^T \mathbf{Z} \right)^{-1} \mathbf{Z}^T \mathbf{Y} \tag{12}$$

3. LTV MODELING BASED ON THE TEMPORAL SMOOTHNESS REGULARIZATION

3.1 LTV model structure with temporal smoothness regularization

Based on the basis model structure, the process output is formulated as:

$$y(t) = \boldsymbol{z}^T(t) \boldsymbol{\varphi}(t) \tag{13}$$

where $\boldsymbol{z}(t)$ is the t-th row vector of the matrix $\mathbf{Z}$ defined in eq. (10). The model coefficient vector $\boldsymbol{\varphi}(t)$ is assumed to be time-varying, which can be determined based on the following criterion:

$$\min_{\boldsymbol{\varphi}(t)} J = \sum_{t=1}^{N} \| y(t) - \boldsymbol{z}^T(t) \boldsymbol{\varphi}(t) \|_2^2 \tag{14}$$

For problem (14), it should be noted that the number of parameters to be optimized exceeds the sample number N. Under the assumption that the model coefficients $\{\boldsymbol{\varphi}(t)\}$ are independent, an overfitted LTV model with poor generalization ability will be obtained. It should be noted that stationary operations are usually necessary requirements in industrial applications, and hence a nonlinear process usually operates at a steady point during a certain period. It implies that changes in the process dynamics would not be overly frequent. To avoid overly frequent model coefficient changes, a temporal smoothness regularization term of model coefficient variations is added (Boyd & Vandenberghe, 2004):

$$\min_{\boldsymbol{\varphi}(t)} J=\sum_{t=1}^{N}\| y(t)-\mathbf{z}^T(t)\boldsymbol{\varphi}(t)\|_2^2+\lambda\sum_{t=1}^{N}\|\boldsymbol{\varphi}(t)-\boldsymbol{\varphi}(t\text{-}1)\|_2^2 \tag{15}$$

where λ is the regulation parameter. The regularization term penalizes overly aggressive model coefficient changes such that model generalization ability is guaranteed. The utilization of the regularization term that penalizes LTV model parameter variations is firstly proposed by Ohlsson, et al. (2010). For the proposed method, the major difference from the method by Ohlsson is:

1. the regularization term is the sum of squared norms rather than norms;
2. the regularization term is in the L_2 norm.

Consequently, the problem formulated in (15) can be solved analytically.

3.2 Numerical algorithm

The optimization objective J in problem (15) is convex, and the optimal solution $\{\boldsymbol{\varphi}(t)\}$ must satisfy the following condition:

$$\frac{\partial J}{\partial \boldsymbol{\varphi}(t)}=\mathbf{0},\ t=1,\ldots,N \tag{16}$$

Let's define:

$$\mathbf{A}_t=\begin{bmatrix} \bar{\mathbf{A}}(1) & -\lambda\mathbf{I} & 0 & \cdots & 0 \\ -\lambda\mathbf{I} & \bar{\mathbf{A}}(2) & -\lambda\mathbf{I} & \cdots & 0 \\ 0 & \ddots & \ddots & \ddots & \vdots \\ \vdots & \ddots & -\lambda\mathbf{I} & \bar{\mathbf{A}}(t-1) & -\lambda\mathbf{I} \\ 0 & \cdots & 0 & -\lambda\mathbf{I} & \bar{\mathbf{A}}(t) \end{bmatrix}_{tmn\times tmn} \tag{17}$$

$$\mathbf{M}_t=\begin{bmatrix} \boldsymbol{\mu}(1) \\ \vdots \\ \boldsymbol{\mu}(t) \end{bmatrix}_{tmn\times 1} \tag{18}$$

where

$$\begin{aligned} \bar{\mathbf{A}}(t) &= 2\lambda\mathbf{I}+\mathbf{z}(t)\mathbf{z}^T(t),\ t=1,\cdots,N-1 \\ \bar{\mathbf{A}}(N) &= \lambda\mathbf{I}+\mathbf{z}(N)\mathbf{z}^T(N) \end{aligned} \tag{19}$$

and

$$\begin{aligned} \boldsymbol{\mu}(1) &= y(1)\mathbf{z}(1)+\lambda\boldsymbol{\varphi}(0) \\ \boldsymbol{\mu}(t) &= y(t)\mathbf{z}(t),\ t=2,\cdots,N \end{aligned} \tag{20}$$

