Quality-Relevant Monitoring and Diagnosis with Dynamic Concurrent Projection to Latent Structures

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Abstract:

In this paper, a data-driven dynamic concurrent projection to latent structures (DCPLS) approach is proposed for quality-relevant fault diagnosis of dynamic processes. First, a novel DCPLS algorithm is proposed for dynamic modeling which captures the dynamic correlations between quality variables and process variables. Quality-specific variations, process-specific variations, and quality-process covariations of dynamic processes are monitored respectively. Secondly, a multi-block extension of DCPLS is designed to compute the contributions according to block partition of the lagged variables, in order to help localize faults. Finally, the application results on strip-thickness relevant fault diagnosis for a practical cold rolling continuous annealing process (CAP) demonstrate the effectiveness of the proposed methods.

Keywords: Dynamic concurrent projection to latent structures, Dynamic process modeling, Fault diagnosis.

1. INTRODUCTION

Data-driven multivariate statistical process monitoring have gained many applications in industrial processes (Qin, 2012; Qin and Zheng, 2013; Zhang and Dudzic, 2006; Kresta et al., 1991; Wise and Gallagher, 1996). They provide an easy way to model correlations between process data (\mathbf{X}) and quality data (\mathbf{Y}) from historical data by projecting the original data into reduced-dimensional latent variables. The principal component analysis (PCA) and projection to latent structures (PLS) algorithms are most commonly used. While PCA-based methods monitor the faults appear in the process variables, PLS-based methods pay more attentions on the quality-relevant faults.

But traditional PLS-based monitoring method in Kresta et al. (1991) divides the measured space in similar way as PCA to have two oblique subspaces, i.e. principal latent subspace and residual subspace. The principal latent subspace includes variations orthogonal to quality which have no contribution to predict quality, meanwhile the residual subspace may be large which makes the corresponding statistic inappropriate. Consequently, total PLS (TPLS) is proposed by further dividing the latent subspace and residual subspace. TPLS-based monitoring, however, uses unnecessary four subspaces for process data (\mathbf{X}) , and leaves some quality variations unpredicted from process variables unmonitored. Concurrent PLS (CPLS) is thus proposed in Qin and Zheng (2013) to give a more comprehensive decomposition of the data space. For a comprehensive treatment and for references to the extensive literature on the subject one may refer to Yin et al. (2012), Qin (2012), and Ding (2012).

The PLS, TPLS as well as CPLS models only reveal static relations between \mathbf{X} and \mathbf{Y} . When the process and quality variables exhibit autocorrelations or dynamic correlations, the normal range defined by these static methods is usually too large to make a high rate of missed detections. Dynamic extensions are straightforward to include a number of lagged values of \mathbf{X} and \mathbf{Y} when deriving the latent structures from the data. For example, the dynamic version of PCA in Ku et al. (1995) modeled the lagged values, and the one in Qin and McAvoy (1996) modeled the lagged values of both \mathbf{X} and \mathbf{Y} . Some other work which did not involve lagged data are also discussed in Kaspar and Ray (1993), and Lakshminarayanan et al. (1997).

The above methods focus on deriving the dynamics relationship between \mathbf{X} and \mathbf{Y} , rather than provide a statistical model for process monitoring. Recent literature of Li et al. (2011b) extended TPLS to dynamic version to achieve a more comprehensive monitoring. But it suffers from the defects similar to the ones in TPLS. Further, while the existing work mainly focuses on process monitoring, they cannot pinpoint the abnormal variables contributed to the fault.

In this paper, we propose a new dynamic CPLS (DCPLS) algorithm to capture the dynamic correlations and autocorrelations between **X** and **Y**. The DCPLS algorithm leads to two new subspaces. One is quality-irrelevant process dynamic variations, the other denotes quality-relevant process-irrelevant dynamic variations. In addition, it is well-known that contribution plot is an effective tool in fault diagnosis used to localize the faulty variables. But for the dynamic modeling version, the column dimensions of augmented process data with the lagged values are usually large. It will display a large number of contributions, which makes it difficult to localize the faulty variables. Consequently, DCPLS is extended to multi-block DCPLS while the original variable and the lagged values are incorporated into a single block.

