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Detecting Process Faults using Singular Spectrum Decomposition

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Abstract: Process faults often lead to process/equipment failure or an emergency abnormal situation and are of greater concern in process industries. Multivariate statistical process monitoring methods using Singular Spectrum Analysis (SSA) have proved to be an effective tool for chemical process monitoring among other multivariate multiscale methods and are extensively studied and widely used for fault detection. In this study, Singular Spectrum Decomposition, a data-adaptive nonparametric method originated from SSA is used for the decomposition of signals into multilevel components which take care of autocorrelation within the process variables. In SSD, unlike SSA, the determination of crucial parameters like the embedding window dimension for building the trajectory matrix and the number of principal components for grouping and reconstructing time series is automated through consideration of the data's frequency content. The proposed approach is applied to detect faults in simulated and industrial data. The evaluation of results showed that the proposed method effectively detects faults in lower scales/levels as compared with the conventional SSA-based method.

Keywords: Singular Spectrum Analysis, Singular Spectrum Decomposition, Principal Component Analysis, Multivariate Statistical Process Monitoring, Fault Detection.

1. INTRODUCTION

The growing complexity of contemporary chemical processes, coupled with the ongoing need for continuous maintenance to optimize operations and address abnormal events, poses a significant challenge for process engineers. Data-driven process monitoring methods play a crucial role in the early detection of process faults, aiming to prevent abnormal conditions from developing and enabling effective corrections at an early stage. Detecting process faults, which have the potential to result in significant process failures, is especially challenging due to their unpredictable and unobservable nature, along with deviations in process variables. To tackle this challenge, multivariate statistical methods, including principal component analysis (PCA) and its various extensions, are employed to detect process faults. Nevertheless, these approaches encounter constraints when confronted with highly nonlinear, auto-correlated, and multiscale data containing embedded background noise. Consequently, there is a necessity to extract genuine fault dynamic features from operational data tainted by noise before initiating statistical analysis for process monitoring (Bakshi,1998; Chiang et al.,2001; Chen et al.,2016). In this study, Singular Spectrum Decomposition (SSD) is utilized to decompose the process signals into multiple levels, proficiently eliminating background noise to improve the precision of process monitoring and fault detection. The study introduces a comprehensive process monitoring framework that merges the multiscale and noise-reduction benefits of SSD with Principal Component Analysis (PCA).

In recent years, singular spectrum analysis (SSA) has emerged as a data-adaptive, nonparametric spectral method for monitoring and detecting faults in chemical processes characterized by nonlinearity and nonstationarity (Aldrich et al., 2007; Krishnannair et al., 2016). The lagged trajectory matrix in SSA involves windowing the process data, and its physical meaningfulness depends on the proper choice of the embedding dimension. Additionally, selecting principal components for grouping and reconstruction of the data requires careful consideration to avoid mode mixing. Despite existing strategies, there is no standardized automated approach for these processes, leading SSA to be primarily used for the reconstruction of specific signal components rather than the meaningful decomposition of process signals. However, SSA has its limitations, including the critical selection of the window length and the need for careful principal component selection to prevent a single component from containing oscillations or patterns associated with different behaviours. Alternatively, similar scales may be distributed across multiple components, a phenomenon known as mode mixing. To address the limitations inherent in Singular Spectrum Analysis (SSA), this study introduces Singular Spectrum Decomposition (SSD), an iterative method for decomposing time series signals in processes.

Singular Spectrum Decomposition (SSD), an innovative iterative time series decomposition method based on SSA, is designed for process fault detection. Unlike SSA, SSD adopts a fully data-driven approach in determining the embedding dimension and selecting principal components for reconstructing specific component series, making it an adaptive decomposition method. SSD operates by extracting energy associated with various intrinsic time scales, circumventing mode mixing, and ensuring precise separation between intermittent components at transition points. In this paper, the limitations of Singular Spectrum Analysis (SSA) in analyzing process signals, particularly in the context of nonstationary data are addressed. Emphasizing the extraction of energy linked to diverse intrinsic time scales, SSD effectively addresses challenges such as mode mixing and ensures accurate separation between intermittent components. Currently, Singular Spectrum Decomposition (SSD) has found successful applications in signal processing. For instance, Bonizzi et al. (2014) have employed SSD in the processing of tidal and tsunami data. Maryam et al. (2018) have suggested the utilization of the SSD technique for screening and extracting gene expression spectra. Additionally, Yan et al.(2017) have integrated SSD with morphological demodulation methods to extract faults in rolling bearings.