The matrix $\mathbf{I}$ is the identity matrix with the size of $mn\times mn$. Based on (16), $\{\boldsymbol{\varphi}(t)\}$ is obtained as:

$$\boldsymbol{\Gamma}=\begin{bmatrix} \boldsymbol{\varphi}(1) \\ \vdots \\ \boldsymbol{\varphi}(N) \end{bmatrix}=\mathbf{A}_N^{-1}\mathbf{M}_N \tag{21}$$

Even though $\mathbf{A}_N$ has a large size, it has a strip structure. Using the skills on matrix computation summarized by Boyd and Vandenberghe (2004) , an iterative algorithm based on the matrix inverse lemma is presented to compute (21) in a cost efficient way. The matrix $\mathbf{A}_t$ can be formulated in a block matrix form:

$$\mathbf{A}_t=\begin{bmatrix} \mathbf{A}_{t-1} & \mathbf{B}_{t-1} \\ \mathbf{B}_{t-1}^T & \bar{\mathbf{A}}(t) \end{bmatrix} \tag{22}$$

The definition of $\mathbf{B}_t$ is:

$$\mathbf{B}_t=\begin{bmatrix} \mathbf{0}_{mn\times mn} & \cdots & \mathbf{0}_{mn\times mn} & -\lambda\mathbf{I} \end{bmatrix}^T \in R^{mn,tmn} \tag{23}$$

Using the matrix inverse lemma for the block matrix, the inverse of $\mathbf{A}_t$ is calculated as follows:

$$\mathbf{A}_t^{-1}=\begin{bmatrix} \mathbf{A}_{t-1}^{-1}+\mathbf{A}_{t-1}^{-1}\mathbf{B}_{t-1}\mathbf{S}_t^{-1}\mathbf{B}_{t-1}^T\mathbf{A}_{t-1}^{-1} & \text{-}\mathbf{A}_{t-1}^{-1}\mathbf{B}_{t-1}\mathbf{S}_t^{-1} \\ \text{-}\mathbf{S}_t^{-1}\mathbf{B}_{t-1}^T\mathbf{A}_{t-1}^{-1} & \mathbf{S}_t^{-1} \end{bmatrix} \tag{24}$$

where

$$\mathbf{S}_t=\bar{\mathbf{A}}(t)-\mathbf{B}_{t-1}^T\mathbf{A}_{t-1}^{-1}\mathbf{B}_{t-1} \tag{25}$$

Noting the formulation of $\mathbf{A}_t^{-1}$ and the definition of $\mathbf{B}_t$, $\mathbf{S}_t$ can be calculated in an iterative form:

$$\mathbf{S}_t=\bar{\mathbf{A}}(t)-\lambda^2\mathbf{S}_{t-1}^{-1} \tag{26}$$

Denote

$$\boldsymbol{\Gamma}_t=\begin{bmatrix} \boldsymbol{\varphi}_t(1) \\ \vdots \\ \boldsymbol{\varphi}_t(t) \end{bmatrix}_{tmn\times 1}=\mathbf{A}_t^{-1}\mathbf{M}_t \tag{27}$$

