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Compressive sparse principal component analysis for process supervisory monitoring and fault detection

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ABSTRACT

This paper presents a novel sparse principal component analysis method, which is named the *compressive sparse principal component analysis (CSPCA)*. CSPCA ensures that the effects of principal components (PCs) with small scores (eigenvalues/variances) on monitoring performance are taken into account during deriving the first PCs, and measurements are adaptively compressed and partially reconstructed without prior knowledge of data sparsity. The proposed method employs the strategy of screening, reconstructing, and detecting for process supervisory monitoring. Data-screening algorithm is employed to sift out data with essential characteristics of abnormal situations at the screening stage. Data selected are adaptively compressed, and abnormal features are highlighted by the partial reconstruction algorithm at the reconstructing stage. A new SPCA is developed by introducing $L_{2,1}$-norm to replace the usual norm in the traditional SPCA, and is employed to analyse data reconstructed at the detecting stage. The effectiveness of the compressive sparse principal component analysis is evaluated on the Pitprops data set and the Tennessee-Eastman process with promising results.

1. Introduction

Multivariate statistical process monitoring (MSPM) methods have attracted increasing attentions. Among these methods, principal component analysis (PCA) is one of the most fundamental methods, which can reduce dimensionality, extract characteristics, and derive principal components (PCs) with large scores for guaranteeing minimal information loss. However, PCA in the process monitoring has two main limitations: (i) Each PC is a linear combination of almost all original variables, and the loadings of PCs are typically nonzero. Consequently, it is difficult to interpret the physical meanings of PCs and to identify essential variables, especially in the high-dimensional situation. (ii) Only principal components with large scores are retained, and PCs with small scores are rejected during seeking PCs. As a result, some essential information, which is contained in principal components with small scores, is ignored so as to impact the algorithm performance, which is demonstrated by Jolliffe in 1982.

In the multivariate statistical analysis field, many methods were proposed to address the first limitation of PCA by incorporating special norms into PCA. Jolliffe and Uddn proposed ScoTLASS to maximize the explained variance on orthogonal loadings for obtaining sparse PCs by introducing LASSO constraint into classic PCA [1]. Zou et al. presented a regression-type sparse PCA (SPCA) to obtain sparse PCs using the lasso/elastic net regularization [2]. Compared to ScoTLASS, SPCA is a computationally efficient method, although complicated objective function. However, The PCs obtained by SPCA is sensitive to the selection of the number of PCs. Witten et al. established a connection between ScoTLASS and SPCA, and developed an efficient method to obtain the first PCs of ScoTLASS [3]. Shen and Huang proposed a sparse PCA via regularized SVD (sPCA-rSVD) to extract PCs through solving the low rank matrix approximation problem [4]. The elements in loading vectors with absolute values smaller than a threshold are artificially set to zero by a threshold method, which is potentially misleading in various respects, as pointed out by Cadima and Jolliffe [5]. Xie et al. proposed a shrinking PCA by introducing the regularization penalty into the original objective function of classic PCA [6]. Qi et al. introduced a 'mixed-norm' to replace the norm of the traditional eigenvalue problem, and extracted uncorrelated PCs (orthogonal loadings) by an iterative algorithm [7]. Most of the methods mentioned above pay more attention to the model space and seek the variables with dominant variances in a data set, which is often suitable for biological or social science data. However, it is unsuitable for monitoring complex industrial process because changes affecting measurements (violating the PCA model) are detected in the

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residual space, and a violation of SPE statistic indicates abnormal operating conditions.

The second limitation of PCA relates to selecting the principal components for impacting the detection sensitivity of PCA-based methods in process monitoring fields. The same limitation exists for most of the spare PCA methods because current spare PCA methods follow a rule based upon the score of the component, i.e. retain components with large scores and reject those with small scores. However, Hotelling [8] and Massy [9] said the last (i.e. smallest scores) component can be significant, and Jolliffe is unequivocal in pointing out a misconception that PCs with small scores are useless [10]. Jolliffe further demonstrates that the components with small scores can be as important as those with large scores, and rejected PCs result in the loss of useful information, which can impact the algorithm performance. Therefore, the selection of sparse principal components is still one of the essential problems in the sparse PCA-based process monitoring field.

On the other hand, statistical process monitoring, in essence, is a process during which the essential features of data are discriminated for evaluating the system performance. It is implied that one just needs to analyse the essential features extracted instead of the raw data for the process monitoring. It is noted that most signals may be expressed using a linear combination of sparse vectors in the transform basis, such as in the wavelet basis. Thus, a sparse signal can be compressed to reduce volumes of data, and then reconstruct a signal from a very limited amount of data, which consists of essential characteristics of the original signal. It is known as the compressive sensing (CS), which builds on the works of Donoho [11] and Candès et al. [12]. According to CS theory, a signal having a sparse-representation in one basis may be reconstructed from a limit amount of measurements in the second basis that is inconsistent with the first one. What is more, the probability of reconstruction failure is zero provided that the sampling size is sufficiently large [12]. Candès and Wakin point out that ‘CS measurement protocols essentially translate analog data into an already compressed digital form so that one can at least in principle obtain super-resolved signals from just a few sensors’ [13]. If process variables monitored can be referred to as ‘sensors’, then it is natural that CS theory can be extended to the statistical process monitoring field. To the best of our knowledge, however, there are few studies focusing on how to apply compressive sensing principles to the process monitoring. One of the important problems is how data with essential features of abnormal situations are extracted and reconstructed without prior knowledge of data sparsity in the process monitoring in the noise situations.

