

Data-driven Key Performance Indicator Fault Detection Approach Based on Sparse Direct Orthogonalization

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Abstract: In recent years, key performance indicator (KPI) detection has attracted much attention in large-scale process plants. Several methods have been developed to solve this issue. However, further studies find that post-processing methods have relatively high false alarm rates (FARs) for quality-unrelated faults. Also, methods combined with preprocessing, like orthogonal signal correction-modified partial least squares (OSC-MPLS), sometimes lack robustness. To deal with this problem, this paper proposes an enhanced pretreatment method, namely sparse direct orthogonalization (SDO), and a novel KPI-related fault detection approach called SDO-MPLS is developed. Compared with OSC-MPLS, the proposed approach has more robust performance and better interpretability, while a numerical case and the Tennessee Eastman process (TEP) are used to demonstrate the effectiveness of the proposed approach.

Keywords: Key performance indicators, Process monitoring, Sparse direct orthogonalization, Modified partial least squares, Fault detection.

1. INTRODUCTION

With the growing scale and complexity of automation applied in chemical plants, the demands for high production quality and safe production environment are increasing rapidly. Data-driven process monitoring and fault diagnosis methods, with less requirements for a priori knowledge, were proposed and developed rapidly based on the great amount of available process history data (Qin, 2012).

Multivariate statistical process monitoring (MSPM) method, one kind of data-driven methods, receives considerably increasing attention in research and application domains currently (Ding, 2013). Principal component analysis (PCA) (Jolliffe, 1986) and partial least squares (PLS) (Höskuldsson, 1988) are two commonly used MSPM techniques and many methods are derived from them. Key performance indicator (KPI) represents key technical factor which is closely relevant to the quality of product (Zhang et al., 2015; Peng et al., 2013). For KPI-related fault detection, the difficulty lies in the fact that it is hard to measure KPIs online.

Therefore, in order to guarantee the safety of production process and stability of product quality, process control approaches usually focus on process variables that can

be measured easily. Process monitoring methods based on PCA can effectively detect and diagnose abnormal data in the process. Nevertheless, Zhou et al. (2010) shows that PCA cannot estimate whether these abnormalities will lead to fluctuations of product quality or other KPIs. Since PCA cannot detect KPI-related faults, PLS algorithm gets more attention in KPI domains. However, when it comes to KPI related detection problems, there are few deficiencies for standard PLS algorithm for the following reasons, as pointed out by Zhou et al. (2010). First, PLS component subspace may contain some elements orthogonal to the KPI space, which have no contribution for prediction. Second, residual subspace may include some components related to the KPI space. Third, the variance of residual subspace may be larger than PLS scores, which makes it inappropriate to use Q statistic. So based on standard PLS, many promising improved methods were proposed for KPI related problems. For example, total projection to latent structures (T-PLS) was proposed by Zhou et al. (2010) to realize a more accurate and detailed decomposition. T-PLS not only contains the redundancy in the scores to explain the predicted quality-related outputs, namely KPIs, but also pays attention to residual part for detecting KPI related faults. A modified partial least squares (M-PLS) was proposed to decrease computation complexity by Yin (2012).

As pointed out by Wang et al. (2015), although coping with KPI-related faults effectively, these approaches fail to reduce the false alarm rates (FARs) for KPI-unrelated

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faults due to the variations in input data which are unrelated to KPIs. Therefore, removing undesired systematic variations from input data in the pretreatment process could be a favorable way to handle this problem. In chemometrics, there are many pretreatment methods aiming at removing the components in input data which are orthogonal to the output, e.g. orthogonal signal correction (OSC) proposed by Wold et al. (1998). Based on these, method combining OSC pretreatment method with M-PLS to improve detection performance was proposed by Wang et al. (2015). In spite of its effectiveness for KPI-unrelated faults, its fault detection rate (FDR) for some certain KPI-related faults is relatively low. Unlike OSC pretreatment, a simpler approach proposed by Andersson which used output signal itself to realize orthogonalization directly, termed as direct orthogonalization (DO) (Andersson, 1999). DO algorithm is built on the basis of PCA. Although DO algorithm has a simple form, it shares drawbacks with PCA, i.e. each principal component is a linear combination of all variables and therefore is difficult to interpret. However, in most cases, data can be accurately described by a few principal components. Thus sparse principal component analysis (SPCA) was proposed by Zou et al. (2006) to achieve variables reduction. SPCA shrinks the loadings to zero to ensure that each component is a combination of only a few of variables.