According the definition of $\boldsymbol{\Gamma}$ in eq. (21), it is obvious that $\boldsymbol{\Gamma}_N=\boldsymbol{\Gamma}$. Using eq. (24), we can obtain:

$$\begin{aligned} \boldsymbol{\varphi}_t(t) &= -\mathbf{S}_t^{-1}\mathbf{B}_{t-1}^T\mathbf{A}_{t-1}^{-1}\mathbf{M}_{t-1}+\mathbf{S}_t^{-1}\boldsymbol{\mu}(t) \\ &= -\mathbf{S}_t^{-1}\mathbf{B}_{t-1}^T\boldsymbol{\Gamma}_{t-1}+\mathbf{S}_t^{-1}\boldsymbol{\mu}(t) \\ &= \lambda\mathbf{S}_t^{-1}\boldsymbol{\varphi}_{t-1}(t-1)+\mathbf{S}_t^{-1}\boldsymbol{\mu}(t) \end{aligned} \tag{28}$$

and

$$\begin{aligned} \begin{bmatrix} \boldsymbol{\varphi}_t(1) \\ \vdots \\ \boldsymbol{\varphi}_t(t-1) \end{bmatrix} &= \boldsymbol{\Gamma}_{t-1}-\mathbf{A}_{t-1}^{-1}\mathbf{B}_{t-1}\boldsymbol{\varphi}_t(t) \\ &= \boldsymbol{\Gamma}_{t-1}-\begin{bmatrix} \lambda\mathbf{A}_{t-2}^{-1}\mathbf{B}_{t-2}\mathbf{S}_{t-1}^{-1} \\ -\lambda\mathbf{S}_{t-1}^{-1} \end{bmatrix}\boldsymbol{\varphi}_t(t) \\ &= \boldsymbol{\Gamma}_{t-1}+\begin{bmatrix} \lambda^{t-1}\mathbf{S}_1^{-1}\mathbf{S}_2^{-1}\cdots\mathbf{S}_{t-1}^{-1} \\ \vdots \\ \lambda^2\mathbf{S}_{t-2}^{-1}\mathbf{S}_{t-1}^{-1} \\ \lambda\mathbf{S}_{t-1}^{-1} \end{bmatrix}\boldsymbol{\varphi}_t(t) \end{aligned} \tag{29}$$

Eq. (29) can be reformulated in an iterated form:

$$\boldsymbol{\varphi}_t(t-d)=\boldsymbol{\varphi}_{t-1}(t-d)+\boldsymbol{\Delta}_t(d) \tag{30}$$

where

$$\boldsymbol{\Delta}_t(1)=\lambda\mathbf{S}_{t-1}^{-1}\boldsymbol{\varphi}_t(t) \tag{31}$$

$$\boldsymbol{\Delta}_t(k)=\lambda\mathbf{S}_{t-k}^{-1}\boldsymbol{\Delta}_t(k-1),\ k=2,\ldots,,t-1 \tag{32}$$

Based on eq. (28) and eq. (30), $\boldsymbol{\Gamma}_t$ can be updated in an iterative manner. Furthermore, the inverse of the large-scale matrix $\mathbf{A}_N$ is avoided and the computational burden is reduced significantly.

4. DATA-DRIVEN MODEL QUALITY ASSESSMENT

4.1 Historical data based benchmark for model quality assessment

The model quality is closely related with control performance. In this article, a historical data based benchmark for model quality assessment is proposed. The benchmark is selected by the user, which is the closed-loop operating data during the period when the control performance is considered to be satisfactory. Consequently, the central ideal of model quality assessment is to evaluate the divergence in the process dynamics during the benchmark period and monitoring period. Combining the benchmark data and monitoring data, the principle for the LTV modeling is reformulated as follows:

$$\min_{\boldsymbol{\varphi}(t),\hat{\boldsymbol{\varphi}}(\hat{t})} J=\sum_{\hat{t}=1}^{\hat{N}} \| \hat{y}(\hat{t}) - \hat{\mathbf{z}}^T(\hat{t})\hat{\boldsymbol{\varphi}}(\hat{t}) \|_2^2 + \lambda \sum_{\hat{t}=1}^{\hat{N}} \| \hat{\boldsymbol{\varphi}}(\hat{t}) - \hat{\boldsymbol{\varphi}}(\hat{t}\text{-}1) \|_2^2$$
$$+\lambda \| \boldsymbol{\varphi}(1) - \hat{\boldsymbol{\varphi}}(\hat{N}) \|_2^2 + \sum_{t=1}^{N} \| y(t) - \mathbf{z}^T(t)\boldsymbol{\varphi}(t) \|_2^2 + \lambda \sum_{t=2}^{N} \| \boldsymbol{\varphi}(t) - \boldsymbol{\varphi}(t\text{-}1) \|_2^2 \tag{33}$$

