

STATISTICAL METHODS FOR PROCESS
MONITORING AND CONTROL

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CONTROL

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*This thesis is dedicated to my beloved parents for their endless support,
encouragement and love.*

Abstract

Nowadays, large-scale datasets are generated in industrial processes as varieties of digital instruments, analytical sensors and data devices are utilized. The data does not transfer to useful knowledge automatically. In the current age of big data, it is critically important to develop data-driven techniques to harness industrial data to make better decisions. Statistical methods can help to make sense of the variety of data from industrial processes. Specifically, this thesis addresses three applications of statistical methods in process engineering in order to obtain different kinds of process knowledge.

With the high-dimensional and correlated process data, multivariate statistical process monitoring methods have been developed to extract useful information from a large amount of process data and detect various types of process faults. Specifically, an independent component analysis (ICA) mixture model based local dissimilarity method is developed for performance monitoring of multimode dynamic processes with non-Gaussian features in each operating mode.

Then, two video analysis based pellet sizing methods are proposed for measuring the pellet size distributions without any off-line and intrusive tests. The videos of free-falling pellets are first taken and then the free-falling tracks of pellets in video frames are analyzed through the two video analysis based pellet sizing approaches. The utility of these two video analysis based pellet sizing methods is demonstrated

through the online measurement and estimation of free-falling nickel pellets in two test videos.

Moreover, a subspace projection based model-plant mismatch detection and isolation method is developed for the closed-loop MPC systems within state-space framework. The model quality indices are developed through subspace projection in order to eliminate the effects of system feedback. The paper machine headbox process with MIMO MPC controller is used to demonstrate the effectiveness of the proposed approach in detecting and isolating different kinds of model-plant mismatches.

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Notation and abbreviations

Chapter 2:

X_1 : Normal benchmark set

X_2 : Monitored set

n : Number of samples

m : Number of variables

R : Covariance matrix of the combined data set

P_0 : Orthogonal matrix

Λ : Diagonal matrix with eigenvalues of R

Y_1, Y_2 : Transformations of X_1 and X_2

S_1, S_2 : Covariance matrices of Y_1 and Y_2

λ_j^1, λ_j^2 : The j th eigenvalue of S_1 and S_2

D_{PCA} : Eigenvalue decomposition based PCA dissimilarity factor

D_{PCA}^λ : Modified angle based PCA dissimilarity factor

$\lambda^{X_1}, \lambda^{X_2}$: Eigenvalues of $X_1^T X_1$ and $X_2^T X_2$

p : Number of PCs

θ_{ij} : Angle between the i -th PC of the benchmark set and the j -th PC of the monitored set

q : Number of ICs

A : Mixing matrix in ICA

$b(t)$: Bias vector

$\text{MMI}(S_{X_1}, S_{X_2})$: Multidimensional mutual information between S_{X_1} and S_{X_2}

$\psi(\cdot)$: The digamma function

$\Gamma(x)$: The Gamma function

l : The number of nearest neighbors identified through data clustering

$\langle \cdot \rangle$: The average over all observations in the data set

$n_{S_{X_1}}, n_{S_{X_2}}$: The numbers of samples in proximity to the nearest neighbors within two IC subspaces

D_{MMI} : The multidimensional mutual information based dissimilarity index

I_1^2, I_2^2 : The ICA based I^2 statistics for the benchmark and monitored data sets

$p(X|\Theta)$: Joint probability density function

$p(x(t)|\Theta)$: Probability density function

K : The number of non-Gaussian classes

C_k : the k -th component

$p(C_k)$: The prior probability

Θ : Parameters of each density function

Φ_k : The m -dimensional diagonal matrix

$s(t)_{k,i}$: The i -th element of the independent component $s(t)_k \in \mathbb{R}^m$ for the k -th class

X_b : Benchmark data set

X_m : Monitored set

M : Number of process variables

N : Number of samples in the benchmark set

R : Number of samples in the monitored set

$X_b^{(k)}$: The k -th subset of benchmark data

N_k : Number of samples from the k -th operating mode

$A_b^{(k)}$: The mixing matrix for the k -th class in the benchmark set

$E_b^{(k)}$: The residual matrix for the k -th class in the benchmark set
 $S_b^{(k)}$: The independent components for the k -th mode
 D_k : The number of ICs in the k -th local ICA model
 $W_b^{(k)}$: The demixing matrix for the k -th class in the benchmark set
 $X_m(i)$: The i -th monitored data set
 $x_c^{(i)}$: The center point for the i -th monitored data set
 $\hat{C}_k$: The identified mode for $x_c^{(i)}$
 $D_{\text{MMI}}^{(k)}(i)$: The ICA mixture model based dissimilarity index
 $I_m^2(i), I_b^{(k)2}$: The ICA based I^2 statistics for the i -th monitored set and the target benchmark set corresponding to the k -th operating mode $\hat{C}_k$
 $\text{MMI}(S_b^{(k)}, S_m(i))$: The multidimensional mutual information between the IC subspaces of the target benchmark set $S_b^{(k)}$ and the i -th monitored set $S_m(i)$
 $D_{\text{MMI},\alpha}^{(k)}$: The estimated control limit value
 h : The bandwidth of kernel function

Chapter 3:

p : p -th frame in the video
 P : Total number of frames in the video
 n : Pellets take the time of n frames time to fall from the top to the bottom of the video region
 i : Pixel row
 j : Pixel column
 I_1 : RGB frame
 I_2 : Gray-scale intensity frame
 I_3 : Background illumination
 I_4 : Filtered gray-scale frame

b : Disk-shaped structuring element
 L : Normalized global threshold
 G_i : Horizontal derivative approximation
 G_j : Vertical derivative approximation
 G : Approximate gradient magnitude
 Θ : Approximate gradient magnitude
 s : s -th sub-curve
 S : Total number of sub-curves in one filtered gray-scale curve
 $J_s = \{j_1, j_2, \dots, j_{n_s}\}$: j -axis training samples for the Gaussian process regression
 $F_s = \{f_s(j_1), f_s(j_2), \dots, f_s(j_{n_s})\}$: Filtered gray-scale training samples for the Gaussian process regression
 n_s : The number of gray-scale samples within the s -th sub-curve
 f_s : The filtered gray-scale values within the s -th sub-curve
 D_s : The training data for the s -th sub-curve
 k : The covariance function of the Gaussian process
 σ_f : The maximum allowable covariance
 l : Gaussian kernel width
 $J_{s*} = \{j_{1*}, j_{2*}, \dots, j_{n_{s*}}\}$: The predicted inputs
 n_{s*} : The width of the s -th gray-scale sub-curve extended to the j -axis
 F_{s*} : The predicted outputs
 K_{s*} : The covariance matrix evaluated between all pairs of training and predicted samples
 K_s : The covariance matrices of the training points
 K_{s**} : The covariance matrices of the training and predicted points
 $\bar{F}_{s*}$: The mean of the prediction
 $\theta_s = \{\sigma_f, l\}$: Model parameters

w : The length of the free falling track
 d : Diameter of pellet
 $N(d)$: The particular diameter d is counted for $N(d)$ times
 $M(d)$: Total number of pellets with the diameter d
 Y_i : The actual percentages of the i -th bin of pellet size
 $\hat{Y}_i$: The predicted percentages of the i -th bin of pellet size
 N : The total number of bins

