Total Projection to Latent Structures for Process Monitoring

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*Partial least squares or projection to latent structures (PLS) has been used in multivariate statistical process monitoring similar to principal component analysis. Standard PLS often requires many components or latent variables (LVs), which contain variations orthogonal to **Y** and useless for predicting **Y**. Further, the **X**-residual of PLS usually has quite large variations, thus is not proper to monitor with the Q-statistic. To reduce false alarm and missing alarm rates of faults related to **Y**, a total projection to latent structures (T-PLS) algorithm is proposed in this article. The new structure divides the **X**-space into four parts instead of two parts in standard PLS. The properties of T-PLS are studied in detail, including its relationship to the orthogonal PLS. Further study shows the space decomposition on **X**-space induced by T-PLS. Fault detection policy is developed based on the T-PLS. Case studies on two simulation examples show the effectiveness of the T-PLS based fault detection methods.* *AIChE J,* 56: 168–178, 2010
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Introduction

Modern industrial processes often possess a large number of measured variables, such as flow-rates, concentrations, temperatures, and pressures. Multivariate statistic process monitoring (MSPM) is effective for detecting and diagnosing faults or abnormal operating situations in many industrial processes, including chemicals, polymers, and microelectronics manufacturing. Two basic multivariate projection methods used in MSPM are principal component analysis (PCA) and partial least squares or projection to latent structures (PLS).[1–6] Process monitoring using PCA or PLS is based on a predefined model built from normal process data. The major advantages of these multivariate projections are their ability to handle large numbers of highly correlated variables, measurement errors, and missing data. Both methods are able to reduce the dimensionality of the monitoring space by projecting measurement data onto a low-dimensional latent space.[1] The processes are then monitored in these subspaces by utilizing multivariate control charts that reflect the information in all measured variables simultaneously.[7]

PCA-based monitoring methods are effective in monitoring all the variations and abnormal situations in process variables (**X**). If one wants to monitor the variations in the process variables that are most influential on quality variables (**Y**), one should perform a PLS decomposition on **X**. PLS model has been used for process monitoring in a way similar to PCA-based methods.[1,8,9] The basic structure and algorithms of PLS have been summarized in the chemometrics literature.[7]

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Although PCA-based monitoring methods are well understood,[10] PLS based methods have not been thoroughly studied. MacGregor et al.[7] proposed the monitoring policy with multiblock PLS and showed how contribution plots were used to identify the fault variables using PLS. Nelson et al.[11] considered the missing data in industrial processes and studied the estimation of scores when the new observation vector had missing data, using PCA and PLS model. Westerhuis et al.[12] proposed the method of calculating generalized contribution plots in process monitoring, including PLS and PCA. Choi and Lee[13] defined new contribution plots of T^2 for multiblock PLS. Recently, Li et al.[14] revealed the geometric properties of PLS for process monitoring and compared monitoring policies using various PLS.

The standard PLS divides the measured variable space into two subspaces.[14] The typical approach is to use T^2 for PLS scores and Q for the **X** residuals. The T^2 index is defined by the Mahalanobis distance whereas the Q index is defined by the Euclidean distance to avoid ill-conditioning due to small eigenvalues. Although it works in many cases, monitoring in two subspaces still faces some problems. On one hand, as there are usually many process variables, PLS uses many components, which makes the predictor model difficult to interpret. These PLS components still include variations orthogonal to **Y** which have no contribution for predicting **Y**. On the other hand, the **X**-residuals from the PLS model are not necessarily small in covariances. There are many cases in which the **X**-residuals contain larger variability of **X** than the PLS scores because PLS does not decompose the **X**-variations in descending order. This makes the use of Q statistic on **X**-residuals inappropriate.

To improve the PLS model, Wold et al.[15] proposed the orthogonal signal correction (OSC) method. The idea was to remove systematic information in **X** not correlated to **Y** before a PLS model was built, to obtain better models. Fearn[16] then reported another way of estimating the orthogonal components. Trygg and Wold[17] put forward the orthogonal projections to latent structures (O-PLS) based on the original nonlinear iterative partial least squares algorithm (NIPALS). The O-PLS method is a preprocessing or filtering method to remove systematic orthogonal variation to **Y** from a given data set **X**. The standard PLS on the filtered data can lead to simpler models. However, the above methods are regression methods, which are not designed for process monitoring.

In this article, we present a total projection to latent structures (T-PLS) and discuss the policy of process monitoring based on the new structure. T-PLS performs further decomposition both in PLS principal space and residual space. The objective for the former is to separate the orthogonal and correlated part to **Y**, and that for the latter is to separate large variations from noise that has very little variation. Then we develop a new monitoring policy based on the T-PLS.

The remainder of this article is organized as follows. Section on PLS for Process Monitoring reviews the PLS algorithm, PLS on **X**-space, and how to use PLS for process monitoring. Section on Total Projection to Latent Structures introduces the T-PLS algorithm and analyzes the T-PLS. Then we develop a complete monitoring policy based on T-PLS detailed in Section on T-PLS Based Fault Detection. Section on Case Study on Simulation Examples uses two simulation examples to illustrate the effectiveness of the new structure. Finally, we present conclusions in last section.

PLS for Process Monitoring

Given input matrix $\mathbf{X} \in \mathbb{R}^{n \times m}$ consisting of n samples with m process variables, and output matrix $\mathbf{Y} \in \mathbb{R}^{n \times p}$ with p quality variables, we can use NIPALS to project (**X**, **Y**) to a low-dimensional space defined by a small number of latent variables ($\mathbf{t}_1, \ldots, \mathbf{t}_A$), where A is the PLS component number. In PLS, the scaled and mean-centered **X** and **Y** are decomposed as:

$$\begin{cases} \mathbf{X} = \sum_{i=1}^{A} \mathbf{t}_i \mathbf{p}_i^T + \mathbf{E} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \\ \mathbf{Y} = \sum_{i=1}^{A} \mathbf{t}_i \mathbf{q}_i^T + \mathbf{F} = \mathbf{T}\mathbf{Q}^T + \mathbf{F} \end{cases} \tag{1}$$

where $\mathbf{T} = [\mathbf{t}_1, \ldots, \mathrm{t}_A]$, $\mathbf{P} = [\mathbf{p}_1, \ldots, \mathbf{p}_A]$, $\mathbf{Q} = [\mathbf{q}_1, \ldots, \mathbf{q}_A]$. $\mathbf{t}_i(i = 1,\ldots, A)$ are score vectors, $\mathbf{p}_i(i = 1,\ldots, A)$ are loading vectors for **X** and $\mathbf{q}_i(i = 1,\ldots, A)$ are loading vectors for **Y**. A brief NIPALS is given in Appendix A. In the NIPALS algorithm, score vectors are calculated by using weight vectors $\mathbf{w}_i$ from deflated **X** data for each dimension. However, $\mathbf{w}_i$ cannot connect $\mathbf{t}_i$ to original **X** data directly. Let $\mathbf{R} = [\mathbf{r}_1,\ldots, \mathbf{r}_A]$, where $\mathbf{r}_1 = \mathbf{w}_1$, for $i > 1$

$$\mathbf{r}_i = \prod_{j=1}^{i-1} \left(\mathbf{I}_m - \mathbf{w}_j \mathbf{p}_j^T\right) \mathbf{w}_i \tag{2}$$

With **R**, the score matrix **T** can be computed directly from original **X**:

$$\mathbf{T} = \mathbf{X}\mathbf{R} \tag{3}$$

Furthermore, **R** and **P** have the following relation[18,19]:

$$\mathbf{P}^T\mathbf{R} = \mathbf{R}^T\mathbf{P} = \mathbf{I}_A \tag{4}$$

In the PLS literature, the case of a single output is referred to as PLS1 and that for multiple outputs is referred to as PLS2. In the general case, the number of PLS components A is usually smaller than the number of **X**-variables, m.

Different from the PCA structure, the PLS induces an oblique projection decomposition on **X** space[14]:

$$\begin{aligned} \mathbf{x} &= \hat{\mathbf{x}} + \tilde{\mathbf{x}} \\ \hat{\mathbf{x}} &= \mathbf{P}\mathbf{R}^T\mathbf{x} \in S_{\mathrm{p}} \equiv \mathrm{Span}\{\mathbf{P}\} \\ \tilde{\mathbf{x}} &= \left(\mathbf{I} - \mathbf{P}\mathbf{R}^T\right)\mathbf{x} \in S_{\mathrm{r}} \equiv \mathrm{Span}\{\mathbf{R}\}^{\perp} \end{aligned}$$

Notice that $\hat{\mathbf{x}}$ is not orthogonal to $\tilde{\mathbf{x}}$ in PLS. From this geometric interpretation, $\hat{\mathbf{x}}$ is the projection of x onto Span{**P**} along $\mathrm{Span}\{\mathbf{R}\}^{\perp}$ and $\tilde{\mathbf{x}}$ is the projection of x onto $\mathrm{Span}\{\mathbf{R}\}^{\perp}$ along Span{**P**}.