where $\{\hat{y}(\hat{t}), \hat{\mathbf{z}}(\hat{t})\}$ and $\{y(t), \mathbf{z}(t)\}$ denote the benchmark data and monitoring data, respectively.

The model coefficients $\{\hat{\boldsymbol{\varphi}}(\hat{t})\}$ and $\{\boldsymbol{\varphi}(t)\}$ reveal the process dynamics during the benchmark period and monitoring periods, respectively. Therefore, model quality can be examined by investing the divergence between $\{\hat{\boldsymbol{\varphi}}(\hat{t})\}$ and $\{\boldsymbol{\varphi}(t)\}$. For each channel at the time instant *t*, the process dynamics is approximated as:

$$G_i(s;t) = \boldsymbol{\theta}_i^T(t)\boldsymbol{F}(s) \tag{34}$$

Noticing eq. (8), $\boldsymbol{\theta}_i(t)$ is formulated using the appropriate elements of $\boldsymbol{\varphi}(t)$ that are corresponding to *i*-th channel. The model quality is evaluated in the L_2 norm:

$$\eta_i(t) = \left\|G_i(s;t) - G_i^0(s)\right\|_2^2 / \left\|G_i^0(s)\right\|_2^2 \tag{35}$$

where $G_i^0(s)$ is the nominal model during the benchmark period. Since the LTV model structure is adopted, $G_i^0(s)$ is specified as:

$$G_i(s;t) = \boldsymbol{\theta}_0^T \boldsymbol{F}(s),\ \boldsymbol{\theta}_0 = \sum_{\hat{t}} \hat{\boldsymbol{\theta}}_i^T(\hat{t}) / \hat{N} \tag{36}$$

where $\{\hat{\boldsymbol{\theta}}_i(\hat{t})\}$ is the model coefficients during the benchmark period and $\boldsymbol{\theta}_0$ is the average of $\{\hat{\boldsymbol{\theta}}_i(\hat{t})\}$. Based on the basis model structure, eq. (35) can be reformulates in the quadratic form:

$$\eta_i(t) = \frac{[\boldsymbol{\theta}_i(t) - \boldsymbol{\theta}_0]^T \mathbf{M} [\boldsymbol{\theta}_i(t) - \boldsymbol{\theta}_0]}{\boldsymbol{\theta}_0^T \mathbf{M} \boldsymbol{\theta}_0} \tag{37}$$

where $\mathbf{M}$ is a constant symmetric matrix with each element being

$$\mathbf{M}_{i,j} = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \mathrm{Re}\left[F_i(j\omega)F_j(-j\omega)\right] d\omega \tag{38}$$

The symbol Re in eq. (3) denotes the real part of a complex number. A higher value of $\eta_i(t)$ indicates more significant model mismatch and higher priority of model maintenance.

The proposed model quality assessment method is data-driven, and the plant model is not necessarily known a priori. Even though the nominal plant model can be used to specify the nominal model coefficient $\boldsymbol{\theta}_0$, it still needs to be pointed out that the nominal plant model is not always available in practice. Moreover, the plant model is usually obtained by the technique system identification, and hence the modeling error is inevitable, which may further affect the reliability of model quality assessment. Nevertheless, these practical issues are handled by the proposed data-driven approach.

4.2 Choice of parameters

For the proposed method, there are two undetermined parameters: the regularization parameter λ and the threshold h for determining model mismatch. The basic idea for determination of these parameters is to resort to the benchmark data, which is described below.