Chapter 4:

$\{A, B, C\}$: State-space representation of the real plant
 $\{\hat{A}, \hat{B}, \hat{C}\}$: State-space representation of the model used in the MPC controllers
 $\{\Delta A, \Delta B, \Delta C\}$: Model-plant mismatches
 k : Sampling instant
 x_k : Real plant state for the k -th sampling instant
 y_k : Real plant output for the k -th sampling instant
 u_k : Plant input for the k -th sampling instant
 o_k : White noise innovation sequence for the k -th sampling instant
 K : Steady state Kalman gain
 $\hat{x}_k$: Model state for the k -th sampling instant
 $\hat{y}_k$: Model output for the k -th sampling instant
 n : The dimension of the system states
 n_y : The dimension of the system outputs
 n_u : The dimension of the system inputs
 $\bar{E}\{\cdot\}$: $\bar{E}\{\cdot\} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=1}^N E\{\cdot\}$
 $u_p(k)$: The past output vector for the k -th sampling instant
 $u_f(k)$: The future output vector for the k -th sampling instant

U_p : The past plant input Hankel matrix
 U_f : The future plant input Hankel matrix
 p : Past horizon
 f : Future horizon
 N : The number of the monitored samples
 Y_p : The past plant output Hankel matrix
 Y_f : The future plant output Hankel matrix
 $\hat{Y}_p$: The past model output Hankel matrix
 $\hat{Y}_f$: The future model output Hankel matrix
 O_p : The past noise disturbance Hankel matrix
 O_f : The future noise disturbance Hankel matrix
 X_p : The past plant state Hankel matrix
 X_f : The future plant state Hankel matrix
 $\hat{X}_p$: The past model state Hankel matrix
 $\hat{X}_f$: The future model state Hankel matrix
 Γ_p : The past extended observability matrix
 Γ_f : The future extended observability matrix
 H_p^d : The past triangular block-Toeplitz matrix
 H_f^d : The future triangular block-Toeplitz matrix
 H_p^s : The past triangular block-Toeplitz matrix
 H_f^s : The future triangular block-Toeplitz matrix
 G_p^s : The past triangular block-Toeplitz matrix
 G_f^s : The future triangular block-Toeplitz matrix
 $A_p(k)$: The subspace equation for the mismatch in A for the past horizon
 $A_f(k)$: The subspace equation for the mismatch in A for the future horizon
 $B_p(k)$: The subspace equation for the mismatch in B for the past horizon

$B_f(k)$: The subspace equation for the mismatch in B for the future horizon

$C_p(k)$: The subspace equation for the mismatch in C for the past horizon

$C_f(k)$: The subspace equation for the mismatch in C for the future horizon

e_k : Model residual for the k -th instant

E_k : The subspace equation of the model residual for the k -th instant

$(\Gamma_f^\perp)^T$: The left null space of Γ_f

$I_{n_y f}$: Identity matrix with the dimension of $n_y f$

$\Pi_{U_f}^\perp$: The orthogonal projector onto the kernel of U_f : $\Pi_{U_f}^\perp = I - U_f^\dagger U_f$

α_f : $\alpha_f = \begin{bmatrix} \Gamma_f : G_f^s \end{bmatrix}$

m : The rank of α_f

$(\alpha_f^\perp)^T$: The left null space of α_f

β_f : $\beta_f = \begin{bmatrix} \Gamma_f : I_{n_y f} \end{bmatrix}$

$(\beta_f^\perp)^T$: The left null space of β_f

X_f : The subspace equation for the future plant state

$\hat{X}_f$: The subspace equation for the past model state

$\hat{\Delta}_f^d$: $\hat{\Delta}_f^d = \begin{bmatrix} \hat{A}^{f-1} \hat{B} : \hat{A}^{f-2} \hat{B} : \dots : \hat{A} \hat{B} : \hat{B} \end{bmatrix}$

$\tilde{\Delta}_f^d$: $\tilde{\Delta}_f^d = \begin{bmatrix} \hat{A}^{f-1} \Delta B : \hat{A}^{f-2} \Delta B : \dots : \hat{A} \Delta B : \Delta B \end{bmatrix}$

$\hat{\Delta}_f^s$: $\hat{\Delta}_f^s = \begin{bmatrix} \hat{A}^{f-1} K : \hat{A}^{f-2} K : \dots : \hat{A} K : K \end{bmatrix}$

ΔA_f : $\Delta A_f = \hat{A}^{f-1} \Delta A + \Delta A_{f-1} \hat{A} + \Delta A_{f-1} \Delta A$

Δ_f^d : $\Delta_f^d = \begin{bmatrix} \Delta A_{f-1} B : \Delta A_{f-2} B : \dots : \Delta A B : 0 \end{bmatrix}$

Δ_f^s : $\Delta_f^s = \begin{bmatrix} \Delta A_{f-1} K : \Delta A_{f-2} K : \dots : \Delta A K : 0 \end{bmatrix}$

θ_f : $\theta_f = \begin{bmatrix} \Gamma_f \hat{A}^f : I_{n_y f} : G_f^s \end{bmatrix}$

$(\theta_f^\perp)^T$: The left null space of θ_f

$\Pi_{U_p}^\perp$: The orthogonal projector onto the kernel of U_p

W_f : The combination of inputs and outputs for the future horizon

W_p : The combination of inputs and outputs for the past horizon

Π_{W_p} : The orthogonal complement of the kernel of W_p

e : e_{ABC} , *i.e.* e_{ABC}^* , e_{AC} , e_C , and e_C^*

R : The corresponding covariance matrix for the index e

$\mu(k)$: The quadratic index

χ_l^2 : Chi-square distribution with l degrees of freedom

l : Degree of freedom

$(1 - \alpha) \times 100\%$: Confidence level for the chi-square distribution

r : Setpoint moves

s : The order of the persistently exciting setpoint

$R_r(\tau)$: $R_r(\tau) = \bar{E}[r(t)r(t - \tau)]$

H_1 : Liquid level in the feed tank

H_2 : Liquid level in the headbox

N_1 : The consistencies in the feed tank

N_2 : The consistencies in the headbox

G_p : The flow rates of the stock entering the feed tank

G_w : The recycled white water

Contents

Abstract	iv
Acknowledgements	vi
Publication List	vii
Notation and abbreviations	ix
1 Introduction	1
1.1 Multivariate Statistical Process Monitoring	3
1.1.1 Tennessee Eastman Chemical Process	4
1.2 Data-driven Soft Sensors	5
1.3 Model Predictive Control	6
1.3.1 MPC Performance Monitoring	8
1.4 Thesis Outline	9
2 Independent Component Analysis Mixture Model Based Dissimilar- ity Method for Performance Monitoring of Non-Gaussian Dynamic Processes with Shifting Operating Conditions	15
2.1 Introduction	16
2.2 Preliminaries	20