For these reasons, in this paper, employing SPCA into DO algorithm will improve decomposition performance, Sparse DO (SDO) algorithm will be proposed, and then a corresponding novel fault detection approach called SDO-MPLS will be developed. Compared with PLS and T-PLS, the proposed approach has lower FARs for KPI-unrelated faults. Moreover, SDO-MPLS keeps low FARs for KPI-unrelated faults and gives better detection rate than OSC-MPLS proposed by Wang et al. (2015). Besides, the SDO preprocessing can reduce the number of latent variables for PLS model to decrease computation load.

2. PRELIMINARIES

In this section, a brief introduction to MPLS, DO and SPCA will be given.

2.1 A Modified Partial Least Square

For a normalized input data matrix $X \in \mathcal{R}^{n \times l}$ and its corresponding output data matrix $Y \in \mathcal{R}^{n \times m}$, a PLS decomposition (Höskuldsson, 1988) can be written as

$$\begin{cases} X = \hat{X} + \tilde{X} = TP^T + \tilde{X} \\ Y = \hat{Y} + \tilde{Y} = TQ^T + \tilde{Y} \end{cases} \quad (1)$$

where T denotes the score matrix, P and Q are the loading matrices to X and Y respectively.

As mentioned before, the standard PLS cannot remove some variations unrelated to Y from \hat{X} (Zhou et al., 2010; Yin, 2012). Meanwhile, \tilde{X} also contains some variations unrelated to Y after decomposition. To remove these variations, a simpler approach, M-PLS, is proposed for KPI-related problems by Yin (2012), where \hat{Y} is given by

$$\hat{Y} = TQ^T = XRQ^T = X\Psi \quad (2)$$

with R representing the weight matrix calculated in PLS. The matrix $\Psi = RQ^T$, representing the correlation between X and Y , is called regression coefficient matrix, which can also be used to make a prediction on the online measured sample x_{new} .

$$y_{pre}^T = y^T = x_{new}^T \Psi \quad (3)$$

Perform singular value decomposition (SVD) on $\Psi\Psi^T$, construct projection matrices and then \hat{X} and \tilde{X} can be obtained by projecting X on $\hat{\Gamma}_\Psi\hat{\Gamma}_\Psi^T$ and $\tilde{\Gamma}_\Psi\tilde{\Gamma}_\Psi^T$,

$$\Psi\Psi^T = [\hat{\Gamma}_\Psi \quad \tilde{\Gamma}_\Psi] \begin{bmatrix} \Lambda_\Psi & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\Gamma}_\Psi^T \\ \tilde{\Gamma}_\Psi^T \end{bmatrix} \quad (4)$$

$$\begin{aligned} \hat{X} &= X\hat{\Gamma}_\Psi\hat{\Gamma}_\Psi^T \in S_{\hat{X}} \equiv span\{\Psi\} \\ \tilde{X} &= X\tilde{\Gamma}_\Psi\tilde{\Gamma}_\Psi^T \in S_{\tilde{X}} \equiv span\{\Psi\}^\perp \end{aligned} \quad (5)$$

where \hat{X} is the subspace that is fully related with the prediction of KPI, and \tilde{X} is orthogonal to \hat{X} which makes no contribution to KPI prediction (Yin, 2012). So we have

$$\hat{Y} = X\Psi = (\hat{X} + \tilde{X})\Psi = \hat{X}\Psi \quad (6)$$

According to Yin et al. (2015), the prediction of KPI is unrelated with \tilde{X} and the KPI prediction on the online sample x_{new} has the following form:

$$y_{new,pre}^T = \hat{x}_{new}^T \Psi = x_{new}^T \hat{\Gamma}_\Psi\hat{\Gamma}_\Psi^T \Psi \quad (7)$$

Based on the properties of SVD decomposition, the monitoring on \hat{x}_{new} can be achieved by taking advantage of T^2 statistics on $\hat{\Gamma}_\Psi^T x_{new}$. Similarly, the monitoring on \tilde{x}_{new} can be realized by applying T^2 statistic on $\tilde{\Gamma}_\Psi^T x_{new}$.

Nevertheless, matrices T , P and Q are calculated based on PLS in these approaches. Accordingly, undesired information in X will affect the succedent calculation more or less. And the increase of fault amplitude will exacerbate the influence from undesired variations, which may lead to unsatisfactory fault diagnosis results (Zhou et al., 2010).