In pursuit of these objectives, this study adopts the trajectory matrix definition for SSD proposed by Bonizzi et al. (2014). This definition plays a crucial role in guaranteeing a consistent reduction in residual energy at each iteration. The process monitoring technique that has been proposed using SSD is combined with PCA to de-correlate the cross-correlation among the process variables. SSD is used to capture the autocorrelation within each variable. In this study, PCA is used for feature extraction of pre-processed signals with SSD. The effectiveness of SSD in fault detection is assessed through the evaluation of simulated numerical data, and a comparative analysis is conducted with the application of SSD in the context of the Base Metal Flotation process, contrasting it with the performance of SSA. The primary goal of this study is to introduce and validate a method that enhances the detection of faults in chemical process systems.

The paper's organization is outlined as follows: Section 2 provides a concise review of SSD, followed by the subsequent section which delves into the process fault detection methodology utilizing SSD. Finally, conclusions are given in the last section.

2. SINGULAR SPECTRUM DECOMPOSITION

SSD, a novel signal decomposition technique derived from SSA, introduces creative improvements. Singular Spectrum Analysis (SSA) dissects the process signals into various additive components like trends or noise through the singular value decomposition (SVD) of a lagged covariance matrix derived from the original process signal. The subsequent reconstruction of the series involves utilizing subsets of eigenvectors and corresponding principal components of the variables through diagonal averaging. The Singular Spectrum Analysis (SSA) algorithm consists of four crucial steps: embedding, singular value decomposition, grouping, and diagonal averaging. These steps have been comprehensively outlined in previous studies, and their methodologies, as reported in works such as Krishnannair et al. (2016), Krishnannair (2017), Golyandina et al. (2001), Vautard et al. (1992), and Aldrich et al. (2007), have been adopted for the purposes of this study. While SSA has demonstrated effectiveness in analyzing and predicting non-stationary time series in previous studies, challenges arise in automatically determining the embedding dimension and selecting principal components with physical meanings for signal reconstruction. In contrast, SSD addresses these challenges by adaptively choosing the fundamental parameters of SSA by focusing on extracting narrow frequency band contents of the signal (Pang et al.,2018). SSD is tailored to break down a signal into its individual components, whereas SSA delves into uncovering the distinct patterns present within the signal. The decomposed singular spectrum components are iteratively derived, and the specific implementation steps for each iteration are as follows:

A. Construction of trajectory matrix

For an input signal $x(n)$ with length of N, setting the embedding dimension to M results in the construction of $M \times N$ matrix $\boldsymbol{X}$. The ith row of this matrix is $x_i = [x(i), \dots, x(N), x(1), \dots, x(i-1)]$. Therefore $\boldsymbol{X}$ can be expressed as $\boldsymbol{X} = [\boldsymbol{x}_1^T, \boldsymbol{x}_2^T, \dots, \boldsymbol{x}_M^T]^T$. For a given series $x(n) = [x_1, x_2, \dots, x_{N-1}, x_N]$, if M is the embedding dimension, the resulting trajectory matrix $\boldsymbol{X}_{SSD}$ would be:

$$\boldsymbol{X}_{\text{SSD}} = (\boldsymbol{X}|\boldsymbol{A}) \qquad (1)$$

Where $\boldsymbol{X}$ is the trajectory of $x(n)$ based on the basic SSA algorithm and the matrix $\boldsymbol{A}$ is

$$\boldsymbol{A} = \begin{bmatrix} x_{k+1} & \cdots & x_N \\ \vdots & \ddots & \vdots \\ x_1 & \cdots & x_{M-1} \end{bmatrix} \qquad (2)$$

In contrast to the fundamental SSA approach, the SSD method enhances the trajectory matrix by introducing an extra block denoted as $\boldsymbol{A}$. This inclusion facilitates the integration of various permutations of the entire time series vector within each row of the adjusted trajectory matrix, referred to as $\boldsymbol{X}_{\text{SSD}}$. Additional insights on this methodology can be explored in references (Bonizzi et al., 2014 , Pang et al., 2018).