2.2.1	Eigenvalue Decomposition Based PCA Dissimilarity Method	20
2.2.2	Modified Angle Based PCA Dissimilarity Method	22
2.2.3	Mutual Information Based ICA Dissimilarity Factor	22
2.3	ICA Mixture Model Based Dissimilarity Approach for Multimode Process Monitoring	24
2.3.1	ICA Mixture Model	24
2.3.2	ICA Mixture Model Based Dissimilarity Method	26
2.4	Application Example	35
2.4.1	Illustrative numerical example	35
2.4.2	Tennessee Eastman Chemical Process	38
2.5	Conclusions	48
3	Multivariate Video Analysis and Gaussian Process Regression Model Based Soft Sensor for Online Estimation and Prediction of Nickel Pellet Size Distributions	55
3.1	Introduction	56
3.2	Image Analysis Based Pellet Sizing Method	61
3.3	Video Analysis Based Pellet Sizing Soft Sensor Methods	63
3.3.1	Pre-processing of Video Frames	64
3.3.2	The First Video Analysis Based Pellet Sizing Method	65
3.3.3	The Second Video Analysis Based Pellet Sizing Method	70
3.4	Comparison of Pellet Size Distribution Prediction Results	79
3.5	Conclusions	81
4	Closed-Loop Subspace Projection Based State-Space Model-Plant Mismatch Detection and Isolation for MIMO MPC Performance	

Monitoring and Diagnosis	90
4.1 Introduction	91
4.2 Problem formulations	93
4.3 Subspace projection based model-plant mismatch detection	96
4.3.1 Detection of model-plant mismatch in system matrix A, B or C	102
4.3.2 Detection of model-plant mismatch in A or C	103
4.3.3 Detection of model-plant mismatch in C	104
4.3.4 Model-plant mismatch isolation based on different model qual- ity indices	105
4.4 Case studies	109
4.5 Conclusions	115
4.6 Acknowledgements	116
5 Conclusions and Future Work	120
5.1 Conclusions	120
5.2 Recommendations for Future Work	122

List of Tables

2.1	Monitored variables in the Tennessee Eastman Chemical process . . .	41
2.2	Six operating modes in the Tennessee Eastman Chemical process . . .	42
2.3	Pre-defined faults in the Tennessee Eastman Chemical process	43
2.4	Three test cases in the Tennessee Eastman Chemical process	45
2.5	Comparison of fault detection results among different types of dissim- ilarity methods	46
3.1	Comparison of the MAPE values of predicted pellet size distributions between the two video analysis based pellet sizing methods for two test videos	82
4.1	Case Studies: Four Test Cases with Different Types of Model-Plant Mismatches in System Matrices	112

List of Figures

1.1	Basic concept for model predictive control (Seborg <i>et al.</i> , 2006). . . .	7
2.1	Illustration of moving window strategy in the ICA mixture model based dissimilarity method	30
2.2	Flow chart of the proposed ICA mixture model based dissimilarity method	33
2.3	Monitoring results in the numerical example	37
2.4	Process flow diagram of the Tennessee Eastman Chemical process . .	39
2.5	Monitoring results of the first test case of the Tennessee Eastman Chemical process	40
2.6	Monitoring results of the second test case of the Tennessee Eastman Chemical process	44
2.7	Monitoring results of the third test case of the Tennessee Eastman Chemical process	47
3.1	Illustrative example of image analysis based pellet sizing method: (a) original image; (b) pellet edge detection results; (c) pellet identification results; and (d) pellet size distribution and cumulative distribution . .	62
3.2	Illustrative procedure of the first video analysis based pellet sizing method	67

3.3	Illustrative example of the first video analysis based pellet sizing method: (a) original image; (b) filtered gray-scale image; (c) black and white image; and (d) edge detection results	68
3.4	Pellet size distribution and cumulative distribution of the first video analysis based pellet sizing method for the first test video	69
3.5	Pellet size distribution and cumulative distribution of the first video analysis based pellet sizing method for the second test video	70
3.6	Illustration of the challenges for the first video analysis based pellet sizing method	71
3.7	Illustration of the second video analysis based pellet sizing method . .	72
3.8	Illustration of the proposed pixel row based scanning of the filtered gray-scale frame in the second video analysis based pellet sizing method	73
3.9	Schematic diagram of the two proposed video analysis based pellet sizing methods	77
3.10	Illustrative example of the second video analysis based pellet sizing method: (a) filtered gray-scale frame with the 41-th pixel row marked; (b) the scanning result of the 41-th row	78
3.11	Predicted sub-curves and the corresponding confidence intervals of the Gaussian process regression models for the 41-th pixel row: (a) Curve 1 with two sub-curves; (b) Curve 2 with three sub-curves	79
3.12	Pellet size distribution and cumulative distribution of the second video analysis based pellet sizing method for the first test video	80
3.13	Pellet size distribution and cumulative distribution of the second video analysis based pellet sizing method for the second test video	81
4.1	Model residual form of closed-loop MPC system in state-space repre- sentation	95

4.2	Schematic diagram of the designed model-plant mismatch isolation logic	107
4.3	Schematic diagram of the paper machine headbox control problem . .	110
4.4	Model-plant mismatch detection results in Case 1	113
4.5	Model-plant mismatch detection results in Case 2	113
4.6	Model-plant mismatch detection results in Case 3	114
4.7	Model-plant mismatch detection results in Case 4	115

Chapter 1

Introduction

This thesis addresses the applications of statistical methods in making sense of industrial process data. The research focuses on how to automatically process and transform the industrial data into useful information and knowledge of the system. With the evolution of a variety of digital instruments, analytical sensors, control systems and data devices, large-scale datasets are generated in industrial processes nowadays. The term of big data is popular in chemical engineering these years, which refers to the large, diverse and complex datasets and results in great opportunities for knowledge discovery. It is critically important to develop data-driven knowledge to take advantage of big data to make better decisions in process industry. In this thesis, several applications of statistical methods are discussed from different aspects to highlight the knowledge acquisition from industrial process data. Though these methods are not presented in big data setting, they may be scalable to big data scope in future research.