2.2 Direct Orthogonalization

DO algorithm is a simple pretreatment method to remove irrelevant variations from X (Andersson, 1999). Instead of using constrained bi-linear model, DO algorithm takes advantage of Y itself to realize the orthogonalization directly. Compared with OSC, DO algorithm replaces constrained resolution algorithm with eigenproblem-based technique, which owns lower computation load and more stable convergence (Andersson, 1999).

Algorithm 1: DO Algorithm (Andersson, 1999)

S1: Orthogonalize X w.r.t. Y , where $\hat{X} = X - Yw^T$, $w = X^T Y (Y^T Y)^{-1}$.

S2: Perform PCA on \hat{X} , $\hat{T}\hat{P}^T = \hat{X}$.

S3: Extract independent variations from X : $\tilde{T} = X\hat{P}$, $X^{DO} = X - \tilde{T}\hat{P}^T$.

S4: $t_{new} = x_{new}^T \hat{P}$.

S5: $x_{new}^{DO} = x_{new} - t_{new} \hat{P}^T$.

It can be seen that DO algorithm is built on the basis of PCA. Its basic idea is to find a direction vector w , satisfying the projection of input matrix X on this vector

is orthogonal to Y , while ensuring that w can extract the maximum variation information of X (Andersson, 1999).

2.3 Sparse Principal Component Analysis

The linear combinations of all variables serve as principal components in PCA, which makes it difficult to interpret. Nevertheless, only a few of principal components are able to describe data precisely in many cases. Thus SPCA is proposed by Zou et al. (2006), which shrinks some loadings to guarantee that each component only consists of a small amount of variables. SPCA method reconstructs PCA into regression problem with a quadratic penalty and attach sparsity by adding lasso penalty.

Algorithm 2: SPCA Algorithm (Zou et al., 2006)

- S1: Let A equals to $V[:, 1 : k]$, which represents the loadings matrix of the first k principal components.
 S2: When $A = [\alpha_1 \ \alpha_2 \ \dots \ \alpha_k]$ is fixed, solve the following regression problem for $j = 1, 2, \dots, k$ $\beta_j = \arg \min_{\beta} (\alpha_j - \beta)^T X^T X (\alpha_j - \beta) + \lambda \|\beta\|_2^2 + \lambda_{1,j} \|\beta\|_1$ where λ is non-negative.
 S3: When $B = [\beta_1 \ \beta_2 \ \dots \ \beta_k]$ is given, compute the SVD decomposition of $X^T X B = U \Sigma V^T$.
 S4: Update $A = UV^T$.
 S5: Repeat Steps 2-4 until convergence.
 S6: $\hat{V}_j = \beta_j / \|\beta_j\|, j = 1, \dots, k$

3. A SPARSE DO-MODIFIED PLS BASED FAULT DETECTION METHOD

Considering the limited interpretability of PCA, SDO algorithm is proposed in this section first to improve the performance in the pretreatment process in the sense of removing irrelevant variations. Then we combine SDO as the pretreatment process with M-PLS to propose a novel KPI-related fault detection method called SDO-MPLS. For SDO, we first write DO into a ridge regression optimization problem and then define a SDO optimization problem by adding l_1 penalty in DO.

3.1 Sparse Direct Orthogonalization

Inspired by SPCA (Zou et al., 2006), DO introduced in last section can be written as a ridge regression optimization problem equivalently, i.e.

$$\begin{aligned} Z &= X - Yw^T = (1 - Y(Y^T Y)^{-1} Y^T) X \\ &= (1 - YY^\dagger) X \end{aligned} \quad (8)$$

$$\begin{aligned} \arg \min_{A, B} \|Z - ZAB^T\|_F^2 + \lambda \|B\|_F^2 \\ \text{s.t. } A^T A = I \end{aligned} \quad (9)$$

where B is $p \times K$ and $\|B\|_F^2 = \sum_{k=1}^K \|B\|_2^2$. Due to the fact that loading vectors in B are orthogonal, let $A_k = [\alpha_1 \ \alpha_2 \ \dots \ \alpha_k]$ and $B_k = [\beta_1 \ \beta_2 \ \dots \ \beta_k]$, the criterion can be written as following:

$$\begin{aligned} \arg \min_{\alpha_k, \beta_k} \|Z - Z\beta_k \alpha_k^T\|_F^2 + \lambda \|\beta_k\|_2^2 \\ \text{s.t. } A_k^T A_k = I \end{aligned} \quad (10)$$