The parameter λ manages the balance between the fitting error and model generalization ability. The parameter λ is tuned based on the cross-validation approach using the benchmark data. In this study, the leave-one-out cross validation (LOOCV) method is applied, the central idea of which is to use only one collected sample as the validation set and the remaining samples as the training set (Arlot & Celisse, 2010). Nevertheless, it should be noted that conventional LOOCV methods primarily aim at time-invariant models and thus needs to be modified for the LTV model structure. Let the *q*-th sample be the validation set, and the LTV model is trained according to the following criteria:

$$\min_{\hat{\boldsymbol{\varphi}}(t)} J(q) = \sum_{\hat{t}=1,\hat{t}\neq q}^{\hat{N}} \| \hat{y}(\hat{t}) - \hat{\mathbf{z}}^T(\hat{t})\hat{\boldsymbol{\varphi}}(\hat{t}) \|_2^2 + \lambda \sum_{\hat{t}=1}^{q-1} \| \hat{\boldsymbol{\varphi}}(\hat{t}) - \hat{\boldsymbol{\varphi}}(\hat{t}\text{-}1) \|_2^2$$
$$+\lambda \sum_{\hat{t}=q+2}^{\hat{N}} \| \hat{\boldsymbol{\varphi}}(\hat{t}) - \hat{\boldsymbol{\varphi}}(\hat{t}\text{-}1) \|_2^2 \tag{39}$$

Comparing eq. (39) and eq. (15), the sample at time instant *q* and the corresponding model coefficient vector $\hat{\boldsymbol{\varphi}}(q)$ would not be involved in training the model. The validation error is defined as follows:

$$e(q,\lambda) = \hat{y}(q) - \hat{\mathbf{z}}^T(q) \frac{\hat{\boldsymbol{\varphi}}(q+1) + \hat{\boldsymbol{\varphi}}(q-1)}{2} \tag{40}$$

From eq. (40), the *q*-th prediction is estimated using the interpolation between $\hat{\boldsymbol{\varphi}}(q+1)$ and $\hat{\boldsymbol{\varphi}}(q-1)$. The regularization parameter λ is determined such that sum of the squared validation error is minimized:

$$\min_{\lambda} \sum_{q} \left[e(q,\lambda)\right]^2 \tag{41}$$

Using the benchmark data, the threshold h can be determined based on the 3-sigma principle:

$$h = \bar{\eta}(\hat{t}) + 3\sigma[\eta(\hat{t})] \tag{42}$$

where $\{\eta(\hat{t})\}$ are the model quality indices in the benchmark periods, while $\bar{\eta}$ and σ are the mean and standard deviation of $\{\eta(\hat{t})\}$, respectively.

5. CASE STUDIES

The proposed method is validated through a simulation case study, which is a binary distillation column developed by Wood and Berry (1973):

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{12.8e^{-s}}{16.7s+1} & \dfrac{-18.9e^{-3s}}{21s+1} \\ \dfrac{6.6e^{-7s}}{10.9s+1} & \dfrac{-19.4e^{-3s}}{14.4s+1} \end{bmatrix} \begin{bmatrix} R \\ S \end{bmatrix} + \begin{bmatrix} \dfrac{3.8e^{-8.1s}}{14.9s+1} \\ \dfrac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} F \tag{43}$$

The process involves of two controlled variables, two manipulated variables and one disturbance variable. Descriptions of the variables are listed in Table 1.