Big data is used to describe the large, diverse, complex datasets, which are generated from different types of instruments, sensors or computer-based transactions.

A three dimensional problem, known as volume, variety and velocity (3Vs), is popularly used to describe the big data characteristics (Manyika *et al.*, 2011; Zikopoulos *et al.*, 2011). It is evident that industrial process data has at least 3V's of big data. The continued advancements in sensing and the decreasing storage costs are two major factors that result in increasing data volume. They are also the driving forces of the statistical methodologies, especially the multivariate control techniques and time-series methods. Not only the measurements, but also different process variables contribute to the large volume of industrial data (Venkatasubramanian *et al.*, 2003; Miletic *et al.*, 2004). Further, the industrial data variety is mainly reflected in the range of data sources and types. An increasing number of statistical methods are developed for analysing multivariate processes with hybrid and continuous process data. With the development of sensing technology, process data is no longer restricted by traditional measurements. It becomes more challenging when non-numeric data is included. For example, the use of image data for process monitoring is a promising area of statistical research. A wide variety of quality characteristics, such as product geometry, surface patterns and dimensional data can be monitored by real time imaging of the process (MacGregor *et al.*, 2005; Torabi *et al.*, 2005). In addition, the velocity of data depends on the system dynamics. As industrial equipment becomes highly instrumented and connected, more and more data streams need to be analyzed. Faster responsiveness to high velocity data is necessary for plant security, inventory managing, product planning and optimization. In brief, the major challenge of big data analysis lies in translating such data into knowledge in real time. Statistical methods can make sense of the variety of data from industrial processes and more importantly, traditional statistical methods for regular data are the basis of big data analysis in many ways. This thesis discusses the statistical methods through the following three aspects:

- (1) Performance monitoring of non-Gaussian dynamic processes with shifting operating conditions;
- (2) Data-based soft sensor for online estimation of nickel pellet size distributions;
- (3) Model-plant mismatch detection for multi-input multi-output (MIMO) model predictive control (MPC) performance monitoring.

The current chapter presents an overview of multivariate statistical process monitoring, data-driven soft sensors, basic concept of MPC and MPC performance monitoring. Furthermore, the thesis outline is presented.

1.1 Multivariate Statistical Process Monitoring

Process monitoring and diagnosis are essential for detecting abnormal operating conditions, process upsets, equipment malfunctions, sensor failures, and other faults in industrial plants. Thousands of process variables are measured and recorded continuously in industrial plants so the process monitoring becomes a challenging task. Meanwhile, the huge amounts of process data can be employed to build various kinds of models for process monitoring. Traditionally, univariate statistical process control (SPC) techniques have been used for monitoring industrial processes. Nevertheless, the highly correlated process measurements in industrial plants often result in the failure of univariate methods.

Multivariate statistical process monitoring (MSPM) techniques like principal component analysis (PCA) and partial least squares (PLS) have been widely used for fault detection and diagnosis in industrial practice (Kosanovich *et al.*, 1996; Kano *et al.*, 2002). These kinds of methods first project the multivariate and collinear data onto a lower dimensional subspace. Then the test statistics like T^2 and SPE are developed

to monitor the multivariate data. The effectiveness of these conventional methods requires that the process data approximately follow multivariate Gaussian distributions for the derivation of control limits. However, industrial data often obeys non-Gaussian distribution so that the PCA/PLS based monitoring techniques become ill-suited. On the other hand, ICA is adopted to decompose multivariate data into linear combinations of statistically independent components (IC). ICA imposes independency on latent variables beyond second-order statistics and thus can extract the non-Gaussian features of process data (Albazzaz and Wang, 2004). Moreover, ICA based monitoring statistics like I^2 and SPE have been developed to describe the variability within the independent component and residual subspaces (Lee *et al.*, 2004).

Moreover, unsupervised pattern matching techniques are proposed to identify similar patterns between multivariate time-series data sets. Various PCA based pattern matching methods compare PC subspaces using similarity factors, which are developed from the geometric angles between principal components (Singhal and Seborg, 2006). Alternately, eigenvalue decomposition of the covariance matrices is used to determine the dissimilarity factor between two data sets (Kano *et al.*, 2002). More recently, the dissimilarity method is extended to ICA for comparing two data sets using independent components (Ge and Song, 2007).

1.1.1 Tennessee Eastman Chemical Process

The Tennessee Eastman Chemical process (TEP) is a well-defined simulation of a chemical process that has been commonly used in process control research (Downs and Vogel, 1993). There are five major unit operations in this process including a reactor, a product condenser, a vapor-liquid separator, a recycle compressor and a product stripper. Two liquid products, G and H , are produced from four gaseous

reactants A , C , D and E along with a by-product F . An inert gaseous component, B , is also present in the reactant. A partial condenser is used to cool the reactor product streams, then the product is fed to a vapor/liquid separator for component separation. Further, the vapor stream existing the separator is recycled to the reactor feed stream through a compressor. The process involves 41 measurement variables, which are a mixture of 22 continuous and 19 composition measurements. Each measurement is corrupted by additive noise and the statistical properties of the noise are unknown. The problem statement also defines process constraints, 20 types of process disturbances, and six operating modes corresponding to different production rates and G/H mass ratios in the product stream. The base operating mode is a 50/50 G/H mass ratio and a production rate of 14,072 lb/h. In addition, the process is nonlinear, open-loop unstable, and contains a mixture of fast and slow dynamics. A decentralized control strategy is adopted for closed-loop operation stability (R.N., 1996). In this thesis, the 22 continuous measurement variables are selected for process performance monitoring purpose.

1.2 Data-driven Soft Sensors

Predictive model based soft sensors have been widely adopted for measuring process variables that cannot be directly measured by physical hardware (Kadlec *et al.*, 2009). The traditional mechanistic model based soft sensor requires in-depth process knowledge and tedious development effort, which are not desirable for industrial applications. In contrast, data-driven soft sensor relies on historical process data only and is thus easy for practical implementations (Lin *et al.*, 2007). Early effort of developing data-driven soft sensors has been attempted through multivariate statistical techniques such as PCA and PLS (Zamprognia *et al.*, 2005; Kano *et al.*, 2000), which

can cope with variable co-linearity and identify the statistical models by projecting the original process variables onto the lower-dimensional latent subspace. However, the PCA or PLS based soft sensor models are essentially linear and cannot accurately characterize nonlinear process dynamics. To overcome this drawback, artificial neural network (ANN) and support vector machine (SVM) techniques are adopted for building soft sensor models of nonlinear processes (Ko and Shang, 2011). With attractive merits, soft sensors have received significant attention for measuring quality variables that are normally determined by off-line analysis, including the particle size distribution of grinding circuits and disarranged ores (Ko and Shang, 2011).