Usually T^2 and Q statistics are used in PLS-based monitoring. Given a new sample $\mathbf{x}_{\mathrm{new}}$, we first calculate[7]:

$$\mathbf{t}_{\mathrm{new}} = \mathbf{R}^T\mathbf{x}_{\mathrm{new}} \tag{6}$$

$$\tilde{\mathbf{x}}_{\mathrm{new}} = \left(\mathbf{I} - \mathbf{P}\mathbf{R}^T\right)\mathbf{x}_{\mathrm{new}} \tag{7}$$

then T^2 and Q are calculated by[13]:

Table 1. Total PLS Algorithm for a Single Output (T-PLS)

Center the columns of **X, y** to zero mean and scale them to unit variance.
(1) Run PLSI algorithm on (**X, y**) to estimate **T** $\begin{cases} \mathbf{X}= \mathbf{TP}^T + \mathbf{E} \\ \mathbf{y} = \mathbf{Tq}^T + \mathbf{F} \end{cases}$ where $T \in \mathbb{R}^{n \times A}$, **q, P, T** are obtained by PLSI, A is determined by cross-validation.
(2) $\mathbf{t}_y = \mathbf{Tq}^T$.
(3) $\hat{\mathbf{X}} = \mathbf{TP}^T, \mathbf{p}_y = \hat{\mathbf{X}}^T\mathbf{t}_y \big/ \mathbf{t}_y^T t_y$.
(4) $\hat{\mathbf{X}}_o = \hat{\mathbf{X}} - \mathbf{t}_y\mathbf{p}_y^T = \mathrm{T_o}P_o^T$, run PCA on $\hat{\mathbf{X}}_o$ with $A - 1$ components.
(5) $\mathbf{E} = \mathbf{T}_r P_r^T + \mathrm{E_r}$, run PCA on E with A_r components, where $A_r < m - A$ is determined using the method by.[20]

$$T^2 = \mathbf{t}_{\text{new}}^T \Lambda^{-1} \mathbf{t}_{\text{new}} \sim \frac{A(n^2-1)}{n(n-A)} F_{A,n-A,} \tag{8}$$

$$Q = \|\tilde{\mathbf{x}}_{\text{new}}\|^2 \sim g\chi^2_{h,} \tag{9}$$

where $\Lambda = \frac{1}{n-1}\mathbf{T}^T\mathbf{T}$. $F_{A,n-A}$ is F-distribution with A and $n - A$ degrees of freedom. $g\chi_h^2$ is the χ^2-distribution with scaling factor g and h degrees of freedom.

Total Projection to Latent Structures

PLS uses two subspaces to monitor processes, respectively. One is the principal subspace S_p which is monitored by T^2, reflecting the major variation related to **Y**. The other is the residual subspace S_r which is monitored by Q, reflecting the variation unrelated to **Y**. However, the principal part $\hat{\mathbf{x}}$ in S_p still contains many components, including variations orthogonal to **Y** and useless to predict **Y**. Another problem in process monitoring is with the standard PLS. As the primary objective of PLS is to maximize the covariance between **X** and **Y**, it does not extract the variance in the **X**-space in a descending order. A latter component can capture more variance in **X** than a previous component. After **Y** is best predicted with A components, the residual of **X** can still contain very large variability. Therefore, it is not suitable to use Q-statistic to monitor **X**-residual in PLS. It is necessary to decompose **E** further. In this section, we propose a further decomposition of PLS defined as T-PLS. We first put forward the T-PLS algorithm for a single output, analyze the properties of the T-PLS, then give the T-PLS algorithm for multiple outputs.

T-PLS algorithm for a single output y

The T-PLS algorithm proposed here is a further decomposition based on the PLS algorithm. With reference to O-PLS, T-PLS can be treated as a postprocessing method to decompose the $\mathbf{TP}^T$ and **E** in the standard PLS. The T-PLS algorithm for a single output **y** is listed in Table 1.

Using the T-PLS algorithm, we can model **X**, **y** as follows:

$$\begin{cases} \mathbf{X} = \mathbf{t}_y\mathbf{p}_y^T + \mathbf{T}_o\mathbf{P}_o^T + \mathbf{T}_r\mathbf{P}_r^T + \mathbf{E}_r \\ \mathbf{Y} = \mathbf{t}_y + \mathbf{F} \end{cases} \tag{10}$$

where $\mathbf{E}_r$ can be expressed as follows:

$$\mathbf{E}_r = \mathbf{E}\left(\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T\right) \tag{11}$$

Compared with a PLS model, the T-PLS model is clear for describing the measured **X** and suitable for monitoring different parts of **X**. For a single output **y**, T-PLS needs only one score vector $\mathbf{t}_y$ to predict the quality variable **y**, whereas PLS1 needs several score vectors $\mathbf{t}_i$ ($i = 1, \ldots, A$). In (10), $\mathbf{t}_y$ is directly correlated to **y** in the original **T**, and $\mathbf{T}_o$ is orthogonal to **y** in the original **T**. $\mathbf{T}_r$ is the main part in the original **E**, and $\mathbf{E}_r$ is the residual part in **X** that represents the noise. T-PLS can be simply explained in Figure 1.

Properties of T-PLS

Like the PLS algorithm, the orthogonality among score vectors holds for the T-PLS algorithm, which is shown in the following lemma:

Lemma 1. $\forall \mathbf{t}_i, \mathbf{t}_j \in$ **Cols** $\{\mathbf{t}_y, \mathbf{T}_o, \mathbf{T}_r\}$:

$$\mathbf{t}_i^T\mathbf{t}_j = 0, \quad i \neq j. \tag{12}$$

Proof: According to the properties of PLS,

$$\mathbf{T}^T\mathbf{E} = 0 \tag{13}$$

From the T-PLS algorithm, we can get

$$\mathbf{t}_y^T\hat{\mathbf{X}}_o = \mathbf{t}_y^T\left(\mathbf{I} - \mathbf{t}_y\mathbf{t}_y^T/\mathbf{t}_y^T\mathbf{t}_y\right)\hat{\mathbf{X}} = 0 \tag{14}$$

Thus

$$\mathbf{t}_y^T\mathbf{T}_o = \mathbf{t}_y^T\hat{\mathbf{X}}_o\mathbf{P}_o = 0 \tag{15}$$

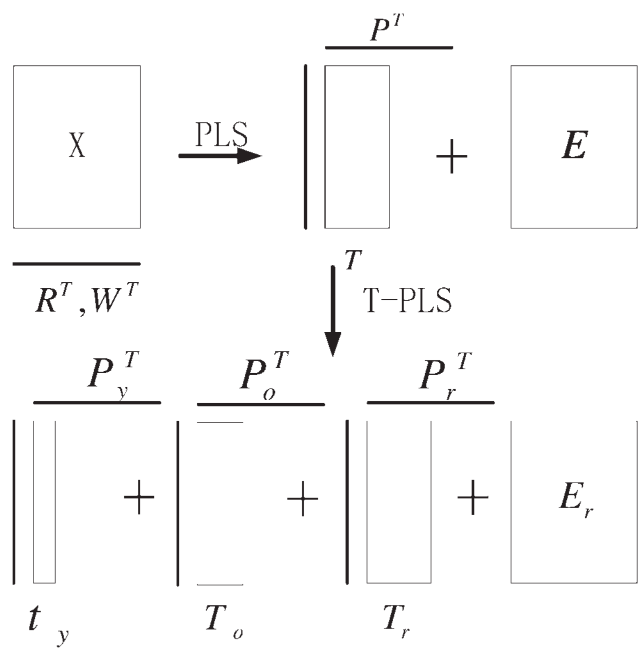

Figure 1. T-PLS.

With orthogonality in PCA model, $\mathbf{t}_i \in \mathbf{T}_o$ and $\mathbf{T}_r$ are all orthogonal to each other. Lemma 1 is proven. ■

As we have pointed out above, $\mathbf{T}_o$ is the orthogonal part to $\mathbf{y}$ in the original $\mathbf{T}$. The following lemma shows the result.

Lemma 2.

$$\mathbf{T}_o^T\mathbf{y} = 0 \tag{16}$$

Proof: Noting that

$$\begin{aligned}\mathbf{T}_o^T\mathbf{y} &= \mathbf{T}_o^T(\mathbf{t}_y + \mathbf{F})\\ &= (\mathbf{T}_o^T\mathbf{t}_y + \mathbf{T}_o^T\mathbf{F}) = \mathbf{P}_o^T\hat{\mathbf{X}}_o^T\mathbf{F}\\ &= \mathbf{P}_o^T\hat{\mathbf{X}}^T\left(\mathbf{I} - \mathbf{t}_y\mathbf{t}_y^T/\mathbf{t}_y^T\mathbf{t}_y\right)\mathbf{F}\\ &= \mathbf{P}_o^T\hat{\mathbf{X}}^T\mathbf{F} = \mathbf{P}_o^T\mathbf{P}\mathbf{T}^T\mathbf{F} = \mathbf{0}\end{aligned}$$

where $\mathbf{T}^T\mathbf{F} = 0$ is a property of the PLS algorithm. Hence, $\mathbf{t}_y^T\mathbf{F} = 0$ and the Lemma is proven. ■