So the ridge regression problem of DO has been defined. For $\alpha_k^T \alpha_k = 1$, there is

$$\begin{aligned} \|Z - Z\beta_k \alpha_k^T\|_F^2 \\ = \text{tr}(Z^T Z) + \text{tr}(Z\beta_k \beta_k^T Z^T) - 2\alpha_k^T Z^T Z \beta_k \\ = \text{tr}(Z^T Z) + \beta_k^T Z^T Z \beta_k - 2\alpha_k^T Z^T Z \beta_k \end{aligned} \quad (11)$$

And the corresponding optimal solution of β_k is

$$\hat{\beta}_k = (Z^T Z + \lambda I)^{-1} Z^T Z \alpha_k \quad (12)$$

when α_k is fixed. Meanwhile, when β_k is fixed,

$$\begin{aligned} \arg \min_{\alpha_k} \|Z - Z\beta_k \alpha_k^T\|_F^2 \\ = \arg \min_{\alpha_k} \text{tr}(Z^T Z + Z\beta_k \alpha_k^T \alpha_k \beta_k^T Z^T - \\ 2\alpha_k^T Z^T Z \beta_k) + \alpha_k^T A_{k-1} \gamma + \delta(\alpha_k^T \alpha_k - 1) \end{aligned} \quad (13)$$

where γ is a vector with a length of $k-1$ and δ is a scalar. Due to the fact that $\alpha_k^T A_{k-1} = 0$ and $\alpha_k^T \alpha_k = 1$, the optimal problem can be changed into $\arg \max_{\alpha_k} (\alpha_k^T U^T U \beta_k)$. Based on Procrustes Rotation proposed by Mardia et al. (1979), then we can compute the SVD of $Z^T Z B$ and get the corresponding optimal solution of A , i.e.

$$(Z^T Z)B = U \Sigma V^T \quad (14)$$

and $\hat{A} = UV^T$. Now similar to SPCA (Zou et al., 2006), we define the sparse decomposition problem of SDO with l_1 penalty as following:

$$\begin{aligned} \{\hat{\alpha}_k, \hat{\beta}_k\} = \arg \min_{\alpha_k, \beta_k} \|(1 - YY^\dagger)X - (1 - YY^\dagger)X\beta_k \alpha_k^T\|_F^2 \\ + \lambda \|\beta_k\|_2^2 + \zeta \|\beta_k\|_1 \end{aligned} \quad (15)$$

Then we can use the coordinate descent method (Bezdek, 1987) to solve the subproblem α_k and β_k alternately until convergence. Therefore, the irrelevant variations in X can be removed by SDO algorithm, i.e.

$$X^{SDO} = X - XBB^T \quad (16)$$

3.2 SDO-MPLS

Similar to OSC (Wold et al., 1998), SDO divides X into two parts, namely X_{sdo} and X_{sdoves} . Then M-PLS is applied to the processed data under SDO filter to realize fault detections. Compared with OSC-MPLS, SDO-MPLS has a more clear interpretation without loss of significant information, which helps to understand the loadings. To realize M-PLS, we need to change input data X in (2) into a matrix after SDO pretreatment X_{sdo} , i.e.

$$\hat{Y} = X_{sdo} \Psi \quad (17)$$

As MPLS introduced in Sec. II, we perform SVD on $\Psi_{sdo} \Psi_{sdo}^T$ and we have

$$\Psi_{sdo} \Psi_{sdo}^T = [\hat{\Gamma}_{sdo} \ \tilde{\Gamma}_{sdo}] \begin{bmatrix} \Lambda_{sdo} & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} \hat{\Gamma}_{sdo}^T \\ \tilde{\Gamma}_{sdo}^T \end{bmatrix} \quad (18)$$

On the basis of projection matrices $\hat{\Gamma}_{sdo}$ and $\tilde{\Gamma}_{sdo}$, X_{sdo} can be decomposed into \hat{X}_{sdo} and \tilde{X}_{sdo} .

$$\begin{aligned} \hat{X}_{sdo} &= X_{sdo} \hat{\Gamma}_{sdo} \hat{\Gamma}_{sdo}^T \\ \tilde{X}_{sdo} &= X_{sdo} \tilde{\Gamma}_{sdo} \tilde{\Gamma}_{sdo}^T \end{aligned} \quad (19)$$