1.3 Model Predictive Control

MPC is one of the most popular forms of advanced control techniques for difficult multivariate control problems and has profound impact on industrial practice. It is reported that there were over 4,500 applications worldwide by the end of 1999, primarily in oil refineries and petrochemical plants (Qin and Badgwell, 2003). With the process model in MPC controllers, the dynamic and static interactions between input, output, and disturbance variables can be captured. The constraints on inputs and outputs can be considered in a systematic manner and the control sequences are calculated by considering optimum set points. Furthermore, the accurate predictions can provide early warnings of possible issues. The basic concept of MPC can be summarized as follows. A reasonably accurate dynamic process model and current measurements can be utilized to predict future system outputs. Then the system input sequences can be calculated based on measurements, set points and predictions. In addition, the inequality constraints on the input and output variables can be considered properly and thus the predicted response moves to the set point optimally.

In MPC applications, the output variables are called controlled variables or CVs, while the input variables are referred to as manipulated variables or MVs. Measured disturbance variables are called DVs (Seborg *et al.*, 2006).

The basic concept for single-input single-output (SISO) MPC is shown in Fig. 1.1 with y , $\hat{y}$ and u representing the actual output, predicted output and manipulated input, respectively. For sampling time k , a set of M values of the input $\{u(k+i-1), i=1, 2, \dots, M\}$ is generated to make the set of P predicted outputs $\{\hat{y}(k+i), i=1, 2, \dots, P\}$ reach the set point in an optimal manner. Only the first move of MVs will be implemented at this sampling time. When new measurements are available, a new sequence of MVs is calculated and the procedure is repeated at each sampling instant. The number of control moves M is known as the control horizon and the number of predictions P is prediction horizon.

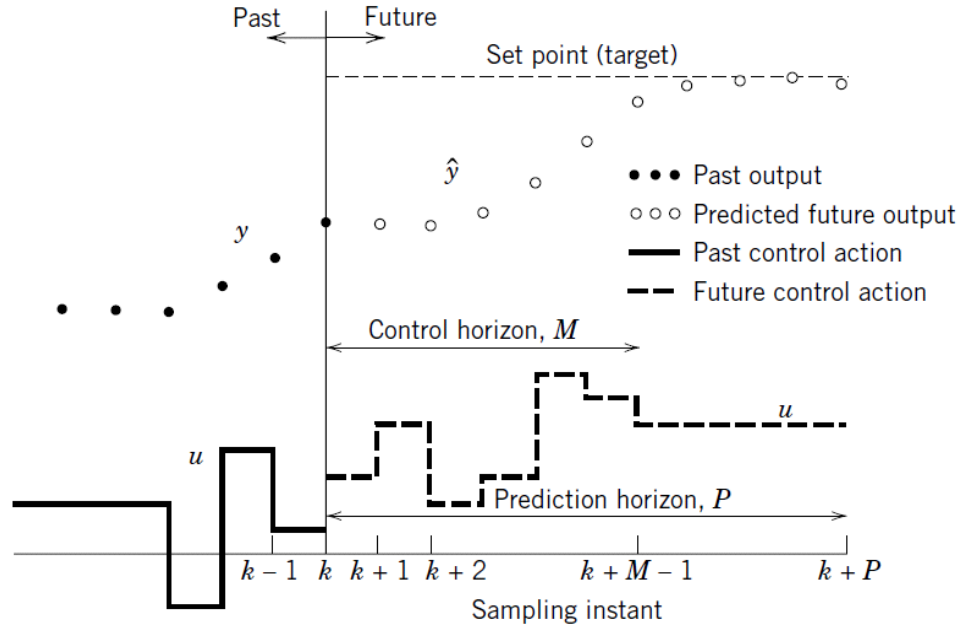


Figure 1.1: Basic concept for model predictive control (Seborg *et al.*, 2006).

1.3.1 MPC Performance Monitoring

The well-performing MPC systems can substantially improve the production capacity, energy conservation, product quality and operational profit in industrial processes (Kano and Ogawa, 2010). However, the performance of industrial MPC applications often degrade dramatically after a period of operation due to various factors such as model-plant mismatch, poor controller tuning, changes of noise disturbances, sensor/actuator faults, abnormal operating events, inappropriate control design, and changes of constraint sets. Hence, research on MPC performance assessment, monitoring and diagnosis has attracted significant attention in the past decades (Huang and Shah, 1999; Joe Qin, 1998; Harris, 1989).

Among the aforementioned factors causing MPC performance deterioration, the model-plant mismatch is a very significant one because the process model is needed in MPC systems for enabling the horizon based predictions of all controlled variables. Even under the normal plant operations, any operational changes can lead to the shifted plant dynamics so that the original controller models may be biased and thus the model-plant mismatch arises. Another type of model-plant mismatch is often due to the improper step testing and inaccurate model identification during the MPC commissioning stage. The unreliable plant models can result in poor predictions on the system outputs, which in turn affect the optimized move sequences of system inputs. Therefore, it is necessary to detect different kinds of model-plant mismatches and resolve the model quality issues rapidly. Usually the entire MIMO model re-identification requires intrusive open-loop plant testing, which can increase the maintenance cost substantially. Thus, it is crucially important to first detect model-plant mismatch and then identify subsystems with the most significant model errors. In this way, only the sub-models that are diagnosed with mismatches need to

be re-identified.

1.4 Thesis Outline

The remainder of the thesis is organized as follows:

Chapter 2 reviews different types of process monitoring methods in process system engineering. With the high-dimensional and correlated process data, multivariate statistical process monitoring methods have been developed to extract useful information from a large amount of process data and detect various types of process faults. Specifically, an ICA mixture model based local dissimilarity method is developed in this chapter for performance monitoring of multimode dynamic processes with non-Gaussian features in each operating mode. The normal benchmark set is assumed to be from different operating modes, each of which can be characterized by a localized ICA model. Thus an ICA mixture model is developed with a number of non-Gaussian components that correspond to various operating modes in the normal benchmark set. Further, the Bayesian inference rules are adopted to determine the local operating modes that the monitored set belongs to and the ICA mixture model based dissimilarity index is derived to evaluate the non-Gaussian patterns of process data by comparing the localized IC subspaces between the benchmark and the monitored sets. Moreover, the process dynamics are taken into account by implementing sliding window strategy on the monitored data set. The developed ICA mixture model based dissimilarity method is applied to monitor the performance of the Tennessee Eastman Chemical process with multiple operating modes and the fault detection results demonstrate the superiority of the proposed method over the conventional eigenvalue decomposition based and geometric angle based PCA mixture dissimilarity methods.