Relationship between T-PLS and O-PLS

In the chemometrics literature, researchers usually use multivariate calibration methods to preprocess process data $\mathbf{X}$.[15–17] The O-PLS algorithm is one of these preprocessing methods.[17] The work by Verron et al. revealed other properties of O-PLS, which connected the O-PLS with standard PLS.[21] We will show the relationship between T-PLS and O-PLS based on the above work. Let $\mathbf{t}_{i,k}$ denote the i-th component extracted after removing k orthogonal components from $\mathbf{X}$ using O-PLS algorithm. $\mathbf{t}_{i+k}$ represents the $(i + k)$th PLS component. Then the following relation is proven by Verron et al.[21]:

$$\forall i > 1, \mathbf{t}_{i,k} = \mathbf{t}_{i+k} \tag{17}$$

This property of O-PLS indicates,

$$\mathrm{Span}\{\mathbf{T}_{\mathrm{ortho}}, \mathbf{t}_{1,k}\} = \mathrm{Span}\{\mathbf{t}_1, \ldots, \mathbf{t}_{k+1}\} \tag{18}$$

where $\mathbf{T}_{\mathrm{ortho}} = [\mathbf{t}_{1,\mathrm{ortho}},\ldots,\mathbf{t}_{k,\mathrm{ortho}}]$ is the orthogonal score matrix in O-PLS. With (10), we can get the following lemma:

Lemma 3. $\forall A > 1$, *suppose that PLS takes A components collected in* $\mathbf{T}$, *and O-PLS takes* $A - 1$ *orthogonal components collected in* $\mathbf{T}_{\mathrm{ortho}}$, *then*

$$\mathrm{Span}\{\mathbf{T}_{\mathrm{ortho}}\} = \mathrm{Span}\{\mathbf{T}_o\} \tag{19}$$

Proof: Noting from (18)

$$\mathrm{Span}\{\mathbf{T}_{\mathrm{ortho}}, \mathbf{t}_{1,k}\} = \mathrm{Span}\{\mathbf{T}\} = \mathrm{Span}\{\mathbf{T}_o, \mathbf{t}_y\} \tag{20}$$

and according to the properties of O-PLS,[17] we have

$$\mathbf{T}_{\mathrm{ortho}}^T\mathbf{y} = 0 \tag{21}$$

As $\mathrm{rank}(\mathbf{T}_{\mathrm{ortho}}) = \mathrm{rank}(\mathbf{T}_o) = A - 1$, if (19) does not hold, there must exist A linearly independent columns in $[\mathbf{T}_o, \mathbf{T}_{\mathrm{ortho}}]$, so that $\mathrm{span}\{\mathbf{T}_{\mathrm{ortho}}, \mathbf{T}_o\} = \mathrm{span}\{\mathbf{T}\}$. Then it can be concluded from (16) and (21) that $\mathbf{T}^T\mathbf{y} = 0$, which is obviously incorrect. Thus, Lemma 3 is proven. ■

As an inference, the following lemma holds.

Lemma 4.

$$\mathbf{t}_{1,k} \propto \mathbf{t}_y \tag{22}$$

Proof: According to the properties of O-PLS, we have

$$\mathbf{t}_{1,k}^T\mathbf{T}_{\mathrm{ortho}} = 0 \tag{23}$$

and from Lemma 1,

$$\mathbf{t}_y^T\mathbf{T}_o = 0 \tag{24}$$

According to (20), we know $\mathbf{t_y}$, $\mathbf{t_{1,k}}$ are both orthogonal complements of $\mathrm{Span}\{\mathbf{T}_o\}$ or $\mathrm{Span}\{\mathbf{T}_{\mathrm{ortho}}\}$ with one dimension. Therefore, $\mathbf{t_{1,k}}$ in O-PLS is proportional to $\mathbf{t}_y$ in T-PLS. ■

Lemmas 3 and 4 indicate that T-PLS has the same result on the decomposition of $\mathbf{T}$ as the O-PLS algorithm. However, T-PLS further decomposes the $\mathbf{X}$-residual $\mathbf{E}$, which is useful for process monitoring.

T-PLS projection structure in X-space

T-PLS algorithm realizes the total decomposition of $\mathbf{X}$ space supervised by $\mathbf{y}$. The following lemma describes the oblique projection structure of *T-PLS:*

Lemma 5. *The T-PLS algorithm induces an oblique decomposition on* $\mathbf{X}$*-space*:

$$\begin{aligned}\mathbf{x} &= \hat{\mathbf{x}}_y + \hat{\mathbf{x}}_o + \hat{\mathbf{x}}_r + \hat{\mathbf{x}}_r\\ \hat{\mathbf{x}}_y &= \mathbf{p}_y\mathbf{q}\mathbf{R}^T\mathbf{x} \equiv \mathbf{C}_1\mathbf{x} \in S_y\\ \hat{\mathbf{x}}_o &= (\mathbf{P} - \mathbf{p}_y\mathbf{q})\mathbf{R}^T\mathbf{x} \equiv \mathbf{C}_2\mathbf{x} \in S_o\\ \hat{\mathbf{x}}_r &= \mathbf{P}_r\mathbf{P}_r^T\left(\mathbf{I} - \mathbf{P}\mathbf{R}^T\right)\mathbf{x} \equiv \mathbf{C}_3\mathbf{x} \in S_{rp}\\ \tilde{\mathbf{x}}_r &= \left(\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T\right)\left(\mathbf{I} - \mathbf{P}\mathbf{R}^T\right)\mathbf{x} \equiv \mathbf{C}_4\mathbf{x} \in S_{rr}\end{aligned} \tag{25}$$

where

$$\mathbf{C}_1 + \mathbf{C}_2 + \mathbf{C}_3 + \mathbf{C}_4 = \mathbf{I}_m \tag{26}$$

Lemma 5 is proven in Appendix B. The meanings of different subspaces are summarized in Table 2.

T-PLS model does not change prediction ability of $\mathbf{y}$ compared with standard PLS model, but it decomposes $\mathbf{X}$-space supervised by $\mathbf{y}$. Moreover, it is easier to interpret and more precise for monitoring. From the properties of PLS and T-PLS, we can conclude that the variations in S_y are most related to $\mathbf{y}$ and the variations in S_o, S_{rp} are unrelated or little related to $\mathbf{y}$. $\tilde{\mathbf{x}}_r$ is thought to be little related to $\mathbf{y}$ in standard PLS based methods.

However, the last assertion about $\tilde{\mathbf{x}}_r$ seems not quite right. PLS uses covariance to decide whether a score vector is correlated to $\mathbf{y}$. As the variance of $\tilde{\mathbf{x}}_r$ is very small or even zero, the covariance of $\tilde{\mathbf{x}}_r$ and $\mathbf{y}$ is accordingly small so that $\tilde{\mathbf{x}}_r$ seems to be uncorrelated to $\mathbf{y}$. In fact, if the correlation coefficient of $\tilde{\mathbf{x}}_r$ and y is not zero, the output y may be

Table 2. Meaning of Different Subspaces

Subspace	Dimension	Description
S_y	1	subspace of **X**-space that is solely responsible in predicting y
S_o	$A-1$	Subspace of **X**-space that is explored by the PLS objective but does not predict y
S_{rp}	A_r	subspace of **X**-space that is not explored by the PLS objective, but has significant variation or excitation in **X**-space
S_{rr}	$m-A-A_r$	subspace of **X**-space that is not excited in the **X**-space of the data

affected by the faults in $\tilde{\mathbf{x}}_r$. This can be explained by the following example.

$$y = x_1 + x_2 + e \tag{27}$$

Suppose the process is described by (27), where e is the noise independent to x_1 and x_2, $x_1 = 2x_2$ in normal situation and $\mathbf{E}(x_1) = \mathbf{E}(x_2) = 0$, $\mathbf{Var}(x_1) = 4\mathbf{Var}(x_2) = 4\sigma^2$. T-PLS for the above system is as follows:

$$\begin{cases} y = \frac{3}{\sqrt{5}}t + \upsilon \\ t = \frac{2}{\sqrt{5}}x_1 + \frac{1}{\sqrt{5}}x_2 \end{cases} \tag{28}$$

where $\dim(S_y) = 1$, $\dim(S_o) = 0$, $\dim(S_{rp}) = 0$, and $\dim(S_{rr}) = 1$.

Assume there is a fault as follows:

$$\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} = \begin{bmatrix} x_1^* \\ x_2^* \end{bmatrix} + \begin{bmatrix} 1 \\ -2 \end{bmatrix} f \tag{29}$$

where * denotes the normal value without faults and f is the fault magnitude. It can be calculated $t = t^*$, which shows that the fault happens in the residual space S_{rr}. We can get from (27) and (28)

$$\begin{aligned} y &= x_1^* + x_2^* + e - f = y^* - f \\ \tilde{y} &= y - \frac{3}{\sqrt{5}}t = y^* - \frac{3}{\sqrt{5}}t^* - f = \tilde{y}^* - f \end{aligned} \tag{30}$$

which shows that output y is affected by the fault that happens in residual space S_{rr}. On the other hand, if (27) is changed to:

$$y = \frac{6}{5}x_1 + \frac{3}{5}x_2 + e \tag{31}$$

The T-PLS (28) will not change, but the result (30) will change to:

$$\begin{aligned} y &= \frac{6}{5}x_1^* + \frac{3}{5}x_2^* + e = y^* \\ \tilde{y} &= y^* - \frac{3}{\sqrt{5}}t^* = \tilde{y}^* \end{aligned} \tag{32}$$

which shows that the output y is not affected by the fault that happens in residual space S_{rr}. Hence, $\tilde{\mathbf{x}}_r$ should be monitored for faults related to **y**.

Table 3. Total PLS Algorithm for Multiple Outputs (T-PLS2)

Center and scale the raw data to give the matrices $\mathbf{X} \in \mathbb{R}^{n\times m}$ and $\mathbf{Y} \in \mathbb{R}^{n\times p}$.