Similar to Zou et al. (2006), the corresponding statistics and thresholds in our case can be determined by

$$\hat{T}_{sdompls}^2 = x_{sdo}^T \hat{\Gamma}_{sdo} \left(\frac{\hat{\Gamma}_{sdo}^T X_{sdo}^T X_{sdo} \hat{\Gamma}_{sdo}}{N-1} \right)^{-1} \hat{\Gamma}_{sdo}^T x_{sdo} \quad (20)$$

$$J_{\hat{T}_{sdompls},th}^2 = \frac{l(N^2-1)}{N(N-l)} F_{\alpha}(l, N-l)$$

$$\tilde{T}_{sdompls}^2 = x_{sdo}^T \tilde{\Gamma}_{sdo} \left(\frac{\tilde{\Gamma}_{sdo}^T X_{sdo}^T X_{sdo} \tilde{\Gamma}_{sdo}}{N-1} \right)^{-1} \tilde{\Gamma}_{sdo}^T x_{sdo}$$

$$J_{\tilde{T}_{sdompls},th}^2 = \frac{(m-l)(N^2-1)}{N(N-m+l)} F_{\alpha}(m-l, N-m+l) \quad (21)$$

$$T_{sdores}^2 = x_{sdores}^T \left(\frac{X_{sdores}^T X_{sdores}}{N-1} \right)^{-1} x_{sdores}$$

$$J_{T_{sdores},th}^2 = \frac{m(N^2-1)}{N(N-m)} F_{\alpha}(m, N-m) \quad (22)$$

Algorithm 3 gives the complete KPI-based SDO-MPLS algorithm. The merits of SDO-MPLS algorithm is that it can remove unexpected irrelevant variations. Furthermore, compared with OSC-MPLS, SDO-MPLS filter data by a few principal components in preprocessing, which helps to enhance the interpretability.

Algorithm 3: KPI-based SDO-MPLS Algorithm

Off-line training

1. Apply SDO to original data to obtain X_{sdo} and X_{sdores} .
2. Implement PLS on X_{sdo} and Y , then calculate the coefficient matrix $\Psi_{sdo} = RQ^T$.
3. Construct $\hat{\Gamma}_{sdo}$ and $\tilde{\Gamma}_{sdo}$ according to $\Psi_{sdo}\Psi_{sdo}^T$.
4. Calculate the thresholds $J_{\hat{T}_{sdompls},th}^2$, $J_{\tilde{T}_{sdompls},th}^2$ and $J_{T_{sdores},th}^2$.

On-line detection

1. Collect and correct online samples.
2. Calculate T^2 statistics, namely $\hat{T}_{sdompls}^2$, $\tilde{T}_{sdompls}^2$ and T_{sdores}^2 .
3. Make the decision based on the diagnostic logic.
 - (a) $\hat{T}_{sdompls}^2 \leq J_{\hat{T}_{sdompls},th}^2$ and $\tilde{T}_{sdompls}^2 \leq J_{\tilde{T}_{sdompls},th}^2$ and $T_{sdores}^2 \leq J_{T_{sdores},th}^2 \rightarrow$ fault-free
 - (b) $\hat{T}_{sdompls}^2 \geq J_{\hat{T}_{sdompls},th}^2 \rightarrow$ KPI-related fault occurs
 - (c) $\tilde{T}_{sdompls}^2 \geq J_{\tilde{T}_{sdompls},th}^2$ or $T_{sdores}^2 \geq J_{T_{sdores},th}^2 \rightarrow$ KPI-unrelated fault occurs

4. SIMULATION

In this section, the effectiveness of the approach proposed in this paper is evaluated by comparing it with standard PLS, T-PLS (Zhou et al., 2010) and OSC-MPLS (Wang et al., 2015) based on numerical example and TEP benchmark. Two commonly used indices, namely FDR and FAR, are considered in the performance evaluation. We mainly focus on the KPI-related subspace because we want to show that the method has both high FDR in KPI-related subspace when KPI-related faults occur and low FAR in KPI-related subspace when KPI-unrelated faults occur (Wang et al., 15).