To address the above issues, we propose the compressive sparse principal component analysis (CSPCA) method with the following advantages: i) CSPCA takes into account the effects of PCs with small scores. ii) CSPCA establishes a connection between the resolution problem of sparse PCs and the selection problem of PCs, and both problems are solved in the unified framework. iii) CSPCA can adaptively reconstruct abnormal data without prior information of the sparsity. iv) CSPCA is a convex optimization problem. CSPCA is employed to monitor process and detect faults. CSPCA consists of the data-screening algorithm, the adaptive reconstruction algorithm and the sensitive sparse PCA at the corresponding stages, respectively. Data-screening algorithm is applied for selecting abnormal data from just-in-time measurements at the screening stage. The adaptive reconstruction algorithm is proposed to compress and reconstruct data selected at the reconstructing stage. Sensitive sparse PCA is developed by introducing $L_{2,1}$-norm to replace L_2-norm of the classic sparse PCA so that the nonconvex resolution problem of PCs is transformed into the convex resolution problem, and the limitations mentioned above are solved at the same time. Subsequently, sensitive sparse PCA algorithm is applied to analysing data reconstructed and detecting abnormal situations at the detecting stage. As illustration, CSPCA is applied to Pitprops data set and Tennessee-Eastman process (TEP).

The rest of this article is organized as follows: Section 2 simply summarizes the compressive sensing principles and various sparse PCA. Section 3 proposes the details of CSPCA method. CSPCA is applied to Pitprops data set and Tennessee-Eastman process (TEP) in Section 4. Finally, conclusions are presented in the last section.

2. Preliminaries

2.1. Compressive sensing

The sparsity and the incoherence are two fundamental principles in the compressive sensing theory, which can ensure that signals can be reconstructed from far few samplings by compressive sensing methods than by traditional methods [13]. Consider a discrete signal $\mathbf{x} = [x_1, \cdots, x_N] \in \mathbf{R}^N$ is expanded in an orthonormal basis matrix $\Psi_i = \left[\psi_1, \cdots, \psi_N\right] \in \mathbf{R}^{N\times N}$ as follows:

$$\mathbf{x} = \sum_{i}^{N} \alpha_i \psi_i \tag{1}$$

where α_i is weighting coefficient sequence of $\mathbf{x}$, and $\alpha_i = \langle \mathbf{x}, \psi_i \rangle$. Clearly, α_i is an equivalent representation of measurements $\mathbf{x}$. The signal $\mathbf{x}$ is called as K-sparse if only K ($K \ll N$) entries of α are nonzero, i.e. the signal $\mathbf{x}$ is linear combinations of K base vectors from basis Ψ. It implies the essential information of $\mathbf{x}$ exists in the K-dimension data instead of the N-dimension data. Moreover, $\mathbf{x}$ is projected into a low dimensional space for obtaining M non-adaptive, linear observations $\mathbf{y} = \Phi\mathbf{x}$ by observation matrix $\mathbf{\Phi} \in \mathbf{R}^{M\times N}$. If $\mathbf{\Phi}$ satisfies the restricted isometry property (RIP) [13] or the null space property (NSP) [14], the information of $\mathbf{x}$ embedded in $\mathbf{y}$ can be recovered with high probability by the reconstruction algorithm. Current reconstruction algorithms mainly include convex optimization based algorithm [15,16], greedy algorithm [17,18], and combinational algorithm [19,20]. Among these algorithms, sparsity adaptive matching pursuit (SAMP) [20] is an improved greedy algorithm, which is able to reconstruct the original signal without prior knowledge of the sparsity. The adaptive partial reconstruction algorithm is proposed based on SAMP in this paper.

2.2. Sparse PCA

We summarized several popular SPCA as follows:

- ScoTALASS [1]: for K-sparse PCs, the coefficient vector is the solution of the following optimization problem,

$$\begin{array}{l} \max\limits_{\mathbf{u}\in\mathbf{R}^p} \mathbf{u}^T \Sigma \mathbf{u} \\ \text{s.t.} \|\mathbf{u}\|_2 = 1 \end{array}, \|\mathbf{u}\|_1 \le \mathrm{t}, \mathbf{u} \perp \mathbf{u}_j, 1 \le \mathrm{j} \le \mathrm{k}-1 \tag{2}$$

where $\mathbf{u}_j$ is the coefficient vector of the jth sparse PCs and t is the tune factor.

- SPCA [2]: solve the regression-type optimization problem as follows:

$$\begin{array}{l} \min\limits_{\mathbf{A},\mathbf{B}} \left\{ \sum\limits_{i=1}^{n} \|\mathbf{x}_i - \mathbf{A}\mathbf{\Gamma}^T\mathbf{x}_i\|_2^2 + \lambda \sum\limits_{j=1}^{k} \|\beta_j\|_2^2 + \sum\limits_{j=1}^{k} \lambda_{1,j} \|\beta_j\|_1 \right\} \\ \text{s.t.} \quad \mathbf{A}^T\mathbf{A} = \mathbf{I} \end{array} \tag{3}$$

where $\mathbf{A} \in \mathbf{R}^{N\times k}, \mathbf{x}_i, \quad i = 1, \cdots, n$ is sampling data. $\mathbf{\Gamma} = \left(\beta_1, \cdots, \beta_k\right)$ with $\beta_i \in \mathbf{R}^p, \quad i = 1, \cdots, k$, $\mathbf{I}$ is the identity matrix. If $\mathbf{A}^*$ and $\mathbf{B}^*$ are