(1) Perform the PLS2 algorithm on **X** and **Y**, $\begin{cases} \mathbf{X} = \mathbf{TP^T} + \mathbf{E} \\ \mathbf{y} = \mathbf{Tq}^T + \mathbf{F} \end{cases}$ where **T, Q, P,** and **R** are obtained in PLS2. PLS component number A is determined by cross-validation.

(2) $\hat{\mathbf{Y}} = \mathbf{TQ}^T = \mathbf{T}_y\mathbf{Q}_y^T$. Run PCA on $\hat{\mathbf{Y}}$ with A_y components, where $A_y = \text{rank}(\mathbf{Q})$.

(3) $\hat{\mathbf{X}} = \mathbf{TP}^T, \mathbf{P}_y^T = \left(\mathbf{T}_y^T\mathbf{T}_y\right)^{-1}\mathbf{T}_y^T\hat{\mathbf{X}}$.

(4) $\hat{\mathbf{X}}_o = \hat{\mathbf{X}} - \mathbf{T}_y\mathbf{P}_y^T = \mathbf{T}_o\mathbf{P}_o^T$. Run PCA on $\hat{\mathbf{X}}_o$ with $A - A_y$ components.

(5) $\mathbf{E} = \mathbf{T}_r\mathbf{P}_r^T + \mathbf{E}_r$ Run PCA on **E** with A_r components, where $A_r < m - A$ is determined using PCA methods.

T-PLS for multiple outputs Y

The T-PLS algorithm for multiple outputs **Y** is given in Table 3. **X** and **Y** can be modeled as follows:

$$\begin{cases} \mathbf{X} = \mathbf{T}_y\mathbf{P}_y^T + \mathbf{T}_o\mathbf{P}_o^T + \mathbf{T}_r\mathbf{P}_r^T + \mathbf{E}_r \\ \mathbf{Y} = \mathbf{T}_y\mathbf{Q}_y^T + \mathbf{F} \end{cases} \tag{33}$$

The T-PLS for multiple outputs (T-PLS2) is basically the same as the T-PLS for a single output (T-PLS1). The only difference is that $\mathbf{t}_y$ in T-PLS1 is replaced by $\mathbf{T}_y$ in T-PLS2 because of the nature of multiple outputs. There are three structure parameters to be decided in T-PLS2. PLS component number A is determined by cross validation. The number of **Y**-related principal components $\mathbf{A_y} = \text{rank}(Q)$ is no greater than p and A. Y-unrelated components number A_r is determined using PCA-based methods.

The properties of TPLS1 also hold for T-PLS2, including Lemmas 1 and 2, which can be proven in a similar way. The relationship between O-PLS and T-PLS for multiple outputs does not hold because O-PLS2 algorithm has different prediction model from PLS2. The **X**-space is partitioned into four subspaces by T-PLS2 in a similar way as shown in Lemma 5 and the meaning of different parts is also the same. The proof can be more involved than T-PLS1 with similar arguments.

T-PLS Based Fault Detection

Conventional PLS-based fault detection methods would plot SPE, T^2 control charts described in Section on PLS for Process Monitoring to monitor a process. Under the assumption that latent vectors are normally distributed with zero

Table 4. Monitoring Statistics and Control Limits

Statistics	Calculation	Control Limit
T_y^2	$t_{y,\text{new}}^T\Lambda_y^{-1}t_{y,\text{new}}$	$\frac{(n+1)}{n}F_{1,n-1,\alpha}$
T_o^2	$\mathbf{t}_{o,\text{new}}^T\Lambda_o^{-1}\mathbf{t}_{o,\text{new}}$	$\frac{(A-1)\left(n^2-1\right)}{n(n-A+1)}F_{A-1,n-A+1,\alpha}$
T_r^2	$\mathbf{t}_{r,\text{new}}^T\Lambda_r^{-1}\mathbf{t}_{r,\text{new}}$	$\frac{A_r\left(n^2-1\right)}{n(n-A_r)}F_{A_r,n-A_r,\alpha}$
Q_r	$\lVert\tilde{\mathbf{x}}_{r,\text{new}}\rVert^2$	$g\chi^2_{h,\alpha}$

n, number of training samples; A, number of PLS principal components; A_y, number of principal components related to **Y**; A_r, number of components unrelated to **Y**.

Table 5. PLS, A = 2

R		P		q^T
0.3260	0.7003	0.3204	0.8192	0.9886
0.3482	−0.3912	0.3513	−0.5702	0.1506
0.6097	0.3272	0.6071	0.1210	
0.6307	−0.4655	0.6344	−0.2485	
0.0548	0.1814	0.0534	0.2645	

mean, the control limits of T^2 and Q can be calculated. T-PLS can also be used for monitoring in a similar way. First, we build a T-PLS model from normal historical process data **X** and **Y**. Then all scores and residuals are calculated from a new sample. Finally, several control plots are constructed with corresponding control limits, which are used for monitoring.

In multivariate statistical process monitoring, two types of statistics are widely used for fault detection. These are the D-Statistic for the systematic part of the process variation and the Q-Statistic for the residual part of process variation which is also called Hotelling's T^2 and SPE statistics in PCA-based methods. In the T-PLS, $\hat{\mathbf{x}}_y$, $\hat{\mathbf{x}}_o$, **and** $\hat{\mathbf{x}}_r$ contain the systematic part of the process variation, thus are suitable to use D-statistics, whereas $\tilde{\mathbf{x}}_r$ represents the residual part of the whole process variation, thus is suitable to use the Q-statistic. For a new measured sample $\mathbf{x}_{new}$, the scores and the residual part are calculated as follows:

$$\mathbf{t}_{y,new} = \mathbf{q}\mathbf{R}^T\mathbf{x}_{new} \in \mathbb{R}^1 \quad (34a)$$

$$\mathbf{t}_{o,new} = \mathbf{P}_o^T\left(\mathbf{P} - \mathbf{p}_y\mathbf{q}\right)\mathbf{R}^T\mathbf{x}_{new} \in \mathbb{R}^{A-1} \quad (34b)$$

$$\mathbf{t}_{r,new} = \mathbf{P}_r^T\left(\mathbf{I} - \mathbf{P}\mathbf{R}^T\right)\mathbf{x}_{new} \in \mathbb{R}^{A_r} \quad (34c)$$

$$\tilde{\mathbf{x}}_{r,new} = \left(\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T\right)\left(\mathbf{I} - \mathbf{P}\mathbf{R}^T\right)\mathbf{x}_{new} \in \mathbb{R}^m \quad (34d)$$

Here we use T-PLS1 structure to calculate the scores and residuals and T-PLS2 structure can be used similarly. Fault detection indices are constructed in Table 4. Assuming the measured sample follows a multivariate normal distribution, control limits for T_y^2, T_o^2, T_r^2 can be obtained using an F-distribution.[22] On the other hand, the control limit for Q is calculated using a χ^2 distribution[22] on the assumption that a residual vector is multivariate normal.

For D-statistics, $\Lambda_y = \frac{1}{n-1}\mathbf{t}_y^T\mathbf{t}_y$ is the variance of t_y which is estimated by the training samples. Λ_o and Λ_r are the covariance matrices of $\mathbf{t}_o$ and $\mathbf{t}_r$. $F_{1,n-1,\alpha}$ means the value of F-distribution with 1 and $n - 1$ degrees at the significance level α. For the Q-statistic, $g = S/2\mu$ and $h = 2\mu^2/S$ are estimated based on the matching moments between a $g\chi_h^2$ distribution and the reference distribution of Q_r, where μ is the sample mean of Q_r and S is the sample variance of Q_r. $g\chi_{h,\alpha}^2$ is the critical value of the χ^2 variable with scaling factor g and h degrees of freedom at significance level α. If the statistics of the new sample fall into these limits, the process is considered to be in control statistically.

Table 6. T-PLS Model, A_y = 1, A = 2, A_r = 1

$\mathbf{p}_y$	$\mathbf{P}_o$	$\mathbf{P}_r$	$\tilde{\mathbf{P}}_r$	
0.3303	−0.7128	−0.3811	−0.4606	0.2226
0.3504	0.5771	0.3785	−0.7435	−0.1657
0.6144	−0.0263	0.5892	0.4203	−0.0251
0.6390	0.3194	−0.5626	0.2395	0.0837
0.0560	−0.2371	−0.2189	0.0315	−0.9567

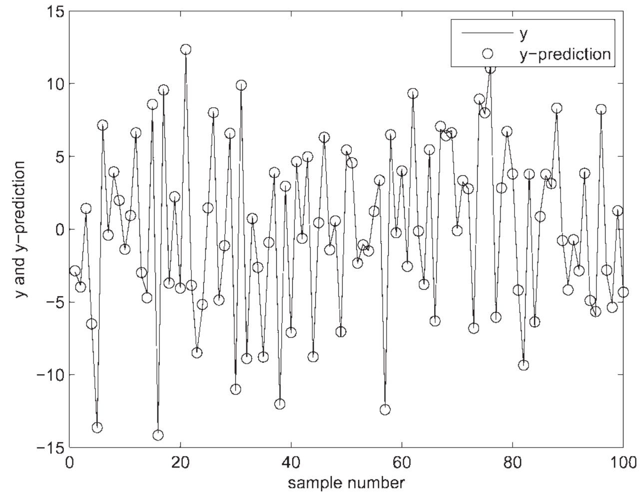

Figure 2. T-PLS model of *y*.