Chapter 3 investigates predictive model based soft sensors that make use of available process measurement data to build predictive models for estimating key product quality variables. Specifically in mining industry, accurate measurement and prediction of pellet size distributions are critically important because they are essential for model predictive control, real-time optimization, planning and scheduling of production. Mechanical sieving is one of the traditional methods for pellet size measurement in industrial practice but cannot be applied in real-time fashion. Alternately, multivariate image analysis based pellet sizing methods may acquire the size information non-intrusively and thus can be implemented for on-line measurement in industrial applications. Nevertheless, the conventional multivariate image analysis based pellet sizing methods cannot effectively deal with the pellet overlapping effects in the still images, which may lead to inaccurate and unreliable measurements of size distributions. In this chapter, two novel video analysis based pellet sizing methods are proposed for measuring the pellet size distributions without any off-line or intrusive tests. The videos of free-falling pellets are taken first and then the free-falling tracks of pellets in video frames are analyzed through the two video analysis based pellet sizing approaches. In the first video analysis method, the Sobel edge detection strategy is adopted to identify and isolate the free-falling tracks in order to estimate the diameters of the corresponding pellets. For the second video analysis approach, the filtered gray-scale video frames are scanned row by row and then the particle diameters are estimated and predicted through the built Gaussian process regression (GPR) models and a fine designed counting rule so as to eliminate the overlapping effects of nickel pellets along the horizontal and vertical directions. The utility of these two video analysis based pellet sizing methods is demonstrated through the measurement and estimation of free-falling nickel pellets in two test videos.

Chapter 4 considers control performance monitoring by using closed-loop operating data. In multivariate MPC systems, the controller performance heavily depends on the prediction accuracy of MIMO process models. Though re-identification of process models can possibly resolve the model quality issues, it is very time-consuming and costly as it may require open-loop step tests in plant operation. Thus, system re-identification without any model-plant mismatch detection or diagnosis is not desirable for industrial MPC systems. This chapter is aimed at precise detection and isolation of significant model-plant mismatches in MIMO model predictive controllers so that the further diagnosis of sub-models with most significant mismatches becomes achievable. In this chapter, a novel subspace projection based model-plant mismatch detection and isolation method is developed for the closed-loop MPC systems within state-space framework. The model quality indices are developed through various kinds of subspace projections in order to eliminate the effects of system feedback. As such, a logic framework is established for isolating different types of model-plant mismatches. One simulated example, the paper machine headbox process with MIMO MPC controller, is used to demonstrate the effectiveness of the proposed approach in detecting and isolating different kinds of model-plant mismatches in a closed-loop fashion.

Finally, the conclusions of the thesis and recommendations for future work are drawn in Chapter 5.

Bibliography

- Albazzaz, H. and Wang, X. Z. (2004). Statistical process control charts for batch operations based on independent component analysis. *Ind. Eng. Chem. Res.*, **43**, 6731–6741.
- Downs, J. and Vogel, E. (1993). A plant-wide industrial process control problem. *Computers & Chemical Engineering*, **17**(3), 245–255.
- Ge, Z. and Song, Z. (2007). Process monitoring based on independent component analysis-principal component analysis (ICA-PCA) and similarity factors. *Ind. Eng. Chem. Res.*, **46**, 2054–2063.
- Harris, T. J. (1989). Assessment of control loop performance. *Can. J. Chem. Eng.*, **67**(5), 856–861.
- Huang, B. and Shah, S. L. (1999). *Performance assessment of control loops: theory and applications*. Springer.
- Joe Qin, S. (1998). Control performance monitoring: a review and assessment. *Comput. Chem. Eng.*, **23**(2), 173–186.
- Kadlec, P., Gabrys, B., and Strandt, S. (2009). Data-driven soft sensors in the process industry. *Comput. Chem. Eng.*, **33**, 795–814.
- Kano, M. and Ogawa, M. (2010). The state of the art in chemical process control in japan: Good practice and questionnaire survey. *J. Proc. Cont.*, **20**(9), 969–982.
- Kano, M., Miyazaki, K., Hasebe, S., and Hashimoto, I. (2000). Inferential control system of distillation compositions using dynamic partial least squares regression. *J. Proc. Cont.*, **10**, 157–166.

- Kano, M., Hasebe, S., Hashimoto, I., and Ohno, H. (2002). Statistical process monitoring based on dissimilarity of process data. *AIChE J.*, **48**(6), 1231–1240.
- Ko, Y.-D. and Shang, H. (2011). A neural network-based soft sensor for particle size distribution using image analysis. *Powder Technol.*, **212**, 359–366.
- Kosanovich, K., Dahl, K., and Piovoso, M. (1996). Improved process understanding using multiway principal component analysis. *Ind. Eng. Chem. Res.*, **35**, 138–146.
- Lee, J.-M., Yoo, C., and Lee, I.-B. (2004). Statistical process monitoring with independent component analysis. *J. Proc. Cont.*, **14**, 467–485.
- Lin, B., Recke, B., Knudsen, J. K. H., and Jørgensen, S. B. (2007). A systematic approach for soft sensor development. *Comput. Chem. Eng.*, **31**, 419–425.
- MacGregor, J., Yu, H., Muñoz, S., and Flores-Cerrillo, J. (2005). Data-based latent variable methods for process analysis, monitoring and control. *Comput. Chem. Eng.*, **29**(6), 1217–1223.
- Manyika, J., Chui, M., Brown, B., Bughin, J., Dobbs, R., Roxburgh, C., and Byers, A. H. (2011). Big data: The next frontier for innovation, competition, and productivity. http://www.mckinsey.com/insights/business_technology/big_data_the_next_frontier_for_innovation.
- Miletic, I., Quinn, S., Dudzic, M., Vaculic, V., and Champagne, M. (2004). An industrial perspective on implementing on-line applications of multivariate statistics. *J. Proc. Cont.*, **14**, 821–836.
- Qin, S. J. and Badgwell, T. A. (2003). A survey of industrial model predictive control technology. *Control Eng. Pract.*, **11**(7), 733–764.