Table 1 Description of the variables in the Wood-Berry process

	description	variable type
x_D	distillate composition	CV
x_B	bottoms composition	CV
R	reflux flow rate	MV
S	steam flow rate	MV
F	feed flow rate	DV

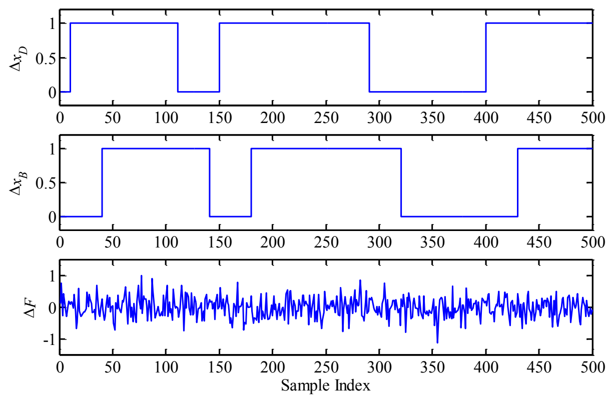

Fig. 1 Set-point changes and the disturbance signal

The channels of R-x_D, R-x_B, S-x_D and S- x_B are denoted as g_{11}, g_{12}, g_{21} and g_{22}, respectively. The disturbance F is set to be unmeasured stochastic disturbance. Furthermore, Gaussian white noise is added to the CV variable. For the purpose of model quality assessment, step changes are introduced to the setpoints of x_D and x_B. The increments in the set-point signal together with the disturbance signal are shown in Fig. 1. The process is controlled by a MPC, and the sampling interval is 0.1 minute.

In the first case, mismatches in the gain are considered. The channel g_{11} has a -50% gain mismatch, while the mismatches in the other channels are $\pm 5\%$. The model matrix is given as follows:

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{6.4e^{-s}}{16.7s+1} & \dfrac{-18.7e^{-3s}}{21s+1} \\ \dfrac{6.5e^{-7s}}{10.9s+1} & \dfrac{-19.3e^{-3s}}{14.4s+1} \end{bmatrix} \begin{bmatrix} R \\ S \end{bmatrix} + \begin{bmatrix} \dfrac{3.8e^{-8.1s}}{14.9s+1} \\ \dfrac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} F \tag{44}$$

To attempt model quality assessment, a total of 1000 samples are collected, and the first half is collected from the nominal period and used as the benchmark. The resulting model quality indices are shown in Fig. 2.

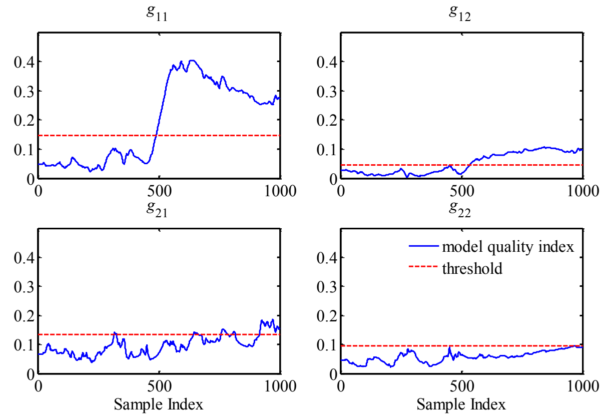

Fig. 2 Model quality assessment in the gain mismatch case

It can be concluded that the channel g_{11} has a more significant degree of model-mismatch and greater impacts on the closed-loop performance. This can be validated by comparing the response data, as shown in Fig. 3. In these two cases, the process outputs of x_D has more significant divergence, while the trajectories of x_B are rather similar. Hence, model re-identification is more necessary to be implemented on the channel g_{11} for controller maintenance purposes.

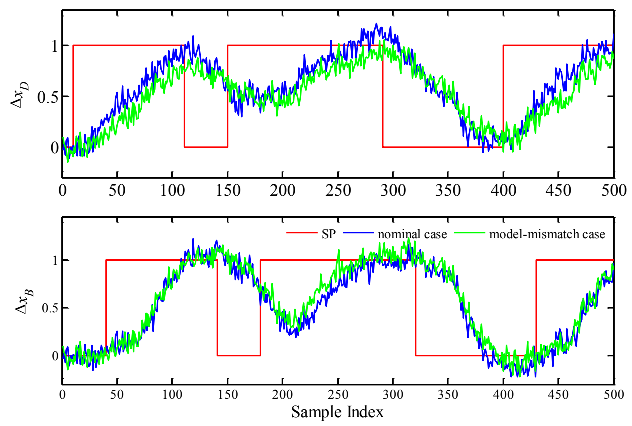

Fig. 3 Closed-loop responses of x_D and x_B in the nominal and gain-mismatch cases