From Figure 1 and Table 4, we can state the relation between PLS and T-PLS. PLS-based monitoring method uses T^2 to detect the faults related to **y**, but T^2 also detects faults in S_o which is orthogonal to **Y** so that it will cause more false alarms. On the other hand, faults in S_r may also affect **y**, which are not detected by T^2, thus it will miss more alarms. In T-PLS, we use T_y^2 and Q_r together to detect faults related to y, which helps to reduce rates of missing alarms and false alarms in most cases. Furthermore, PLS-based method uses Q to detect faults unrelated to y, which cannot monitor faults in S_o. In T-PLS, T_o, T_r, and Q_r are used together to detect faults unrelated to **y**, which covers all the faults unrelated to **y**. Q_r may detect incipient faults compared with Q, because Q_r has little variance in normal situations.

O-PLS has the same decomposition of **T** as T-PLS. However, as a preprocessing method, it drops the information of S_o. Besides, it does not decompose the residual of PLS

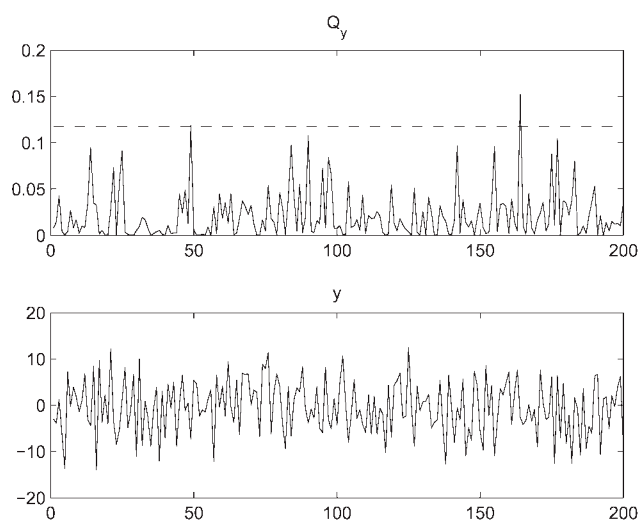

Figure 3. When fault only occurs in S_o, *y* is not affected.

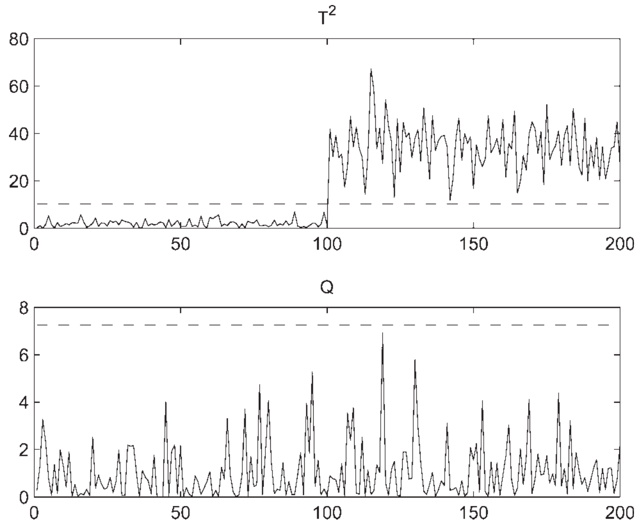

Figure 4. PLS based monitoring when fault occurs in S_o only, $f = 3$.

further. Therefore, if one uses O-PLS to monitor the process, one in fact monitors faults related to **y** by $T_{\mathbf{y}}^2$ of T-PLS and monitors faults unrelated to **y** by Q of PLS.

Case Study on Simulation Examples

To demonstrate the effectiveness of T-PLS for fault detection, two simulation examples are used.

A numerical example

We first consider a synthetic numerical example without feedback as follows.

$$\begin{cases} \mathbf{x}_k = \mathbf{A}\mathbf{z}_k + \mathbf{e}_k \\ y_k = \mathbf{C}\mathbf{x}_k + \upsilon_k \end{cases} \tag{35}$$

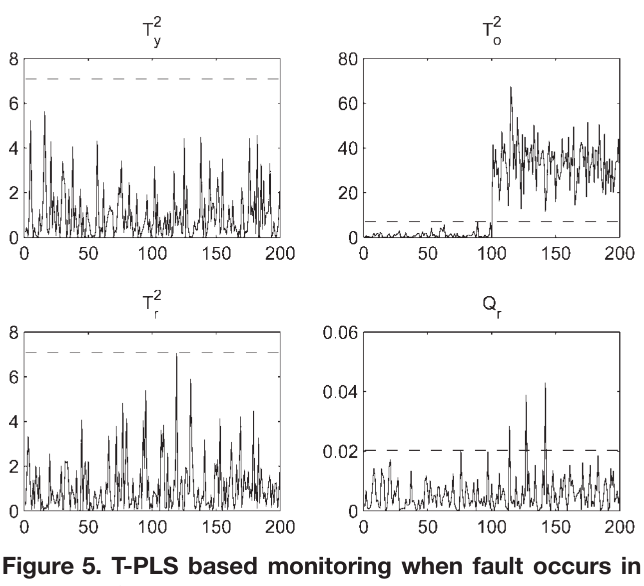

Figure 5. T-PLS based monitoring when fault occurs in S_o only, $f = 3$.

Table 7. False Alarm Rates of Faults Unrelated to y (%)

F	PLS (T^2)	$T-$PLS (T_y^2or Q_r)	PCA (T^2)	PCA (Q)
1	12.0	2.8	8	2.3
2	74.4	1.4	68.9	1.1
3	99.8	2.0	98.9	1.7

where

$$\mathbf{z}_k \in \mathbb{R}^{\mathbf{3}}, z_{k,i} \sim \mathbf{U}([0,1])(i=1,2,3),$$

$$\mathbf{A} = \begin{pmatrix} 1 & 3 & 4 & 4 & 0 \\ 3 & 0 & 1 & 4 & 1 \\ 1 & 1 & 3 & 0 & 0 \end{pmatrix}^T, \mathbf{e}_k \in \mathbb{R}^{\mathbf{5}},$$

$$e_{k,j} \sim \mathbf{N}(0, 0.05^2)\ (j=1,\ldots,5),$$

$$\upsilon_k \sim \mathbf{N}(0, 0.1^2), \mathbf{C} = (2\,2\,1\,1\,0)$$

U([0,1]) means the uniform distribution in the interval [0,1], and **N**(μ, σ^2) means the normal distribution with mean μ and variance σ^2. A fault is added in the following form:

$$\mathbf{x}_k = \mathbf{x}_k^* + \Xi f \tag{36}$$

where **x*** is the normal value without fault, produced by (35), Ξ is the fault direction vector, and f is the fault magnitude.

We use 100 samples under normal operation condition to perform a PLS model ($A = 2$) on (**X**,**y**). The PLS components number $A = 2$ is determined using cross validation, which offers a good prediction of y. PLS matrices are listed in Table 5.

Then we perform the T-PLS1 algorithm based on the PLS. As y is single, $A_y = 1$. We choose $A_r = 1$ for the number of components uncorrelated to y. The T-PLS matrices are shown in Table 6, where $\tilde{\mathbf{P}}_r \in \mathbb{R}^{m \times m-A-A_r}$ is the matrix of basis vectors of S_{rr}, which consists of all left singular vectors of $(\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^{\mathbf{T}})$ related to nonzero singular values.

T-PLS has the same prediction as PLS. Output y is estimated by the model (10) and shown in Figure 2. One hundred faulty samples, produced by (36), are used for fault detection per time. We compare the fault detection using standard PLS and T-PLS, under various fault cases. In the

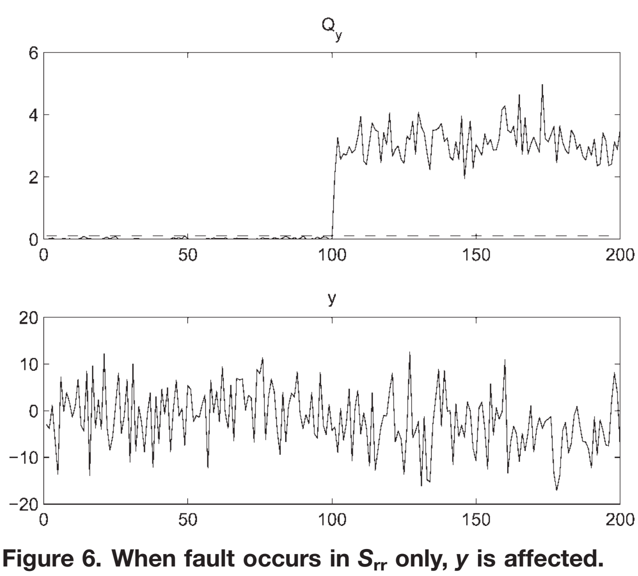

Figure 6. When fault occurs in S_{rr} only, y is affected.