- R.N., L. (1996). Decentralized control of the tennessee eastman challenge process. *Journal of Process Control*, **6**(4), 205–221.
- Seborg, D., Edgar, T. F., and Mellichamp, D. (2006). *Process dynamics & control*. John Wiley & Sons.
- Singhal, A. and Seborg, D. E. (2006). Evaluation of a pattern matching method for the Tennessee Eastman challenge process. *J. Proc. Cont.*, **16**, 601–613.
- Torabi, K., Sayad, S., and Balke, S. (2005). On-line adaptive Bayesian classification for in-line particle image monitoring in polymer film manufacturing. *Comput. Chem. Eng.*, **30**(1), 18–27.
- Venkatasubramanian, V., Rengaswamy, R., Yin, K., and Kavuri, S. N. (2003). A review of process fault detection and diagnosis: Part I: Quantitative model-based methods. *Comput. Chem. Eng.*, **27**, 313–326.
- Zamprogna, E., Barolo, M., and Seborg, D. E. (2005). Optimal selection of soft sensor inputs for batch distillation columns using principal component analysis. *J. Proc. Cont.*, **15**, 39–52.
- Zikopoulos, P., Eaton, C., *et al.* (2011). *Understanding big data: Analytics for enterprise class hadoop and streaming data*. McGraw-Hill Osborne Media.

Chapter 2

Independent Component Analysis Mixture Model Based Dissimilarity Method for Performance Monitoring of Non-Gaussian Dynamic Processes with Shifting Operating Conditions

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Contributions:

The study is performed by Jingyan Chen in consultation with Dr. Jie Yu. The paper is written by Jingyan Chen and edited by Dr. Jie Yu.

2.1 Introduction

Process monitoring is one of the most important tasks in process system engineering to ensure plant safety, product quality, production profit and environment sustainability. Due to the large number of process variables measured and recorded continuously in industrial plants, process monitoring has become a challenging task to not only detect abnormal process behavior as early as possible but also increase fault detection accuracy and mitigate false alarms. With the high-dimensional and correlated process data, multivariate statistical process monitoring (MSPM) methods have been developed to extract useful information from a large amount of process data and detect various types of process faults (Nomikos and MacGregor, 1994; Venkatasubramanian *et al.*, 2003; Miletic *et al.*, 2004; Qin and Yu, 2007; AlGhazzawi and Lennox, 2008; Yu and Qin, 2009c,a).

Principal component analysis (PCA) and partial least squares (PLS) are the most commonly used MSPM techniques, which can cope with data collinearity caused by cross-correlated process variables (Raich and Çinar, 1996; Chen and Liu, 1999; Qin, 2003; Choi *et al.*, 2006). PCA is a multivariate statistical tool that can be used for data compression and information extraction by transforming the original set of correlated process variables into a subset of latent variables. Those principal components are the linear combinations of the original measurement variables and represent the feature directions of the most significant variability in a data set (Kosanovich *et al.*, 1996; Chiang *et al.*, 2001). However, PCA takes into account only second-order statistics so that it lacks the ability to effectively extract non-Gaussian features from industrial data (Lee *et al.*, 2004b; Rashid and Yu, 2012). Moreover, the control limits of Hotelling's T^2 and SPE indices in PCA and PLS based monitoring methods are derived from the assumption that the latent variables follow a multivariate Gaussian

distribution approximately. In industrial practice, however, process data may not always follow Gaussian distribution so that the traditional T^2 and SPE control limits can become ill-suited (Martin and Morris, 1996). Furthermore, the regular PCA and PLS models are essentially static as they are formulated from process data without considering auto-correlations. Nevertheless, chemical processes often show significant dynamic features and non-steady-state transitions on different process variables. Dynamic PCA (DPCA) has been developed to deal with time-varying process dynamics through time-lagged multivariate statistical models on process variables (Ku *et al.*, 1995). However, an excessively large number of variables may be required in such model structures due to the time-shifted process variables. In contrast, a subspace model identification based monitoring approach is proposed for large-scale processes monitoring (Treasure *et al.*, 2004). Although this method needs a considerably smaller number of variables to build dynamic process model, the higher-order statistics are still not taken into consideration for non-Gaussian process features. Alternately, independent component analysis (ICA) based monitoring methods are developed to deal with non-Gaussian processes (Albazzaz and Wang, 2004). ICA is a multivariate statistical technique to extract statistically independent components (ICs) from observed process data so that the latent variables have the minimal statistical dependencies. Effective and significant ICs can also be extracted from explanatory variables by utilizing the multiple linear regression integrated with ICA (Kaneko *et al.*, 2008). In addition, kernel ICA based monitoring technique is introduced to handle nonlinear processes (Lee *et al.*, 2004a). Another modified strategy is to integrate local outlier factor (LOF) with ICA for monitoring process with the mixture of Gaussian and non-Gaussian variables (Lee *et al.*, 2011). Though ICA can deal with non-Gaussian processes through higher-order statistics, it is not well suited for chemical processes with multiple modes caused by the shifting operation conditions.

Meanwhile, machine learning methods such as support vector machines (SVMs) and hidden Markov models (HMMs) are proposed for fault detection and diagnosis (Chiang *et al.*, 2004; Mahadevan and Shah, 2009; Rashid and Yu, 2012; Yu, 2012b,a, 2013; Yu and Rashid, 2013). SVMs have strong capability of nonlinear feature extraction and can isolate faulty samples from the normal measurements with high generalization capacity. However, SVM based monitoring techniques typically do not take into account process dynamics. On the other hand, HMMs are well suited for modeling dynamic sequence of process measurements given their ability to estimate not only the sequential values of process variables but also the dependencies among those variables. Nevertheless, the required computational load of HMM methods can be quite high. Alternately, pattern matching strategies based on dissimilarity factors can monitor multivariate processes by comparing latent variable subspaces and evaluating the similarity between normal benchmark and monitored data sets (Kano *et al.*, 2002; Singhal and Seborg, 2002b, 2005; Rashid and Yu, 2012b). One of the proposed PCA dissimilarity factor depends on the Karhunen-Loeve(KL) expansion and eigenvalue decomposition on the covariance matrices of benchmark and monitored sets (Kano *et al.*, 2002). In contrast, the other type of PCA pattern matching method relies on the geometric angles between each pair of principal components of benchmark and monitored data sets (Singhal and Seborg, 2002a, 2006). These unsupervised pattern matching methods, however, only take into consideration the second-order statistic of covariance and thus may not extract the non-Gaussian process features effectively. A multidimensional mutual information based dissimilarity method is proposed to characterize the dissimilarity between the independent component subspaces of benchmark and monitored sets based upon the statistical dependencies of the extracted subspaces (Rashid and Yu, 2012b). Although the higher-order statistics of entropy and mutual information are taken into account and thus non-Gaussian

process features can be captured, the shifting process operating conditions are not considered.