The selection of the embedding dimension M significantly influence the analysis results. For SSD, M is adaptively chosen as f_{max}/f_s, f_{max} is the dominant frequency in the power spectral density (PSD) of $x(n)$, and f_s represents the sampling frequency.

B. Decomposition

Singular value decomposition is executed on the trajectory matrix $\boldsymbol{X}_{SSD}$, defined as

$$\boldsymbol{X}_{SSD} = \sum_{i=1}^{M} \lambda_i \, u_i v_i^T \qquad (3)$$

where $\boldsymbol{u}_i$ and $\boldsymbol{v}_i$ are the left and right singular vectors and λ_i's are singular values.

C. Grouping and Reconstruction

As expressed in (3), the trajectory matrix $\boldsymbol{X}_{SSD}$ can be represented as the sum of M principal components. The $L(L < M)$ principal components, whose left eigenvectors exhibit a dominant frequency in the range of $[f_{max} - \Delta f$, $f_{max} + \Delta f]$ are selected to reconstruct a desired singular spectrum component. Δf is estimated through Gaussian interpolation of the power spectral density (PSD) of the input signal. Assuming that the selected L principal components contribute to a new matrix $\widetilde{\boldsymbol{X}}$, the corresponding estimated component is obtained by conducting diagonal averaging on the sum of L matrices, each obtained by taking the outer product of the corresponding eigenvectors. That is $\widetilde{\boldsymbol{X}_{SSD}} = \sum_{k=1}^{L} \widetilde{\boldsymbol{u}_{\iota_k}} \widetilde{\boldsymbol{u}_{\iota_k}^T} \boldsymbol{X}_{SSD}$, where $\widetilde{u_\iota}$s are the corresponding eigenvectors. The transition to a one-dimensional series can be obtained by averaging each ij -th the element of $\widetilde{\boldsymbol{X}}$ over all i and j. This can be achieved as follows:

$$i + j = \begin{cases} k + 1 \; and \; k + 1 + N, & when \; i + J < N \\ k + 1 & when \; i + j \geq N \end{cases} \tag{4}$$

The estimated singular spectrum component is then subtracted from $x(n)$. This process is iteratively performed on the residual until a stopping criterion is met. The decomposition process is stopped when the normalized mean square error between the residual and the original signal is less than 1%. For further details on SSD, refer to Bonizzi et al.,(2014) and Pang et al.,(2018).

3. PROCESS MONITORING METHODOLOGY

The suggested approach for process monitoring utilizing Singular Spectrum Decomposition (SSD) involves breaking down each process variable into various singular spectrum components. A Principal Component Analysis (PCA) model is established for each component derived from SSD to identify faults. Initially, SSD is employed on each variable to generate multiple singular spectrum components at various resolutions/scales. Subsequently, for each scale, the respective SSD components of all variables are amalgamated into a unified matrix, enabling the application of PCA for fault detection. The process monitoring methodology based on Singular Spectrum Analysis (SSA) adheres to analogous procedural steps as the SSD-based method. More clearly, the SSD based monitoring methodology consists of decomposing each variable into multiple levels of components by using SSD which is followed by the development of a PCA model using the reconstructed variables at each level. In SSA based monitoring methodology, the variables are decomposed into multiple components using SSA followed by the development of a PCA model of SSA components at each scale.

The suitable count of principal components to be retained is determined for each component within every scale, and control limits for monitored indices such as Hottelling's T^2 and Q statistics are computed. These limits are established using parameters derived from the dataset collected during normal operating conditions, following the methodology outlined by Kresta et al., (1991). If, at a specific scale T^2 or Q for the reconstructed new dataset is outside the calculated control limits, the process is judged to be out of control. The reliability percentage is calculated by considering the number of samples that exceed the control limit in the new dataset.

4. RESULTS AND DISCUSSION

In this section, the validation of the proposed methodology is conducted by applying Singular Spectrum Decomposition (SSD) and Singular Spectrum Analysis (SSA) to datasets that represent both a nonlinear dynamic process and a base metal flotation plant.