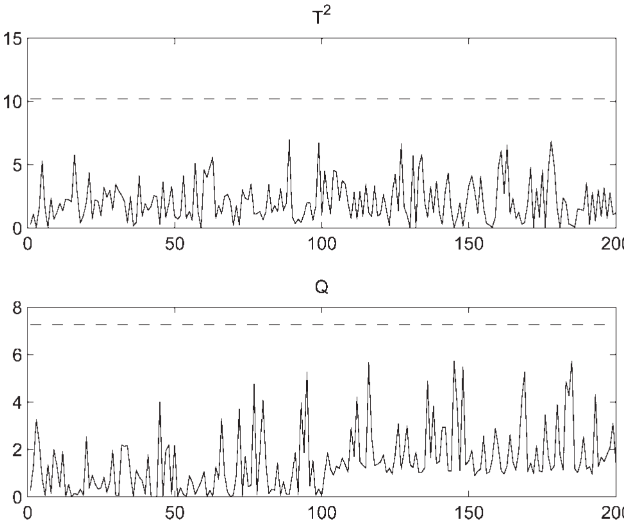

Figure 7. PLS based monitoring when fault occurs in S_{rr} only, $f = 1$.

following figures, the first 100 samples are normal samples and the last 100 samples are faulty samples. Moreover, to show the relation of PCA and T-PLS, T^2 and Q statistics in PCA are also involved in the comparisons.

To reflect whether the fault affects the output y, another Q-statistic of Y-residual **F** is defined as follows:

$$Q_y = \|y - \hat{y}\|^2 \sim g\chi^2_{h,\alpha} \quad (37)$$

$g\chi^2_{h,\alpha}$ is the control limit, where the calculation is similar as Q_r. This statistic is used for the classification of faults but not for fault detection.

Fault Occurs in S_o Only. Let $\Xi = \mathbf{p}_o$, thus the fault occurs in S_o only. It is observed from Figure 3 that this fault does not affect y. Figures 4 and 5 show the fault detection results using PLS and T-PLS, respectively, with $f = 3$. PLS based methods alarm in T^2, whereas T-PLS based statistics alarm in T_o^2 but

Table 8. Fault Detection Rates of Faults Related to y (%)

f	PLS (T^2)	$T-$PLS (T_y^2 or Q_r)	PCA (T^2)	PCA (Q)
1	0	100	0	100
2	0	100	0	100
3	0	100	0	100

does not alarm in T_y^2. The results of the simulation indicate that T-PLS could tell the faults related to **Y** from the faults unrelated to **Y**. This property holds regardless of the fault magnitude, as shown in Table 7. Therefore, T_y^2 in T-PLS could reduce the false alarm rate of the faults unrelated to y. Furthermore, it is observed that this kind of fault could be detected by T^2 but not by Q in PCA-based monitoring.

Fault Occurs in S_{rr} Only. Let Ξ be the first column of $\mathbf{P}_r$, thus the fault occurs in S_{rr} only. It is observed in Figure 6 that faults in S_{rr} break the old correlation between **X** and **y,** which shows y is affected by this fault. When $f = 1$, PLS-based methods could not detect faults as shown in Figure 7, whereas T-PLS based statistic Q_r detects faults sensitively as shown in Figure 8. Table 8 lists the fault detection rates under different fault magnitudes. The results of simulation show T-PLS based policy could improve the detection rate in this case, compared with PLS-based policy. It is observed further that this fault could be detected by Q but not detected by T^2 in PCA-based monitoring.

Fault Occurs in S_y Only. Let $\Xi = \mathbf{p}_y$, thus fault occurs in S_y only. This fault affects y, but not affects *y*-residual as shown in Figure 9. Table 9 lists the fault detection rates based on PLS, T-PLS, and PCA structure. The results of the simulation indicate that T-PLS based method gives higher fault detection rates than PLS for this kind of fault. From Table 9, it is observed that the fault could be detected by T^2 but not detected by Q in PCA-based methods.

Fault Occurs in S_{rp} Only. Let $\Xi = \mathbf{P}_r$, thus fault occurs in S_p only. This fault does not affect y as shown in Figure 10. It is observed that both T-PLS and PLS based fault detection does not alarm using T_y^2 and T^2, respectively, in Table 10. Moreover, this fault is observed to be detected by T^2 but not detected by Q in PCA-based methods.

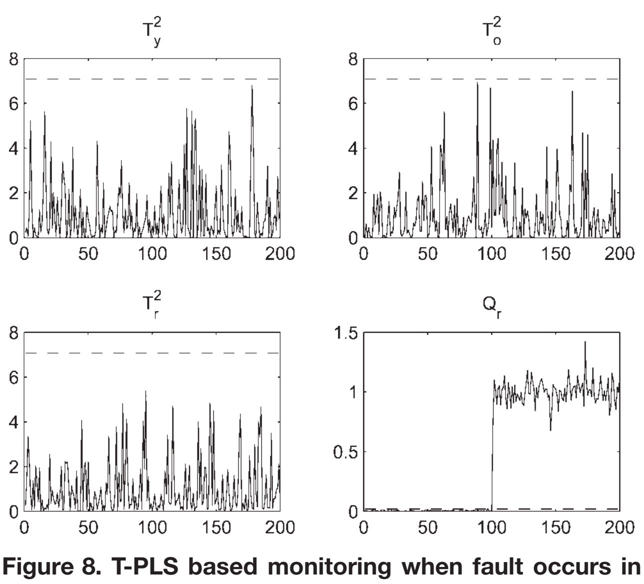

Figure 8. T-PLS based monitoring when fault occurs in S_{rr} only, $f = 1$.

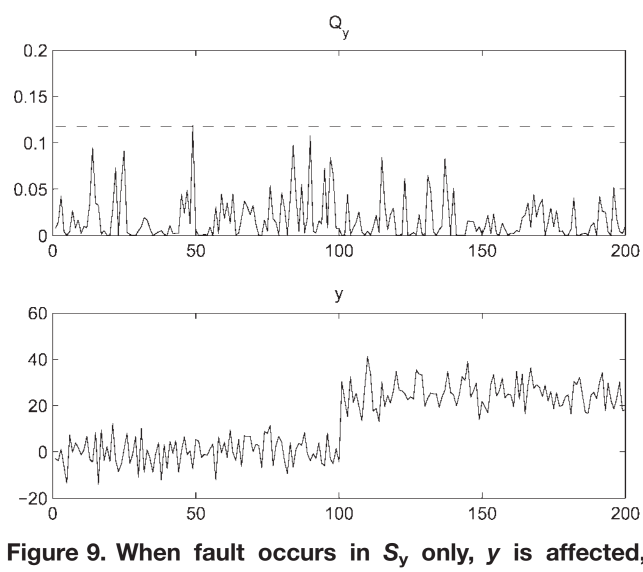

Figure 9. When fault occurs in S_y only, y is affected, $f = 10$.

Table 9. Fault Detection Rates of Faults Related to y (%)

f	PLS (T^2)	$T-$PLS (T_y^2 or Q_r)	PCA (T^2)	PCA (Q)
2	0.5	4.8	0	2.1
4	7.8	19.7	4.7	2.7
6	34.2	45.8	29.7	1.5
8	64.9	76.3	59.5	1.5
10	86.4	94.1	83.7	2.0

In this simulation, PLS used T^2 to monitor the faults related to y, whereas T-PLS used T_y^2 and Q_r to monitor the faults related to y. It was observed in the numerical examples that for faults related to y, which might be in S_y and S_{rr}, T-PLS produced a higher fault detection rate than PLS under the same fault magnitude. For faults in S_o, T-PLS was observed to have lower false alarm rate than PLS. From the simulations, T-PLS seems better than PLS for monitoring the faults related to y.

From the simulation, it is also observed that T^2 monitors S_y, S_o, S_{rp} together approximately, and Q monitors the S_{rr} approximately. That is because PCA-based monitoring method only tells whether there is a fault, but not sure whether the fault affects quality data. T^2 statistic in PCA monitors the systematic variations in the process and Q statistic monitors the residual part in process which has small variance.

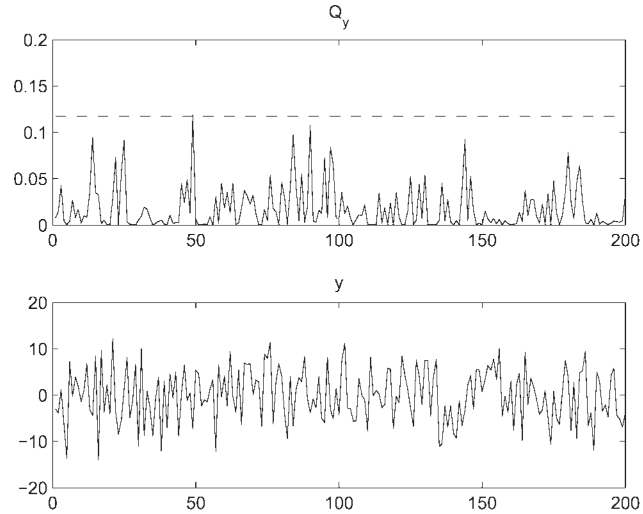

Figure 10. When fault occurs in S_{rp} only, y is not affected, $f = 5$.