This paper is organized as follows. In Section 2, dynamic CPLS modeling and monitoring method is proposed. Then the DCPLS method is extended to multi-block DCPLS to help localize the faulty variable in Section 3. In Section 4, the proposed methods are applied to a practical continuous annealing process. Finally, conclusions are summarized and further work is discussed in Section 5.

2. DYNAMIC CONCURRENT PLS MODELING AND MONITORING

2.1 Concurrent PLS Modeling

The data collected are $\mathbf{X} \in \mathbb{R}^{n \times m}$ and $\mathbf{Y} \in \mathbb{R}^{n \times p}$, where $\mathbf{X} \in \mathbb{R}^{n \times m}$ consists of *n* samples with *m* process variables and $\mathbf{Y} \in \mathbb{R}^{n \times p}$ consists of *n* samples with *p* output variables. After mean-centering and variance scaling, the partial least squares decomposition is used to project \mathbf{X} and \mathbf{Y} to low dimensional spaces (MacGregor et al., 1994)

$$\begin{cases} \mathbf{X} = \mathbf{T}\mathbf{P}^T + \mathbf{E} \\ \mathbf{Y} = \mathbf{T}\mathbf{Q}^T + \mathbf{F} \end{cases}$$
(1)

where $\mathbf{T} \in \Re^{n \times A}$ is score matrix, $\mathbf{P} \in \Re^{m \times A}$ and $\mathbf{Q} \in \Re^{p \times A}$ are loading matrices, A is the number of latent variables, and \mathbf{E} and \mathbf{F} denote the residuals for \mathbf{X} and \mathbf{Y} , respectively.

In PLS, the latent subspace \mathbf{T} contains variations orthogonal to \mathbf{Y} . Furthermore, because the PLS algorithm does not capture input variations in a descending order, the residual subspace \mathbf{E} may include some large variations. To overcome the problems, CPLS decomposes the unpredicted output variations into two separate subspaces, and combines the output-irrelevant part in the PCS and the RS into one subspace relevant to inputs only (Qin and Zheng, 2013; Qin, 2012). The CPLS algorithm is seen as follows (Qin and Zheng, 2013),

$$\begin{cases} \mathbf{X} = \mathbf{T}_c \mathbf{P}_c^T + \widetilde{\mathbf{X}}_c = \mathbf{T}_c \mathbf{P}_c^T + \mathbf{T}_x \mathbf{P}_x^T + \widetilde{\mathbf{X}} \\ \mathbf{Y} = \mathbf{T}_c \mathbf{Q}_c^T + \widetilde{\mathbf{Y}}_c = \mathbf{T}_c \mathbf{Q}_c^T + \mathbf{T}_y \mathbf{Q}_y^T + \widetilde{\mathbf{Y}} \end{cases}$$
(2)

where $\mathbf{T}_c \in \Re^{n \times A_c}$ represents variations in **X** that are useful to predict **Y**, $\mathbf{T}_x \in \Re^{n \times A_x}$ denotes the ones in **X** that are not useful to predict **Y**, $\mathbf{T}_y \in \Re^{n \times A_y}$ denotes the ones in **Y** unpredictable by **X**, $\mathbf{P}_c \in \Re^{m \times A_c}$, $\mathbf{P}_x \in \Re^{m \times A_x}, \ \mathbf{Q}_c \in \Re^{p \times A_c}$ and $\mathbf{Q}_y \in \Re^{p \times A_y}$ are loading matrices for the score matrices, $\widetilde{\mathbf{X}}_c$ and $\widetilde{\mathbf{Y}}_c$ denote output-irrelevant input and unpredictable output, and $\widetilde{\mathbf{X}}$ and $\widetilde{\mathbf{Y}}$ represent the input-residual and output-residual respectively. A_c , A_x and A_y are the numbers of \mathbf{Y} -relevant principal components, \mathbf{Y} -irrelevant principal components, and \mathbf{X} -irrelevant principal components, respectively.