4.1 Numerical example

The synthetic numerical example in (Zhou et al., 2010; Wang et al., 2015), widely used in the performance test of KPI-based MSPM methods, is adopted in this paper, i.e.

$$\begin{cases} x_k = Au_k + e_k \\ y_k = cx_k + v_k \end{cases} \quad (23)$$

where A is a 3×5 matrix, $u_k \in R^3$, $e_k, x_k \in R^5$ and

$$c_k = [2 \ 2 \ 1 \ 1 \ 0] \quad (24)$$

In case that there are faults, suppose that the faults are added in process variable space as following:

$$x_k = x_k^* + \Xi f \quad (25)$$

where x_k^* represents the normal sample value, Ξ and f are the fault direction and magnitude respectively.

KPI-related faults: From the expression of the numerical case (Wang et al., 2015), it is obvious that those faults will influence KPIs a lot when their directions are chosen as $\Xi = [2 \ 2 \ 1 \ 1 \ 0]$. In other words,

$$y_k = cx_k + v_k = c(x_k^* + \Xi f) + v_k \neq cx_k^* + v_k \quad (26)$$

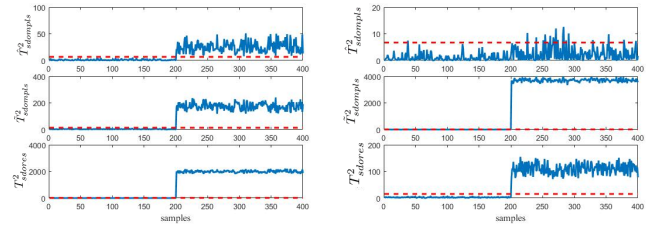


Fig. 1. SDO-MPLS for KPI-related faults in numerical example

Fig. 2. SDO-MPLS for KPI-unrelated faults in numerical example

f	PLS (%)	TPLS(T^2) (%)	TPLS(Q) (%)	OSC-MPLS (%)	SDO-MPLS (%)
2.0	79	4.5	100	4.5	13.5
4.0	100	16.5	100	17.5	46.5
6.0	100	34.5	100	36	85.5
8.0	100	67.5	100	69	100
10.0	100	85	100	86	100

For the comparison of FDRs among PLS, T-PLS, OSC-MPLS and SDO-MPLS methods, fault magnitudes have been set to 2.0, 4.0, 6.0, 8.0, 10.0 respectively. Considering KPI-related faults, the performance of these methods is shown in Table 1. It can be seen that FDR of each method increases with growing fault magnitude and FDR of SDO-MPLS reaches 100% when fault magnitude ≥ 8.0 . However, T-PLS(T^2) and OSC-MPLS own FDRs which are less than 100% even if magnitude reaches 10.0. On the other hand, PLS and T-PLS(Q) keep outstanding performance no matter how large fault magnitude is. Although the FDR of SDO-MPLS is lower than those of PLS and T-PLS(Q) when fault magnitude is less than 8.0, it is valid for KPI-related fault detections and is superior to T-PLS(T^2) and OSC-MPLS. The detection result of SDO-MPLS approach with $f = 8.0$ is shown in Fig.1.

KPI-unrelated faults: As for KPI-unrelated cases (Wang et al., 2015), faults with direction $\Xi = [0 \ 0 \ 0 \ 0 \ 1]$ can be chosen, which leads to

$$y_k = cx_k + v_k = c(x_k^* + \Xi f) + v_k = cx_k k + v_k \quad (27)$$

It is observed that such faults have no contribution to KPI, which shows the KPI irrelevance. Similarly, PLS, T-PLS, OSC-MPLS and SDO-MPLS approaches are applied to detect KPI-unrelated faults under same magnitudes. The detection results of SDO-MPLS method is plotted in Fig. 2 and FARs for KPI-unrelated faults by different approaches are given in Table 2.

Table 2. FAR for KPI-unrelated faults under different magnitudes

f	PLS (%)	TPLS(T^2) (%)	TPLS(Q) (%)	OSC-MPLS (%)	SDO-MPLS (%)
2	0	0	100	0	0
4	10.5	2	100	2	1.5
6	31	7.5	100	7	6.5
8	54	16.5	100	17	16.5
10	75.5	30	100	30	27.5

As seen from Table 2, PLS method fails to achieve low FAR when the magnitude of KPI-unrelated faults is relatively large. Although SDO-MPLS approach does not perform the best for KPI-related faults as shown in Table 1, it holds the lowest FAR among these approaches as fault magnitude grows. Also, T-PLS(T^2) and OSC-MPLS share relatively low FAR with the growing fault strength, but their FDR are lower than that of SDO-MPLS as shown in Table 1. Conversely, T-PLS(Q) falsely handles with many KPI-unrelated faults as shown in Table 2.