Tennessee Eastman Benchmark

The Tennessee Eastman Process (TEP) was created by the Eastman Chemical Company to provide a realistic industrial process for evaluating process control and monitoring methods.[23] The process consists of five major units: a reactor, condenser, compressor, separator, and stripper; and it contains eight components: A, B, C, D, E, F, G, and H. The gaseous reactants A, C, D, and E and the inert B are fed to the reactor where the liquid products G and H are formed. The species F is a by-product of the reactions. The reactions in the reactor are:

$$\begin{aligned} A(g)+C(g)+D(g) &\rightarrow G(\text{liq}) \\ A(g)+C(g)+E(g) &\rightarrow H(\text{liq}) \\ A(g)+E(g) &\rightarrow F(\text{liq}) \\ 3D(g) &\rightarrow 2F(\text{liq}) \end{aligned} \tag{38}$$

The detailed description of the process can be found in Chapter 8 of Chiang et al.[24] The process used here is operated under closed-loop control. The simulation code for the TEP in closed loop can be found on the web site http://brahms.scs.uiuc.edu. TEP has been widely used as a benchmark process for evaluating the process diagnosis methods such as PCA, multiway PCA, support vector machine, and Fisher discriminant analysis (FDA). PLS-based methods were also applied to the TEP.[25–27] Chiang et al. reviewed the fault detection and diagnosis method of the multivariate statistics such as PCA, FDA, PLS, and canonical variate analysis (CVA) and compared them using the case study of TEP.[26]

Model and Fault Description. The TEP contains two blocks of variables: the XMV block of 12 manipulated variables and XMEAS block of 41 measured variables. Process measurements are sampled with interval of 3 min. Nineteen composition measurements are sampled with time delays that vary from 6 min to 15 min. This time delay has a potentially critical impact on product quality control within the plant.[25] It implies that the fault effect on product quality cannot be detected until the next sample of **Y** is available. During this time, the products are produced with uncontrolled quality. PLS-based monitoring methods can detect the fault more correlated to **Y** compared with PCA, thus received wide applications in industrial cases. There are 15 known faults in TEP.[24] Faults 1–7 are associated with step changes in a process variable, e.g., in the cooling water inlet temperature. Faults 8–12 are associated with an increase in the variability of some process variables. Fault 13 is a slow drift in the reaction kinetics. Faults 14–15 are associated with sticking valves.

In this study, the component G in stream 9, i.e., XMEAS (35), is chosen as quality variable y with a time delay of 6

Table 11. Fault Detection Rate of TEP Using PLS, O-PLS, and T-PLS (%)

Process Faults with Known Cause			Fault Detection Rate		
Faults ID	Fault Description	Type	PLS	O-PLS	T-PLS
IDV (1)	A/C Feed Ratio, B Composition constant (Stream 4)	Step	81.4	14.4	99.3
IDV (2)	B composition A/C Ration Constant (Streams 4)	Step	98.0	85.8	97.0
IDV (5)	Condenser cooling water inlet temperature	Step	29.6	15.5	99.5
IDV (6)	A Feed Loss Step (Stream 1)	Step	99.4	97.3	99.8
IDV (8)	A, B, C Feed composition (Stream 4)	Random Variation	96.5	66.9	93.4
IDV (10)	C Feed temperature	Random Variation	72.9	33.8	79.1
IDV (12)	condenser cooling water inlet temperature	Random Variation	98.3	70.9	95.6
IDV (13)	Reaction kinetics	Slow drift	94.1	80.5	95.3

Table 12. False Alarm Rate for TEP Using PLS, O-PLS, and T-PLS (%)

Process Faults with Known Cause			Fault Alarm Rate		
Faults ID	Fault Description	Type	PLS	O-PLS	T-PLS
IDV (0)	Normal situation	–	9.8	3.6	5.6
IDV (3)	D Feed Temperature (Stream 2)	Step	10.3	3.8	5.9
IDV (4)	Reactor cooling water inlet temperature	Step	51.8	16.5	33.5
IDV (9)	D Feed temperature	Random variation	7.9	3.6	5.3
IDV (11)	Reactor cooling water inletting water inlet temperature	Random variation	47.3	18.1	32.3
IDV (15)	Condenser cooling water valve	Sticking	6.8	3.1	5.0

min. 22 process measurements and 11 manipulated variables, i.e., XMEAS (1–22) and XMV (1–11), are chosen as **X**. We use 480 normal samples to build a PLS and T-PLS model. First, the samples are centered to zero mean and scaled to unit variance. Six components are kept for PLS according to cross validation. A_y is set to 1 for single output y and $A_r = 17$ is selected according to PCA-based methods.

Fault Detection Using PLS and T-PLS. Here we use 13 faulty sample sets and one normal sample set for fault detection. Each set consists of 960 samples. It is difficult to compare PLS and T-PLS in TEP because faults might take place in all subspaces of T-PLS. Thus it is necessary to identify whether a kind of fault is related to y or not. Thus we use output y and Q_y as the classifiers. If y is affected by the fault, output y or Q_y exceeds the corresponding control limit. Let n_y represent the number of faulty samples which affect y and n_t represent the total number of faulty samples. The fault is considered to be related to y if $n_y/n_t > 0.1$. According to this criterion, eight faults are related to y, while five faults are unrelated to y. The normal situation without any faults is regarded as the latter. The detection of faulty samples related to y is an effective alarm, whereas the detection of faulty samples unrelated to y is considered as a false alarm. Tables 11 and 12 list the fault detection rates and false alarm rates using PLS and T-PLS of 14 faults.

From Tables 11 and 12, we observe that T-PLS has higher detection rates and lower false alarm rates than PLS in most simulated cases. In a few cases (e.g., IDV 2 and 8), PLS has a marginally higher detection rate. Moreover, the results show that O-PLS has lower detection rates for faults related and unrelated to y than other two methods. It is because O-PLS does not separate the different variations of **X** appropriately according to the fault effect on y.

Conclusions

In this article, the T-PLS algorithm is proposed. The purpose of T-PLS is to acquire a further decomposition on **X**-space, which is more suitable for process monitoring. The T-PLS is proven to be an oblique space decomposition of **X**-Space. The properties of each subspace in T-PLS are analyzed in detail, including the relationships between T-PLS and O-PLS methods.

Table 10. False Alarm Rates of Faults Unrelated to y (%)

f	PLS (T^2)	$T-$PLS(T_y^2 or Q_r)	PCA (T^2)	PCA (Q)
2	0	2	10.8	1.3
4	0	2.4	72.2	1.9
6	0	3	99.5	2.7

The statistical process monitoring methods based on T-PLS are developed to monitor the process operating performance. Both theoretical analysis and simulation results show better performance of T-PLS than PLS and O-PLS. For faults related to quality variables **Y,** T-PLS based methods can give lower false alarm rate and missing alarm rate than PLS-based methods in most simulated cases.

Acknowledgments

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Notation

A = number of PLS components that are used
A_y = number of **Y**-related principal components in T-PLS
A_r = number of **Y**-unrelated components in T-PLS
$\mathbf{X} \in \mathbb{R}^{n \times m}$ = matrix of process data (m process variables and n samples)
$\mathbf{Y} \in \mathbb{R}^{n \times p}\ y \in \mathbb{R}^{n \times 1}$ = matrix of quality data (p quality variables and n samples)
$\mathbf{P} \in \mathbb{R}^{m \times A}\mathbf{p} \in \mathbb{R}^{m \times 1}$ = loading matrix (vector) for X in PLS
$\mathbf{Q} \in \mathbb{R}^{p \times A}\mathbf{q} \in \mathbb{R}^{1 \times A}$ = loading matrix (vector) for Y in PLS
$\mathbf{W} \in \mathbb{R}^{m \times A}$ = weights matrix (vector) for deflated **X** in PLS
$\mathbf{R} \in \mathbb{R}^{m \times A}$ = weights matrix (vector) for original **X** in PLS
$\mathbf{T} \in \mathbb{R}^{n \times A}$ = score matrix in PLS
$\mathbf{E} \in \mathbb{R}^{n \times m}$ = residual matrix for **X** in PLS
$\mathbf{F} \in \mathbb{R}^{n \times p}$ = residual matrix for **Y** in PLS
$\mathbf{Q}_y \in \mathbb{R}^{p \times A_y}$ = regression coefficient for T-PLS2
$\mathbf{T}_y \in \mathbb{R}^{n \times A_y}\mathbf{t_y} \in \mathbb{R}^{n \times 1}$ = score matrix (vector) of Y-related part in **T**
$\mathbf{T}_o \in \mathbb{R}^{n \times A - A_y}$ = score matrix of Y-orthogonal part in **T**
$\mathbf{T}_r \in \mathbb{R}^{n \times A_r}$ = score matrix of Y-unrelated part in **E**
$\mathbf{P}_y \in \mathbb{R}^{m \times A_y}\mathbf{p_y} \in \mathbb{R}^{m \times 1}$ = loading matrix (vector) for Y-related part of **X** in T-PLS
$\mathbf{P}_o \in \mathbb{R}^{m \times A - A_y}$ = loading matrix (vector) for Y-related part of **T** in T-PLS
$\mathbf{P}_r \in \mathbb{R}^{m \times A_r}$ = loading matrix (vector) for Y-related part of **T** in T-PLS
$\mathbf{E}_r \in \mathbb{R}^{n \times m}$ = residual matrix for **X** in T-PLS

Literature Cited

1. Wise BM, Gallagher NB. The process chemometrics approach to process monitoring and fault detection. *J Process Control*. 1996;6:329–348.
2. Qin SJ. Statistical process monitoring: basics and beyond. *J Chemom*. 2003;17:480–502.
3. Lu N, Yao Y, Gao F, Wang F. Two-dimensional dynamic PCA for batch process monitoring. *AIChE J*. 2005;51:3300–3304.
4. Lee J, Qin S, Lee I. Fault detection and diagnosis based on modified independent component analysis. *AIChE J*. 2006;52:3501–3514.
5. Shi J, Liu X. Product quality prediction by a neural soft-sensor based on MSA and PCA. *Int J Autom Comput*. 2006;3:17–22.
6. Harkat M, Djelel S, Doghmane N, Benouaret M. Sensor fault detection, isolation and reconstruction using nonlinear principal component analysis. *Int J Autom Comput*. 2007;4:149–155.