2.2 Dynamic Concurrent PLS Modeling

For a dynamic process, the current values of the variables will depend on the past ones. Thus there is a need to capture the dynamic correlations between \mathbf{Y} and (\mathbf{X}) , and the lagged values of them. Assume the dynamic orders are known as priori knowledge, i.e. *a* for process variables and *b* for quality variables, the lagged data matrix of both quality and process data is obtained to have the following dynamic concurrent PLS modeling algorithm.

Step 1. Collect historical process and quality data, i.e. **X** and **Y**.

$$\mathbf{X} = \begin{bmatrix} x_1(1) & x_2(1) & \cdots & x_m(1) \\ x_1(2) & x_2(2) & \cdots & x_m(2) \\ \vdots & \vdots & \ddots & \vdots \\ x_1(n) & x_2(n) & \cdots & x_m(n) \end{bmatrix}_{n \times m}$$
$$\mathbf{Y} = \begin{bmatrix} y_1(1) & y_2(1) & \cdots & y_p(1) \\ y_1(2) & y_2(2) & \cdots & y_p(2) \\ \vdots & \vdots & \ddots & \vdots \\ y_1(n) & y_2(n) & \cdots & y_p(n) \end{bmatrix}_{n \times p}$$

Step 2. Construct augmented \mathbf{X}_g and \mathbf{Y}_g .

$$\mathbf{X}_{g} = [\mathbf{X}_{1}, \mathbf{X}_{2}, ..., \mathbf{X}_{m}]$$
$$\mathbf{Y}_{g} = [\mathbf{Y}_{1}, \mathbf{Y}_{2}, ..., \mathbf{Y}_{p}]$$

where

$$\mathbf{X}_{i} = \begin{bmatrix} x_{i}(k) & x_{i}(k-1) & \cdots & x_{i}(k-a+1) \\ x_{i}(k+1) & x_{i}(k) & \cdots & x_{i}(k-a+2) \\ \vdots & \vdots & \ddots & \vdots \\ x_{i}(k+n-1) & x_{i}(k+n-2) & \cdots & x_{i}(k+n-a) \end{bmatrix}$$
$$(i = 1, 2, ..., m)$$
$$\mathbf{Y}_{j} = \begin{bmatrix} y_{j}(k) & y_{j}(k+1) & \cdots & y_{j}(k+b-1) \\ y_{j}(k+1) & y_{j}(k+2) & \cdots & y_{j}(k+b) \\ \vdots & \vdots & \ddots & \vdots \\ y_{j}(k+n-1) & y_{j}(k+n) & \cdots & y_{j}(k+n+b-2) \end{bmatrix}$$
$$(j = 1, 2, ..., p)$$

Step 3. Perform CPLS in Section 2.1 on $(\mathbf{X}_g, \mathbf{Y}_g)$ to have the projection matrices in DCPLS as \mathbf{Q} , \mathbf{Q}_c , \mathbf{R}_c , \mathbf{P}_x , R_c^{\dagger} and \mathbf{Q}_y similar to the ones of CPLS.

Step 4. The five dynamic latent structures, i.e., processspecific subspace \mathbf{T}_x , quality-specific subspace \mathbf{T}_y , processquality covariation \mathbf{T}_c , potentially process-relevant subspace $\tilde{\mathbf{X}}$, and potentially quality-relevant subspace $\tilde{\mathbf{Y}}$, are built respectively.

Relative to the five subspaces defined for CPLS in Eq. (2), the ones of DCPLS can exhibit dynamic correlations and autocorrelations between **X** and **Y**.

2.3 DCPLS-Based Monitoring

To monitor the five latent subspaces, the statistics and corresponding control limits are computed accordingly similar to the ones in Qin and Zheng (2013). The detailed algorithm is described as follows.

