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Monitoring of operating point and process dynamics via probabilistic slow feature analysis

Feihong Guo [a], Chao Shang [a], Biao Huang [b], Kangcheng Wang [a], Fan Yang [a,*], Dexian Huang [a]

[a] Tsinghua National Laboratory for Information Science and Technology (TNList) and Department of Automation, Tsinghua University, Beijing 100084, China
[b] Department of Chemical and Materials Engineering, University of Alberta, Edmonton, Alberta T6G 2G6, Canada

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ABSTRACT

Traditional multivariate statistical process monitoring (MSPM) approaches aim at detecting deviations from the routine operating condition. However, if the process remains well controlled by feedback controllers in spite of some deviations, alarms triggered in this context become no longer necessary. In this regard, slow feature analysis (SFA) has been recently applied to MSPM tasks by Shang et al. (2015), which allows for seperate distributions of both nominal operating points and dynamic behaviors. Since a poor control performance is always characterized by dynamics anomalies, one can discriminate nominal operating deviations with acceptable control performance, from real faults that deserve more attentions, according to the temporal dynamics of processes. In this work, we propose a new process monitoring scheme based upon probabilistic SFA (PSFA). Compared to deterministic SFA, its probabilistic extension takes the measurement noise into considerations and allows for missing data imputation conveniently, which is beneficial for process monitoring. Apart from generic T^2 and SPE metrics for monitoring the operating point, a novel S^2 statistics is considered for exclusively monitoring temporal behaviors of processes. Two case studies are provided to show the efficacy of the proposed monitoring approach.

1. Introduction

In recent years, multivariate statistical process monitoring (MSPM) approaches have played an indispensable role in chemical, semiconductor, and food industries, with the intent to furnish useful information about process status, and further assist decision-making of operators on maintainence actions [1,2,3]. The general principle of MSPM is to first characterize the distribution of process data collected in nominal operating conditions, and then raise alarms online once process measurements transgress the routine data distribution. In particular, latent variable modeling techniques, notably principal component analysis (PCA), and partial least squares (PLS), are most-used statistical ones, which account for data colinearity by projecting data into a low-dimensional subspace [4,5,6,7,8].

Most traditional MSPM methods are prone to ideal assumptions for routine process operations. Any deviation from the designed operating condition will be signaled as faulty, no matter where the newly created operating point lies. Under this circumstance, the process tends to shift occasionally to a new operating point due to various impacts, including both active set-point adjustments and passive disturbances; however, thanks to the compensation of control systems, the process may get well controlled as usual. On this occasion, the original routine condition delineated by traditional MSPM approaches will be inevitably violated and alarms get raised hereafter. Nonetheless, such alarms are essentially unnecessary and even detrimental, for the reason that the process still operates acceptably. For process practitioners, it is challenging to identify real faults of direct interest from a myriad of alarms, which entails a considerable labor overhead to deal with.

To this end, a novel process monitoring scheme based on slow feature analysis (SFA) has been put forward recently [9], which tames the aforementioned problem with effect. As an unsupervised model proposed in 2002 [10], SFA basically extracts slowly varying components that underlie multi-dimensional time series data, termed as *slow features*. Thanks to the statistical properties of slow features, SFA is amenable to individual approximations to both the steady distribution $P(\boldsymbol{x})$ and the temporal distribution $P(\dot{\boldsymbol{x}})$, for which conventional statistical models fall short of describing. For process monitoring purposes, deviations from nominal operating point can be detected according to the steady state distribution $P(\boldsymbol{x})$, while process dynamics anomalies can be identified by monitoring the disruptions of the temporal distribution $P(\dot{\boldsymbol{x}})$. The rationale of SFA-based monitoring strategy is to treat process dynamics as an indicator of control performance. It is generally recognized that real faults typically come with poor control performance as well as drastic dynamic behaviors. As a consequence, once deviations from routine operating conditions are detected by traditional MSPM approaches, one can further examine whether the process is under control or not by monitoring process dynamics $P(\dot{\boldsymbol{x}})$, thereby

* Corresponding author.
E-mail address: yangfan@tsinghua.edu.cn (F. Yang).

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removing unnecessary alarms. In this way, alarms on behalf of real faults can be unmasked in a sophisticated manner, yielding interpretable fault information for process practitioners.

Recently, SFA has been generalized to its probabilistic version, i.e., probabilistic SFA (PSFA) [11], which has been applied to dynamic soft sensor modeling [12]. Different from its deterministic counterpart, PSFA takes the form of linear Gaussian state-space models, in which slow features are assumed as hidden states evolving as independent first-order auto-regressive (AR1) processes *a priori*. Most importantly, for monitoring system design, PSFA is potentially advantageous to deterministic SFA due to the following reasons. First, deterministic SFA provides no allowance for measurement noises. It straightforwardly computes the time difference $\dot{\boldsymbol{x}}$ of sequential measurements, which will significantly amplify the noise effect with the presence of measurement noises, resulting in an irrational estimation of slow features. In contrast, measurement noises are taken into considerations by PSFA in a fully probabilistic framework, which can be well mitigated by applying the well-known Kalman filter to the inference of slow features [12]. Second, missing data are fairly frequent in process measurements [13], which will add significant difficulties in monitoring statistics design [14]. For PSFA, it is convenient to impute missing data by means of Kalman filter, which is beyond the capability of deterministic SFA.