4.2 TEP benchmark

In this section, TE benchmark process (Downs et al., 1993) is utilized to illustrate KPI-based MSPM methods and their corresponding performance. It has been widely applied in the analysis of KPI-based MSPM methods (Yin et al., 2012; Yin et al., 2015; Wang et al., 2015).

TEP consists of five major parts: reactor, condenser, compressor, separator and stripper. Eight components, A, B, C, D, E, F, G and H, are taken into account, including four gaseous inputs, two products from four reactants in the process, an inert and a by-product. Totally, there are 52 variables in TEP benchmark, namely 11 manipulated variables and 41 process variables (Downs et al., 1993). In order to build X , all of the manipulated variables and 22 process variables are chosen from 52 measurements. According to these variables, E(XMEAS(35)) serves as the KPI (Yin et al., 2015), which is the product analysis of component E. As for classification of faults on KPI relations, Q statistic of Y-residual has been widely applied in (Yin et al., 2015), i.e.

$$Q_y = \|y - \hat{y}\|^2 \sim g\chi_{h,\alpha}^2 \quad (28)$$

where $g\chi_{h,\alpha}^2$ is the control limit. Based on the fluctuation of y and corresponding Q_y between fault-free and faulty samples, it can be observed that KPI-related faults include IDV(1), IDV(2), IDV(5), IDV(6), IDV(7), IDV(8), IDV(10), IDV(12), IDV(13), IDV(14), IDV(16), IDV(17), IDV(18) and IDV(20). Meanwhile, IDV(3),

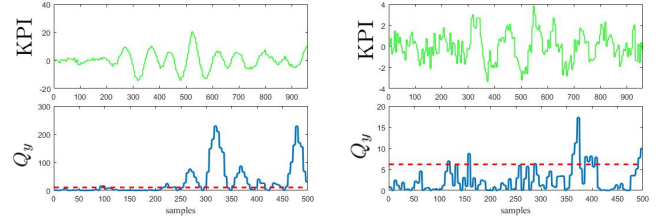


Fig. 3. KPI-related fault: IDV 8; Fig. 4. KPI-unrelated fault: IDV 11

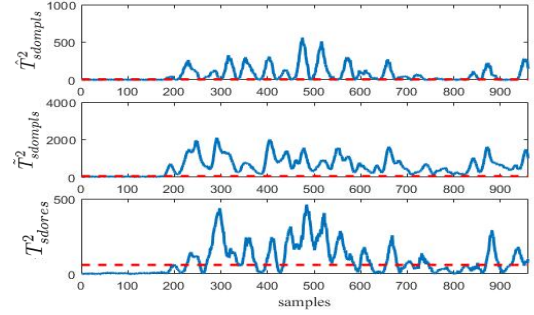


Fig. 5. SDO-MPLS for KPI-related faults in TEP

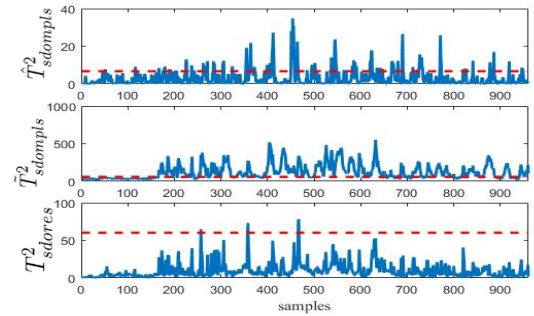


Fig. 6. SDO-MPLS for KPI-unrelated faults in TEP

IDV(4), IDV(9), IDV(11), IDV(15) and IDV(19) belong to KPI-unrelated faults (Wang et al., 2015). Considering KPI-related fault IDV(8) and KPI-unrelated fault IDV(11), Fig. 3 and Fig. 4 reflect the change of y and Q_y between fault-free and faulty samples. From the figures, it is shown that y in IDV(8) fluctuates sharply but the expectation and variance of y in IDV(11) change slightly. Fig. 5 and Fig. 6 reflect the fault detection results of SDO-MPLS when applied in these two faults. FDRs for KPI-related faults and FARs for KPI-unrelated faults in the TEP benchmark are shown in Table 3 and 4 respectively.