In the second case, model mismatches in the delay and time constant are considered. The process model is formulated in eq. (45). The time constant of g_{21} is increased from 10.9 to 22, and the delay of g_{22} is increased from 3 to 7. For the other channels, there is no model mismatch.

$$\begin{bmatrix} x_D \\ x_B \end{bmatrix} = \begin{bmatrix} \dfrac{12.8e^{-s}}{16.7s+1} & \dfrac{-18.9e^{-3s}}{21s+1} \\ \dfrac{6.6e^{-7s}}{22s+1} & \dfrac{-19.4e^{-7s}}{14.4s+1} \end{bmatrix} \begin{bmatrix} R \\ S \end{bmatrix} + \begin{bmatrix} \dfrac{3.8e^{-8.1s}}{14.9s+1} \\ \dfrac{4.9e^{-3.4s}}{13.2s+1} \end{bmatrix} F \quad (45)$$

The same set-point change as the gain mismatch case is introduced. The model quality indices are displayed in Fig. 4. Model mismatches in channels g_{21} and g_{22} are isolated accurately. Furthermore, it is concluded that the model-mismatch in g_{21} has greater impacts on the closed-loop performance due to larger values of the model quality index, which can be validated by the closed-loop response in Fig. 5. Therefore, the sub model g_{21} has a higher priority to be maintained.

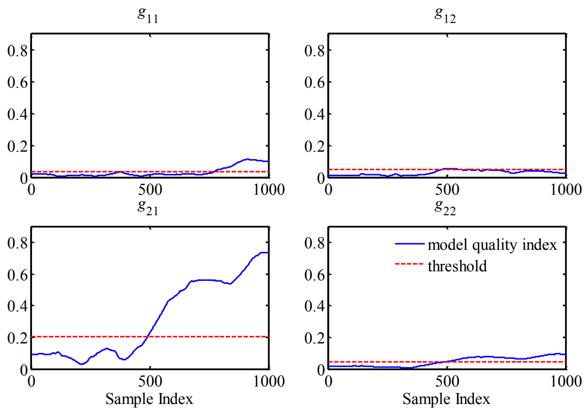

Fig. 4 Model quality assessment in the time constant and delay mismatch case

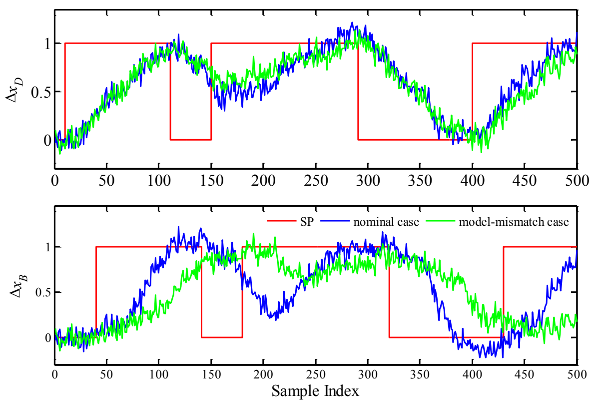

Fig. 5 Closed-loop responses of x_D and x_B in the nominal case and model-mismatch cases

6. CONCLUSIONS

In this article, the temporal smoothness regularization approach is applied to evaluate model quality and detect plant-model mismatch. The process dynamics is approximated by the LTV model structure based on the basis-model approach with temporal smoothness regularization term. The central idea of the smoothness regularization is to penalize overly aggressive model parameter changes such that model generalization ability is guaranteed. The model quality index is defined as the difference in L_2 norm between the nominal model and the current model, which is a practical indicator for detection of plant-model mismatches. Representative cases are studied, and results indicate that the proposed method is able to provide reasonable guides for controller maintenance purposes.

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