4.1 Case Study 1: Nonlinear Dynamic Process

A five-variable nonlinear dynamic process proposed by Chen and Liao (2002) is used to investigate the efficiency of the proposed monitoring method. The model is represented by

$$\mathbf{x}(t) = \boldsymbol{\mathcal{A}}\mathbf{x}(t-1) + \boldsymbol{\mathcal{B}}\mathbf{u}^2(t-1) \tag{5}$$

$$\mathbf{u}(t) = \boldsymbol{\mathcal{C}}\mathbf{u}(t-1) + \boldsymbol{\mathcal{D}}\mathbf{w}(t-1) \tag{6}$$

$$\mathbf{y}(t) = \mathbf{x}(t) + \mathbf{v}(t) \tag{7}$$

where the coefficient matrices are given by

$$\boldsymbol{\mathcal{A}} = \begin{bmatrix} 0.118 & -0.191 & 0 \\ 0.847 & 0.264 & 0.9 \\ 0.214 & -0.11 & 0 \end{bmatrix} \qquad \boldsymbol{\mathcal{B}} = \begin{bmatrix} 0.05 & 0.1 \\ 0.05 & 0.05 \\ 0 & 0.05 \end{bmatrix}$$

$$\boldsymbol{\mathcal{C}} = \begin{bmatrix} 0.811 & -0.226 \\ 0.477 & 0.415 \end{bmatrix} \qquad \boldsymbol{\mathcal{D}} = \begin{bmatrix} 0.193 & 0.689 \\ -0.320 & -0.749 \end{bmatrix}$$

$\mathbf{u}(t)$, $\boldsymbol{y}(t)$and $\mathbf{x}(t)$ are input, output and state variables at time t, $\mathbf{v}(t)$ and $\mathbf{w}(t)$ are uncorrelated zero mean Gaussian noise, with variance of 0.5 and 5 respectively. The inputs $\mathbf{u}(t)$ and outputs $\mathbf{y}(t)$ are measured and used to monitor the system. The first 500 samples generated by the above equations are taken as normal data. A fault condition (Case 1) is generated by changing the 1×2 element of $\boldsymbol{\mathcal{B}}$ to -0.1. Fig. 1 displays the data pertaining to abnormal conditions. Specifically, the initial 160 samples correspond to the normal condition, while the subsequent 340 samples capture the manifestation of abnormalities in the data.

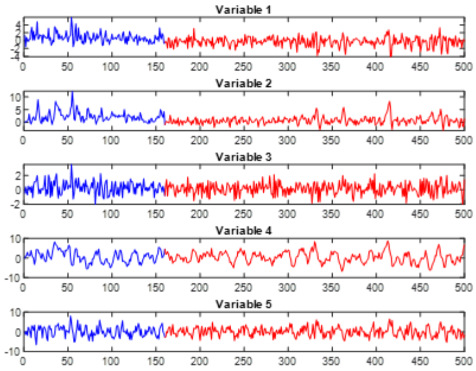

Fig. 1.Data for abnormal operating conditions(first 160 samples represent the normal operation and last 340 samples represent the abnormality in the data).

For the SSA decomposition, an embedding window of size M=6 was chosen by identifying the maximum value of the decorrelation point. This point is where the autocorrelation function of each variable first passes through zero. The SSD method decomposes each variable into multiple components, and the minimum number of components obtained through SSD decomposition for each variable was selected for grouping and signal reconstruction. Consequently, seven singular spectrum components were utilized for reconstructing the signal into multiple levels in the SSD approach. The PCA model was then employed to monitor the SSA and SSD components at various scales. The PCA model retained principal components that accounted for a minimum of 90% of the variance in the data.

Table 1 presents the estimated reliability of Hotelling's T^2 and Q statist for both SSD and SSA in normal and fault cases. In Case 0, the reliability percentage was calculated using the instances where the number of samples exceeded the control limits in the first 160 samples from the abnormal data. Conversely, for Case 1, the reliability percentage was determined based on the last 340 samples from the abnormal data that exceeded the control limits. It is noteworthy that the control limits for both statistics were established at a 95% confidence level. In the specified fault condition, the reliability percentage of the SSD approach surpassed that achieved with the SSA approach. Nevertheless, it is noteworthy that the performance of SSA was also impacted by its limited applicability in nonlinear processes. The outcomes demonstrate the superiority of the proposed method over the SSA approach in this particular case study.