Concerning FDR for KPI-related faults, PLS method works well except in IDV(5), as shown in TABLE 3. At the same time, the Q statistic of T-PLS obtains outstanding performance in many KPI-related faults but IDV(7). However, the T^2 statistic of T-PLS cannot detect IDV(14) whose FDR is only 6.7%. As for OSC-MPLS, it does not perform well in some cases, e.g., IDV (16) and IDV (20). Compared with T-PLS and OSC-MPLS, SDO-MPLS guarantees that FDRs for KPI-related faults will

Table 3. FDR for KPI-related faults in the TEP benchmark.

Fault no	PLS (%)	TPLS(T^2) (%)	TPLS(Q) (%)	OSC-MPLS (%)	SDO-MPLS (%)
IDV(1)	100	36.9	99.1	37.5	59.7
IDV(2)	97.9	55.1	69.5	48.7	31.7
IDV(5)	30.5	25.8	60.2	71.4	23.7
IDV(6)	99.7	97.4	100	93.2	97.9
IDV(7)	74.8	44.1	31.5	30.9	40.4
IDV(8)	96.2	74.0	68.8	66.6	76.3
IDV(10)	85.2	58.5	74.5	25.2	51.9
IDV(12)	99.8	77.8	73.0	71.3	77.4
IDV(13)	95.0	86.1	93.4	81.7	85.8
IDV(14)	99.4	6.7	83.1	76.4	54.1
IDV(16)	67.9	40.8	71.0	17.7	33.9
IDV(17)	83.3	27.1	84.7	47.9	25.6
IDV(18)	90.5	88.7	89.9	82.2	89.0
IDV(20)	55.6	25.9	56.8	7.2	20.3

Table 4. FAR for KPI-unrelated faults in the TEP benchmark

Fault no	PLS (%)	TPLS(T^2) (%)	TPLS(Q) (%)	OSC-MPLS (%)	SDO-MPLS (%)
IDV(3)	9.3	12.1	0.5	3.8	8.3
IDV(4)	51.4	10.7	45.4	3.9	6.4
IDV(9)	7.3	9.7	0.5	1.5	5.7
IDV(11)	55.9	13.1	28.9	23.5	16.0
IDV(15)	13.4	6.5	0.6	4.7	7.1
IDV(19)	11.9	7.4	58.3	3.6	5.7

exceed 20% though it does not have the highest FDRs totally.

When it comes to faults unrelated to KPI, PLS, T-PLS, OSC-MPLS and SDO-MPLS approaches are applied to detect them similarly. As seen from TABLE 4, PLS method obtains high FAR in many cases which proves once again that PLS is not valid for KPI-related fault detection. Although T^2 statistic of T-PLS performs well when dealing with KPI-unrelated faults, it can be seen that Q statistic of T-PLS cannot maintain its superiority for KPI-unrelated faults. FAR of T-PLS(Q) for IDV (11) even exceeds 50% in TABLE IV. Meanwhile, OSC-MPLS works well and its performance outweighs those of PLS and T-PLS. SDO-MPLS shares similar low FARs with OSC-MPLS in most cases. Furthermore, it is noteworthy that SDO-MPLS has remarkable lower FAR than OSC-MPLS under IDV (11) circumstance.

From the table listed above, it is observed that PLS and T-PLS do not work well for KPI-unrelated fault detection. Although OSC-MPLS has low FARs in most KPI-unrelated fault cases, its FAR exceeds 20% for IDV (11) as shown in TABLE IV, which is relatively high for others. According to above detailed analysis, it can be concluded that SDO-MPLS shows better fault detection performances for KPI-related process monitoring and fault detection, in the sense that reducing FAR for KPI-unrelated faults without sacrificing FDR for KPI-related faults.

5. CONCLUSION

In this paper, an improved KPI-related fault detection method, namely SDO-MPLS, is proposed. We first propose SDO to remove undesired variations from input space.

Further, M-PLS is implemented to decompose input space into two orthogonal ones. Compared with PLS and T-PLS, the proposed approach has lower FARs for KPI-unrelated faults. When it comes to OSC-MPLS, SDO-MPLS is more robust and reduces FAR for KPI-unrelated faults without sacrificing FDR for KPI-related faults. The superiority of the performances for SDO-MPLS is finally demonstrated by a numerical case and TEP benchmark.

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