Step 1. Collect monitored process and quality samples, i.e. \mathbf{x} and \mathbf{y} . To project the monitor sample into the subspace in Section 2.2, the original sample is augmented in the way similar to \mathbf{X} and \mathbf{Y} . The augmented sample \mathbf{x}_g and \mathbf{y}_g is constructed from \mathbf{x} and \mathbf{y} as follows.

$$\mathbf{x}_{g} = \left[\mathbf{x}_{1}, \mathbf{x}_{2}, ..., \mathbf{x}_{m}\right]^{T}$$
$$\mathbf{y}_{g} = \left[\mathbf{y}_{1}, \mathbf{y}_{2}, ..., \mathbf{y}_{p}\right]^{T}$$

where

$$\mathbf{x}_{i} = [x_{i}(k) \ x_{i}(k-1) \cdots x_{i}(k-a+1)]$$

$$(i = 1, 2, ..., m)$$

$$\mathbf{y}_{j} = [y_{j}(k) \ y_{j}(k+1) \cdots y_{j}(k+b-1)]$$

$$(j = 1, 2, ..., p)$$

Step 2. For a sample \mathbf{x}_g and \mathbf{y}_g , the DCPLS scores and residuals are calculated as follows.

$$\mathbf{t}_c = \mathbf{Q}_c^T \mathbf{Q} \mathbf{R}^T \mathbf{x}_{\mathrm{g}} = \mathbf{R}_c^T \mathbf{x}_{\mathrm{g}}$$
(3)

$$\mathbf{t}_x = \mathbf{P}_x^T \tilde{\mathbf{x}}_c; \quad \tilde{\mathbf{x}}_c = (\mathbf{I}_x - \mathbf{R}_c \mathbf{R}_c^{\dagger}) \mathbf{x}_g \tag{4}$$

$$\widetilde{\mathbf{x}} = \left(\mathbf{I}_x - \mathbf{P}_x \mathbf{P}_x^T\right) \widetilde{\mathbf{x}}_c \tag{5}$$

$$\mathbf{t}_y = \mathbf{Q}_y^T \tilde{\mathbf{y}}_c; \quad \tilde{\mathbf{y}}_c = (\mathbf{y}_g - \mathbf{Q}_c \mathbf{R}_c^T \mathbf{x}_g) \tag{6}$$

$$\widetilde{\mathbf{y}} = \left(\mathbf{I}_y - \mathbf{Q}_y \mathbf{Q}_y^T\right) \widetilde{\mathbf{y}}_c \tag{7}$$

where \mathbf{I}_x and \mathbf{I}_y are the identity matrices of $(m \times a) \times (m \times a)$ and $(p \times b) \times (p \times b)$, respectively, $\mathbf{R}_c = \mathbf{R} \mathbf{Q}^T \mathbf{Q}_c$, and \mathbf{R}_c^{\dagger} is the pseudo-inverse.

The fault detection statistics for the five subspaces in DCPLS can be computed to have three T^2 statistics for \mathbf{t}_c , \mathbf{t}_x and \mathbf{t}_y , i.e. T_c^2 , T_x^2 and T_y^2 , and two Q statistics for $\tilde{\mathbf{x}}$ and $\tilde{\mathbf{y}}$, i.e. Q_x and Q_y .

Step 3. The control limits for DCPLS can be derived similarly to those of the CPLS in Qin and Zheng (2013) using the results of Box (1954).

Step 4. The five statistics defined in Step 2 for DCPLS can be compared to the corresponding control limits computed in Step 3 to achieve comprehensive process monitoring **X**-specific, **Y**-specific, **X**-**Y** co-variation, potentially **X**-relevant, and potentially **Y**-relevant subspaces respectively.

It is noted that the above algorithm can give complete monitoring to abnormal dynamic variations, but fault detection delay is inevitable and the length is relied on the time-delay orders of the augmented data matrix. There is an tradeoff between the improvement and the time-delay. Further, one should keep in mind that a single abnormality sample from the fault detection statistic denotes an abnormal dynamic variation in a time interval.

3. MULTI-BLOCK DCPLS-BASED DIAGNOSIS

After an abnormality is detected, it is often necessary to pinpoint the variables which are related to the abnormality and interpret the monitoring results further. Although one can derive contribution plots for the CPLS algorithm to achieve fault diagnosis similar to the ones for TPLS in Li et al. (2011a), it often displays many variable contributions due to the fact that the augmented input matrix may be many times (5-50) the amount of the original input. To conduct this problem, the following multi-block DCPLS is proposed based on the multi-block partition for the augmented data matrices ($\mathbf{X}_q, \mathbf{Y}_q$).