In this regard, we develop a systematic monitoring scheme based on PSFA, which enables a concurrent monitoring of both operating point and process dynamics. Based on existing results with regard to PSFA, in this article, we suggest using the Akaike information criterion (AIC) to select the number of slow features in PSFA. In addition, the missing data issue of PSFA is approached by investigating into properties of Kalman filter equations. Although linear Gaussian state-space models have already been used for process monitoring [15], the temporal dynamics of hidden states is not fully exploited in designing monitoring statistics. The independence between probabilistic slow features allows the definition of S^2 statistics based on temporal derivatives to be clearly made, as well as the corresponding control limits to be readily obtained. The novel S^2 statistics abstracts dynamic behaviors of the process, in addition to the T^2 and SPE statistics that are responsible for describing operating points. In the face of operating point deviations detected by T^2 and SPE statistics, the S^2 control chart equips operators with interpretable information about dynamic behaviors of the process, which is especially beneficial for reducing unnecessary alarms in industrial practice.

The layout of this article is given as follows. The methodological details of SFA and the related monitoring scheme proposed in [9] are briefly introduced in Section 2. The mathematical formulation of PSFA is given in Section 3, and a model selection strategy is also suggested. In Section 4, the online estimation issue of slow features, especially in the case of missing data, is discussed, and the PSFA-based monitoring policy is further presented. Sections 5 and 6 contain case studies to demonstrate the efficacy of the proposed method, followed by conclusions in the final section.

2. Slow feature analysis and the corresponding monitoring scheme

2.1. Slow feature analysis model

Assume that there are m input variables in total, amounting to an m-dimensional input vector $\boldsymbol{x}\in\mathbb{R}^m$. Mathematically, SFA decomposes the original input $\boldsymbol{x}$ into a linear combination of slow features $\boldsymbol{s}$:

$$\mathbf{x} = \mathbf{Rs}. \tag{1}$$

Statistical properties of slow features can be represented as $\mathbb{E}\{s_j\} = \mathbb{E}\{\dot{s}_j\} = 0, \mathbb{E}\{s_i s_j\} = \delta_{ij}, \quad \mathbb{E}\{\dot{s}_j^2\} = \omega_j \quad (1 \le j \le m)$, where δ_{ij} stands for the Kronecker delta function [9,10]. It can be seen that SFA not only describes the steady state distribution $P(\boldsymbol{x})$ but also delineates the temporal distribution $P(\dot{\boldsymbol{x}})$ explicitly. This is just what generic statistical models like PCA and independent component analysis (ICA) fail to achieve.

In order to derive an SFA model from time series data $\mathbf{x}(t)$, one could resort to the SFA algorithm [10], which consists of two consecutive steps of singular value decomposition (SVD). The input data $\mathbf{x}$ are assumed to have zero mean in each dimension. By performing SVD decomposition first on the covariance matrix of original input as $\mathbb{E}\{\mathbf{x}\mathbf{x}^{\mathrm{T}}\} = \mathbf{U}\boldsymbol{\Lambda}\mathbf{U}^{\mathrm{T}}$, the original input $\mathbf{x}$ can be sphered as $\mathbf{z} = \boldsymbol{\Lambda}^{-\frac{1}{2}}\mathbf{U}^{\mathrm{T}}\mathbf{x}$ such that $\mathbb{E}\{\mathbf{z}\mathbf{z}^{\mathrm{T}}\} = \mathbf{I}_m$. Next, a second SVD on the covariance of $\dot{\mathbf{z}}$ yields $\mathbb{E}\{\dot{\mathbf{z}}\dot{\mathbf{z}}^{\mathrm{T}}\} = \mathbf{P}\boldsymbol{\Omega}\mathbf{P}^{\mathrm{T}}$, where $\boldsymbol{\Omega} = \mathrm{diag}\{\omega_1, \cdots, \omega_m\}$ with diagonal elements arranged in an ascending order. Finally, matrix $\mathbf{R}$ is calculated as

$$\mathbf{R} = \mathbf{U}\boldsymbol{\Lambda}^{\frac{1}{2}}\mathbf{P} \in \mathbb{R}^{\mathrm{m}\times\mathrm{m}}. \tag{2}$$