Table 1. Reliability of SSA and SSD in nonlinear dynamic process.

Method	Statistic	Case 0	Case 1
SSA	T^2	10%	14%
	Q	8%	16%
SSD	T^2	9%	75%
	Q	6%	67%

4.2 Case Study 2: Base Metal Flotation Process

In this investigation, the study focused on five features, referred to as image variables, extracted from digital images depicting surface froths in the zinc roughers of a complex base metal flotation plant. These image variables include the small number emphasis feature (SNE), second moment (SM), average grey level of the image (AGL), entropy (ENT), and froth instability (INSTAB).

The concentrator plant comprised several integrated unit operations, including a semi-autogenous (SAG) mill, a ball mill, a hydrocyclone for classifying pulp from the ball mill, a flotation feed buffer tank, and flotation rougher banks. The textural features of the flotation froths were assessed using the neighboring grey level dependence matrix method as outlined by Bezuidenhout et al. (1997).

The reference models for SSA and SSD were constructed using a dataset comprising 284 samples obtained during normal operating conditions (referred to as Case 0). Model evaluation was conducted using a separate set of 299 samples collected under faulty conditions (referred to as Case 1). The variables representing normal and abnormal conditions are depicted in Fig.2.

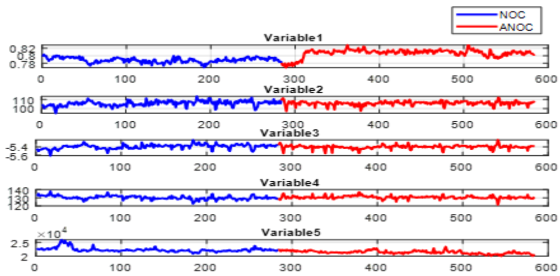

Fig. 2. Variables from normal (NOC) and abnormal operating conditions (ANOC) in the base metal flotation plant.

The fundamental SSA-based process monitoring scheme was implemented with a sliding window of size M=43, determined based on the sample autocorrelation functions of the variables. In the SSD approach, the signal was decomposed into three singular spectrum components, as the minimum number of decompositions achieved through each variable was three in this case study. Hence, three singular spectrum components were employed for the reconstruction of signals in the application of the PCA model for fault detection. The reliability percentage of Hotelling's T^2 and Q statistics SSA and SSD for in fault case and the normal case are listed in Table 2.

While the basic SSA successfully identified the onset of the fault condition, the reliability percentage of both Hotelling's T^2 and Q statistics reached 100% with the SSD approach. In this study, the performance of SSD proved to be equally effective as that of SSA.

Table 2. Reliability of PCA, SSA, EMD and EMD-SSA in Base Metal Flotation Plant process.

Method	Statistic	Case 0	Case 1
SSA	T^2	6%	100%
	Q	7%	94%
SSD	T^2	3%	100%
	Q	3%	100%

6. CONCLUSIONS

In this study, both SSA and SSD were utilized for fault detection in chemical processes. The research showed that the proposed approach is more effective in detecting faults compared to SSA, leveraging the capabilities of SSD. SSA and SSD are employed to extract multiscale components, and PCA is subsequently applied to each SSA/SSD component for fault detection. Results from simulated and industrial studies revealed an improved performance of SSD in nonlinear process monitoring when compared to SSA. Both SSA and SSD demonstrated similarly superior performance, as observed in the industrial case study.

The presented SSD method provides an adaptive energy-frequency-based decomposition of data into multiple components. Its data-driven and adaptive characteristics, coupled with its effective use of data, position SSD as a valuable alternative for decomposing and analyzing noisy, nonlinear, and nonstationary process signals. Unlike SSA, the SSD method automates the selection of the window length and the principal components of the corresponding trajectory matrix for grouping and reconstructing a specific component at a particular scale, introducing an adaptive dimension. Additionally, the updated definition of the trajectory matrix improves feature identification in the data and leads to a reduction in residual energy after each iteration. Furthermore, this study marks the inaugural application of SSD for chemical process monitoring and fault detection.

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