Step 1. Rearrange the elements in \mathbf{x}_g to incorporate the variable and the lagged values to establish block sample \mathbf{x}_i .

Step 2. Five block statistics are defined according to variable partition for the augmented data with lagged values.

a) the block contributions $BC_i(Q_x)$ (i = 1, 2, ..., m) for Q_x are defined as

$$BC_i\left(Q_x\right) = \left\|\mathbf{\tilde{x}}_i\right\|^2 \tag{8}$$

where $\tilde{\mathbf{x}}_i$ is composed of elements of $\tilde{\mathbf{x}}$ defined in (5) corresponding to the i^{th} process variable.

b) the block contributions $BC_{j}\left(Q_{y}\right)\left(j=1,2,...,p\right)$ for Q_{y} are defined as

$$BC_j(Q_y) = \|\tilde{\mathbf{y}}_j\|^2 \tag{9}$$

where $\tilde{\mathbf{y}}_j$ is composed of elements of $\tilde{\mathbf{y}}$ defined in (7) corresponding to the j^{th} quality variable.

c) The block contributions for T^2 involve approximations by neglecting cross-terms in the quadratic indices. The block contributions for T_c^2 and T_x^2 are defined as

$$BC_i\left(T^2\right) = \left\|\mathbf{\Gamma}_{x,i}\mathbf{x}_i\right\|^2 \tag{10}$$

where $\Gamma_{x,i}$ is a matrix composed of the corresponding diagonal block of Γ_x given in Table 1.

The block contributions for T_y^2 is defined as

$$BC_{j}\left(T_{y}^{2}\right) = \left\|\mathbf{\Gamma}_{y,j}\tilde{\mathbf{y}}_{c,j}\right\|^{2} \tag{11}$$

where $\Gamma_{y,j}$ is a matrix composed of the corresponding diagonal block of $\Gamma_y = \mathbf{I}_y - \mathbf{Q}_y \mathbf{Q}_y^T$.

Table 1. $\Gamma_{\mathbf{x}}$ for the Two T^2 Statistics of \mathbf{X} .

$Index_x$	$\Gamma_{\mathbf{x}}$
T_c^2	$\mathbf{R}_c \mathbf{\Lambda}_c^{-0.5} \mathbf{R}_c^T$
T_x^2	$(\mathbf{I}_x - \mathbf{R}_c \mathbf{R}_c^{\dagger}) \mathbf{P}_x \mathbf{\Lambda}_x^{-0.5} \mathbf{P}_x^T (\mathbf{I}_x - \mathbf{R}_c \mathbf{R}_c^{\dagger})$

Step 3. For easy visualization, relative block contributions of the DCPLS are applied to scale the statistics based on their respective control limits derived similarly as Qin et al. (2001). It is utilized to analyze the fault effects on auto-correlation and cross-correlation for each variable in the process and quality space concurrently.

4. CASE STUDIES ON STRIP-THICKNESS MONITORING AND DIAGNOSIS OF CONTINUOUS ANNEALING PROCESSES

The section apply the proposed methods to strip-thickness relevant monitoring and diagnosis of continuous annealing process (CAP).

4.1 Description of Continuous Annealing Process

The physical layout of the CAP is shown in Fig. 1. The raw material, i.e. cold-rolling steel strip, is annealed in furnace zone, where temperature and tension control are realized when the strip goes through the furnace section. Further, the temper mill is used to improve the flatness and thickness of the strip to have the final products, i.e. tinning black plates.

For the CAP, practitioners are more concerned with the faults relevant to abnormal product quality. But the existing work in Liu et al. (2012) mainly focussed on process faults using measured rolling speeds and currents. As stripthickness is an important quality index, it is essential to monitor the strip-thickness relevant fault. The stripthickness is mainly affected by the distributed 17 striptensions, 21 furnace temperatures, 8 striptemperatures and 6 speeds and currents of the temper mill. They are selected as process variables, while the strip-thickness is quality variable.