Slow features $\mathbf{s}$ can thus be computed as $\mathbf{s} = \mathbf{P}^{\mathrm{T}}\mathbf{z} = \mathbf{P}^{\mathrm{T}}\boldsymbol{\Lambda}^{-\frac{1}{2}}\mathbf{U}^{\mathrm{T}}\mathbf{x} = \mathbf{R}^{-1}\mathbf{x}$. Therefore, the statistical properties of $\mathbf{s}$ can be easily calculated as

$$\begin{aligned} \mathbb{E}\{\mathbf{s}\mathbf{s}^{\mathrm{T}}\} &= \mathbf{P}^{\mathrm{T}}\mathbb{E}\{\mathbf{z}\mathbf{z}^{\mathrm{T}}\}\mathbf{P} = \mathbf{I}, \\ \mathbb{E}\{\dot{\mathbf{s}}\dot{\mathbf{s}}^{\mathrm{T}}\} &= \mathbf{P}^{\mathrm{T}}\mathbb{E}\{\dot{\mathbf{z}}\dot{\mathbf{z}}^{\mathrm{T}}\}\mathbf{P} = \boldsymbol{\Omega}. \end{aligned} \tag{3}$$

In a nutshell, SFA simultaneously diagonalizes the covariance matrices of both $\mathbf{s}$ and $\dot{\mathbf{s}}$, as implied by (3). In particular, each SF s_j is characterized by its *slowness* that $\mathbb{E}\{\dot{s}_j^2\} = \omega_j \quad (1 \le j \le m)$. A small ω_j indicates a slowly varying SF, and vice versa. According to different slowness of SFs, s can be futher partitioned into two groups:

$$\begin{aligned} \mathbf{s} &= \begin{bmatrix} \mathbf{s}_{\mathrm{d}} \\ \mathbf{s}_{\mathrm{e}} \end{bmatrix}, \\ \mathbf{s}_d &= \mathbf{P}_{1:\mathrm{M}}^{\mathrm{T}}\boldsymbol{\Lambda}^{-\frac{1}{2}}\mathbf{U}^{\mathrm{T}}\mathbf{x}, \\ \mathbf{s}_e &= \mathbf{P}_{(M+1):m}^{\mathrm{T}}\boldsymbol{\Lambda}^{-\frac{1}{2}}\mathbf{U}^{\mathrm{T}}\mathbf{x}, \end{aligned} \tag{4}$$

where $\mathbf{P}_{1:M}$ denotes the first M columns of $\mathbf{P}$, and $\mathbf{P}_{(M+1):m}$ denotes the remaining ones. Accordingly, $\mathbf{s}_d$ encapsulates M slowest features on behalf of dominant variations of time series data, and $\mathbf{s}_e$ represents residuals with fast variations (notice that $\omega_1 < \omega_2 < \cdots < \omega_m$). For determining M reasonably, Ref. [9] suggests an objective criterion based on the slowness of input reconstructions.

2.2. Monitoring statistics design based on slow features

The Hotelling's T^2 statistics is firstly applied to both $\mathbf{s}_d$ and $\mathbf{s}_e$ to measure the steady variations of slow features. A pair of statistics are defined on the basis of $\mathbf{s}_d$ and $\mathbf{s}_e$ as [9]

$$\begin{aligned} T^2 &= \mathbf{s}_d^{\mathrm{T}}\mathbf{s}_d \sim \chi_M^2, \\ T_e^2 &= \mathbf{s}_e^{\mathrm{T}}\mathbf{s}_e \sim \chi_{m-M}^2, \end{aligned} \tag{5}$$

where the property $\mathbb{E}\{\mathbf{s}\mathbf{s}^{\mathrm{T}}\} = \boldsymbol{I}$ is utilized. Besides, because the statistical property of temporal variations is also described by $\mathbb{E}\{\dot{\mathbf{s}}\dot{\mathbf{s}}^{\mathrm{T}}\} = \Omega$, another pair of statistics can be defined based on the temporal difference $\dot{\mathbf{s}}$ as: [9].

$$\begin{aligned} S^2 &= \dot{\mathbf{s}}_d^{\mathrm{T}}\boldsymbol{\Omega}_d^{-1}\dot{\mathbf{s}}_d \sim \frac{M\left(N^2-2N\right)}{(N-1)(N-M-1)} F_{M,N-M-1}, \\ S_e^2 &= \dot{\mathbf{s}}_e^{\mathrm{T}}\boldsymbol{\Omega}_e^{-1}\dot{\mathbf{s}}_e \sim \frac{(m-M)\left(N^2-2N\right)}{(N-1)(N-m+M-1)} F_{m-M,N-m+M-1}, \end{aligned} \tag{6}$$

where N denotes the number of available process samples, $\boldsymbol{\Omega}_d = \mathrm{diag}\{\omega_1, \cdots, \omega_M\}$ and $\boldsymbol{\Omega}_e = \mathrm{diag}\{\omega_{M+1}, \cdots, \omega_m\}$.

Thanks to the statistical properties of slow features, both groups of statistics have clear physical interpretations themselves. The T^2 and T_e^2 statistics abstract the steady position of operating conditions $P(\dot{\mathbf{x}})$, whereas S^2 or S_e^2 charts characterize temporal behaviors of process data $P(\dot{\mathbf{x}})$. In practice, once either T^2 or T_e^2 exceeds the threshold