7. MacGregor JF, Jaeckle C, Kiparissides C, Koutoudi M. Process monitoring and diagnosis by multiblock PLS methods. *AIChE J*. 1994;40:826–838.
8. Khan A, Moyne J, Tilbury D. Virtual metrology and feedback control for semiconductor manufacturing processes using recursive partial least squares. *J Process Control*. 2008;18:961–974.
9. Kaneko H, Arakawa M, Funatsu K. Development of a new soft sensor method using independent component analysis and partial least squares. *AIChE J*. 2009;55:87–98.
10. Alcala C, Qin S. Reconstruction-based contribution for process monitoring. *Automatica*. 2009;45:1593–1600.
11. Nelson PRC, Taylor PA, MacGregor JF. Missing data methods in PCA and PLS: score calculations with incomplete observations. *Chemom Intell Lab Syst*. 1996;35:45–65.
12. Westerhuis JA, Gurden SP, Smilde AK. Generalized contribution plots in multivariate statistical process monitoring. *Chemom Intell Lab Syst*. 2000;51:95–114.
13. Choi SW, Lee IB. Multiblock PLS-based localized process diagnosis. *J Process Control*. 2005;15:295–306.
14. Li G, Qin SJ, Zhou DH. Geometric properties of partial least squares for process monitoring. *Automatica*. In press.
15. Wold S, Antti H, Lindgren F, Öhman J. Orthogonal signal correction of near-infrared spectra. *Chemom Intell Lab Syst*. 1998;44:175–185.
16. Fearn T. On orthogonal signal correction. *Chemom Intell Lab Syst*. 2000;50:47–52.
17. Trygg J, Wold S. Orthogonal projections to latent structures (O-PLS). *J Chemom*. 2002;16:119–128.
18. Dayal BS, MacGregor JF. Improved PLS algorithms. *J Chemom*. 1997;11:73–85.
19. De Jong S. SIMPLS: an alternative approach to partial least squares regression. *Chemom Intell Lab Syst*. 1993;18:251–263.
20. Qin SJ, Dunia R. Determining the number of principal components for best reconstruction. *J Process Control*. 2000;10:245–250.
21. Verron T, Sabatier R, Joffre R. Some theoretical properties of the O-PLS method. *J Chemom*. 2004;18:62–68.
22. Nomikos P, Macgregor JF. Multivariate SPC Charts for Monitoring Batch Processes. *Technometrics*. 1995;37:41–59.
23. Downs JJ, Vogel EF. A plant-wide industrial process control problem. *Comput Chem Eng*. 1993;17:245–255.
24. Chiang LH, Russell E, Braatz RD.*Fault Detection and Diagnosis in Industrial Systems*. London: Springer, 2001.
25. Wilson DJH, Irwin GW. PLS modelling and fault detection on the Tennessee Eastman benchmark. In: American Control Conference, 1999. Proceedings of the 1999. Vol. 6. 1999:3975–3979.
26. Chiang LH, Russell EL, Braatz RD. Fault diagnosis in chemical processes using Fisher discriminant analysis, discriminant partial least squares, and principal component analysis. *Chemom Intell Lab Syst*. 2000;50:243–252.
27. Lee G, Han CH, Yoon ES. Multiple-fault diagnosis of the Tennessee Eastman process based on system decomposition and dynamic PLS. *Ind Eng Chem Res*. 2004;43:8037–8048.

Appendix A: X-deflated PLS algorithm

Center the columns of **X, Y** to zero mean and scale them to unit variance. Set $i = 1$ and $\mathbf{X}_1 = \mathbf{X}$.

(1) Set $\mathbf{u}_i$ to any column of **Y**.
(2) $\mathbf{w}_i = \mathbf{X}_i^T \mathrm{u}_i / \| \mathbf{X}_i^T \mathrm{u}_i \|$.
(3) $\mathbf{t}_i = \mathbf{X}_i \mathbf{w}_i$.
(4) $\mathbf{q}_i = \mathbf{Y}^T \mathbf{t}_i / \mathbf{t}_i^T \mathbf{t}_i$.
(5) $\mathbf{u}_i = \mathbf{Y}\mathbf{q}_i$. If $\mathbf{t}_i$ converges, go to Step vi, else return to Step ii.
(6) $\mathbf{p}_i = \mathbf{X}^T \mathbf{t}_i / \mathbf{t}_i^T \mathbf{t}_i$.
(7) $\mathbf{X}_{i+1} = \mathbf{X}_i - \mathbf{t}_i \mathbf{p}_i^T$. Set $i = i + 1$ and return to step i. Terminate if $i > A$.

Appendix B: Proof of Lemma 5

Proof: First, we show the matrices $\mathbf{C}_i$ ($i = 1, 2, 3, 4$) are all idempotent. Noting (4) and the following equations from the properties of T-PLS

$$\mathbf{q}\mathbf{R}^T\mathbf{p}_y = \mathbf{q}\mathbf{R}^T\mathbf{P}\mathbf{T}^T\mathbf{t}_y/(\mathbf{t}_y^T\mathbf{t}_y) = 1$$

$$(\mathbf{I} - \mathbf{P}\mathbf{R}^T)\mathbf{P}_r\mathbf{P}_r^T = \mathbf{P}_r\mathbf{P}_r^T$$

Thus, we can get

$$\mathbf{C}_1^2 = \mathbf{p}_y\mathbf{q}\mathbf{R}^T\mathbf{p}_y\mathbf{q}\mathbf{R}^T = \mathbf{p}_y\mathbf{q}\mathbf{R}^T = \mathbf{C}_1 \quad \text{(B1)}$$

$$\begin{aligned}\mathbf{C}_2^2 &= (\mathbf{P} - \mathbf{p}_y\mathbf{q})\mathbf{R}^T(\mathbf{P} - \mathbf{p}_y\mathbf{q})\mathbf{R}^T \\ &= (\mathbf{P} - \mathbf{p}_y\mathbf{q})(\mathbf{I} - \mathbf{R}^T\mathbf{p}_y\mathbf{q})\mathbf{R}^T \\ &= (\mathbf{P} - \mathbf{p}_y\mathbf{q} - \mathbf{P}\mathbf{R}^T\mathbf{p}_y\mathbf{q} + \mathbf{p}_y\mathbf{q})\mathbf{R}^T \\ &= (\mathbf{P} - \mathbf{p}_y\mathbf{q})\mathbf{R}^T = \mathbf{C}_2\end{aligned} \quad \text{(B2)}$$

$$\begin{aligned}\mathbf{C}_3^2 &= \mathbf{P}_r\mathbf{P}_r^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T)\mathbf{P}_r\mathbf{P}_r^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T) \\ &= \mathbf{P}_r\mathbf{P}_r^T\mathbf{P}_r\mathbf{P}_r^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T) = \mathbf{C}_3\end{aligned} \quad \text{(B3)}$$

$$\begin{aligned}\mathbf{C}_4^2 &= (\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^T)(\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^T) \\ &= (\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^T - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^T) \\ &= (\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^T) = \mathbf{C}_4\end{aligned} \quad \text{(B4)}$$

The above results indicate $\mathbf{C}_i$ (i = 1–4) are all projection matrices and their range spaces are all projection subspaces. Furthermore, $\mathbf{C}_i$s have the following relationships:

$$\mathbf{C}_1\mathbf{C}_2 = \mathbf{p}_y\mathbf{q}\mathbf{R}^T(\mathbf{P} - \mathbf{p}_y\mathbf{q})\mathbf{R}^T = (\mathbf{p}_y\mathbf{q} - \mathbf{p}_y\mathbf{q})\mathbf{R}^T = 0 \quad \text{(B5)}$$

$$\begin{aligned}\mathbf{C}_1\mathbf{C}_3 &= \mathbf{p}_y\mathbf{q}^T\mathbf{R}^T\mathbf{P}_r\mathbf{P}_r^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T) \\ &= \mathbf{p}_y\mathbf{q}^T\mathbf{R}^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T)\mathbf{P}_r\mathbf{P}_r^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T) \\ &= 0\end{aligned} \quad \text{(B6)}$$

$$\begin{aligned}\mathbf{C}_1\mathbf{C}_4 &= \mathbf{p}_y\mathbf{q}\mathbf{R}^T(\mathbf{I} - \mathbf{P}_r\mathbf{P}_r^T)(\mathbf{I} - \mathbf{P}\mathbf{R}^T) \\ &= \mathbf{p}_y\mathbf{q}\mathbf{R}^T(\mathbf{I} - \mathbf{P}\mathbf{R}^T) - \mathbf{C}_1\mathbf{C}_3 = 0\end{aligned} \quad \text{(B7)}$$

Other properties can be proven in a similar way. The whole relationships can be summarized as:

$$\mathbf{C}_i\mathbf{C}_j = \mathbf{C}_j\mathbf{C}_i = 0 \quad (i \neq j) \quad \text{(B8)}$$

Furthermore, the sum of $\mathbf{C}_i$ satisfies the following equation:

$$\mathbf{C}_1 + \mathbf{C}_2 + \mathbf{C}_3 + \mathbf{C}_4 = \mathbf{P}\mathbf{R}^T + (\mathbf{I} - \mathbf{P}\mathbf{R}^T) = \mathbf{I} \quad \text{(B9)}$$

It can be concluded that S_y, S_o, S_p, S_r are not overlapped and form the whole **X**-space. ■

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