Further, the manufacturing line is a typical multivariate dynamic process. The dynamics comes from the inertias of the carrying roll and thermal inertia of the strip, and the ones caused by closed-loop control of measured tensions and temperatures. It is desirable to monitor and diagnose strip thickness-specific and process-specific abnormalities to achieve complete monitoring and diagnosis, which makes itself suitable for DCPLS based method.

4.2 Results and Discussions

The proposed DCPLS method and multi-block DCPLS methods are applied to a real CAP. The studied process section consists of 54 process variables and 1 quality variable, i.e., m = 54, p = 1. The original quality variable, i.e. strip-thickness and some contributed process variables can be seen from Fig. 2. The variation of strip-thickness cannot be straightforward analyzed on how it is affected by the process variables. n = 2000 samples are used to model the normal operation situation. The sampling time is 0.1 seconds. The data are modeled by applying the DCPLS algorithm in Section 2.2. After that, decentralized fault diagnosis strategies discussed in Sections 2 and 3 are demonstrated using 400 samples that include a strip-thickness relevant fault.

As this work discusses quality-relevant fault diagnosis, the proposed method is only compared with CPLS method which is indeed a two layer concurrent monitoring method, but not with one layer PCA and dynamic PCA based methods due to limited space. Process monitoring results using CPLS and DCPLS approaches are shown in Fig. 3 and Fig. 4. The five statistics in the CPLS but not the two statics in PLS is used because of the oblique decomposition of quality and process spaces for PLS algorithm. For this application with only 1 quality variable, Q_y is null with four statistics shown in Fig. 3. From Fig. 3 and Fig. 4, the fault situation can be detected by both CPLS and DCPLS, with higher fault magnitude for DCPLS. From the Fig. 3, complete monitoring is achieved to see some excursions appear around Sample 200 in T_c^2 , and some other significant ones appear around Samples 327 and 381. It seems the strip-thickness is not affected around the last two time intervals. But from the monitoring results of DCPLS as shown in Fig. 4, the faults caused by deviation of autocorrelation and dynamic correlation are observed from T_c^2 and Q_x of DCPLS as shown in Fig. 4. The proposed DCPLS avoids some missed alarms which demonstrate the advantages of the DCPLS method. Further, the estimated quality curve in Fig. 5 seems that there may be large portion of variations in unpredicted quality. The deviation of the actual and predicted value of the strip-thickness in Fig. 5 denotes the quality-specific variations which cannot be estimated from the process measurements. For this application, the thickness variation can be caused by the unmeasured process variation, e.g. gas flow in the furnace zone. But from Fig. 5 one cannot identify the faulty variables contributed to the process and quality faults.

The multi-block DCPLS based contribution plot is shown in Fig. 6. From T_c plot in Fig. 6, the contributed variables for the faulty sample No. 320 is variable No. 24, i.e. temperature of No. 2 cooling furnace, and the abnormalities appears at variables No. 43 and No. 52 for T_x in Fig. 6 can be considered not relevant to strip-thickness. By detailed analysis, the large contributions of variables No. 43 and No. 52 are indeed caused by some process-specific variation, i.e. the unreasonable temperature cooling operation.

5. CONCLUSIONS

The paper proposed a dynamic concurrent modeling and diagnosis method for continuous annealing processes. It provides an easy way to achieve comprehensive monitoring and helps localize faults. The proposed method can be further generalized to other dynamic processes which are desirable to monitor and diagnose quality and process variations concurrently.

The following aspects can be considered in the future work: i) The dynamic time-delay of the lagged data is determined based on priori knowledge in this work. It is helpful to derive the time-delay length directly using the process data; ii) Due to the large column dimensions of augmented process matrix, the computation load will increase a lot. It is desirable to achieve fast implementation of the dynamic modeling algorithm. The Map-Reduce based distributed computation framework can be a research direction.

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Fig. 1. The layout of continuous annealing process.



Fig. 2. The original quality variable and selected contribution process variables.

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Fig. 3. CAP process monitoring results using CPLS.

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Fig. 4. CAP process monitoring results using DCPLS.

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Fig. 5. Actual strip-thickness and predicted strip-thickness



- Fig. 6. CAP strip-thickness relevant diagnosis results using MBDCPLS.
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