In order to deal with multimode processes, multi-PCA based monitoring approach is proposed with multiple PCA models developed for different operating conditions (Zhao *et al.*, 2004). However, the priori process knowledge and preliminary clustering step are needed to classify the historical data into different operating modes. A mixture PCA model is developed to deal with the multimode process monitoring, which takes advantage of PCA and heuristic smoothing clustering techniques (Chen and Liu, 1999). Gaussian mixture model (GMM) combined with PCA and discriminant analysis (DA) have been integrated for fault detection and isolation, which does not require the normally distributed process data (Choi *et al.*, 2004). As an alternative solution, a Bayesian inference based GMM method has been proposed to characterize different operating modes with various Gaussian components in GMM. Then, a Mahalanobis distance and Bayesian posterior probability based monitoring index is designed to assess process performance under shifting modes (Yu and Qin, 2008, 2009b; Yu, 2012c). In PCA mixture model and GMM based monitoring frameworks, the process data with each operating mode are assumed to follow a multivariate Gaussian distribution approximately. Therefore, they may not be well suited for the scenario where there exists significant within-mode process non-Gaussianity.

In this study, ICA mixture model (ICAMM) is integrated with mutual information based non-Gaussian dissimilarity index for monitoring multimode dynamic processes that have non-Gaussianity within single operating mode. First, a normal benchmark data set is selected to build the ICA mixture model so that the non-Gaussian structure is retained in each component. Then, a sliding window strategy is carried out to obtain a series of subsets of monitored data with the same length as the benchmark set for handling process dynamics. Each sample in the subset of monitored data is classified

into a local ICA component through the maximized posterior probability. Further, the mutual information based dissimilarity index between the local ICA subspaces of the benchmark and monitored data sets is estimated for detecting the abnormal operating events of the process.

The remainder of this article is organized as follows. The conventional PCA and ICA dissimilarity based process monitoring methods are reviewed in Section 2. Then the ICA mixture model based dissimilarity approach is developed in Section 3 for multimode dynamic process monitoring. In Section 4, the superiority of the new approach is demonstrated through its comparison with PCA mixture model based dissimilarity methods in the application example of the Tennessee Eastman Chemical process. Finally, the conclusions of this work are drawn in Section 5.

2.2 Preliminaries

2.2.1 Eigenvalue Decomposition Based PCA Dissimilarity Method

The eigenvalue decomposition based PCA dissimilarity method has been developed for process monitoring and fault detection (Kano *et al.*, 2002). Consider a normal benchmark set $X_1 \in \mathbb{R}^{n \times m}$ and a monitored set $X_2 \in \mathbb{R}^{n \times m}$, where n is the number of samples and m is the number of variables. The covariance matrix of the combined data set is given by

$$R = \frac{1}{2n-1} \begin{bmatrix} X_1 \\ X_2 \end{bmatrix}^T \begin{bmatrix} X_1 \\ X_2 \end{bmatrix} \quad (2.1)$$

The eigenvalue decomposition on R leads to

$$RP_0 = P_0\Lambda \quad (2.2)$$

where P_0 is an orthogonal matrix and Λ is a diagonal matrix with the eigenvalues of R . The data matrices X_1 and X_2 can be transformed as

$$Y_1 = \sqrt{\frac{n-1}{2n-1}} X_1 P_0 \Lambda^{-1/2} \quad (2.3)$$

and

$$Y_2 = \sqrt{\frac{n-1}{2n-1}} X_2 P_0 \Lambda^{-1/2} \quad (2.4)$$

Let S_1 and S_2 be the covariance matrices of Y_1 and Y_2 , respectively. Then the following relationship holds

$$1 - \lambda_j^1 = \lambda_j^2 \quad (2.5)$$

where λ_j^1 and λ_j^2 are the j th eigenvalue of S_1 and S_2 , respectively. Thus, the following eigenvalue decomposition based PCA dissimilarity factor D_{PCA} can be defined for evaluating the dissimilarity of the benchmark and monitored data sets

$$D_{PCA} = \frac{4}{m} \sum_{j=1}^m (\lambda_j^1 - 0.5)^2 \quad (2.6)$$

The larger D_{PCA} value indicates that the monitored set has more different pattern from the normal benchmark set and thereby is more likely to be abnormal.

2.2.2 Modified Angle Based PCA Dissimilarity Method

The modified angle based PCA dissimilarity method can also be used for process monitoring (Singhal and Seborg, 2002a). The dissimilarity index for the benchmark and monitored data sets X_1 and X_2 is defined as follows

$$D_{PCA}^\lambda \triangleq \frac{\sum_{i=1}^p \sum_{j=1}^p (\lambda_i^{X_1} \lambda_j^{X_2}) \sin^2 \theta_{ij}}{\sum_{i=1}^p \lambda_i^{X_1} \lambda_j^{X_2}} \quad (2.7)$$

where λ^{X_1} and λ^{X_2} correspond to the eigenvalues of $X_1^T X_1$ and $X_2^T X_2$, respectively. In addition, p denotes the number of PCs retained in the PCA model and θ_{ij} is angle between the i -th PC of the benchmark set and the j -th PC of the monitored set. This dissimilarity factor takes into account the variance along each principal component direction.

2.2.3 Mutual Information Based ICA Dissimilarity Factor

In addition to the PCA based dissimilarity factors, a multidimensional mutual information based ICA dissimilarity index D_{MMI} is proposed for non-Gaussian process monitoring (Rashid and Yu, 2012b). At the t -th sampling instant, the measurement sample $x(t) = [x(t)_1, x(t)_2, \dots, x(t)_m]^T$ with m process variables can be expressed as linear combinations of q unknown independent components

$$x(t) = As(t) + b(t) \quad (2.8)$$

where $A \in \mathbb{R}^{m \times q}$ is an unknown mixing matrix, $b(t)$ is the bias vector and $s(t) = [s(t)_1, s(t)_2, \dots, s(t)_q]^T$ represent q independent components. The fast fixed-point ICA algorithm (FastICA) can be used to estimate the mixing matrix A and independent

components $s(t)$ from the measurement data (Hyvärinen and Oja, 2000).

Two sets of ICs, $S_{X_1} \in \mathbb{R}^{q \times n}$ and $S_{X_2} \in \mathbb{R}^{q \times n}$, can be obtained from the normal benchmark set X_1 and the monitored set X_2 , respectively. Thus the multidimensional mutual information between S_{X_1} and S_{X_2} is expressed as

$$\text{MMI}(S_{X_1}, S_{X_2}) = \psi(l) - \frac{1}{l} - \langle \psi(n_{S_1}) + \psi(n_{S_2}) \rangle + \psi(n) \quad (2.9)$$

where $\psi(\cdot)$ is the digamma function given by

$$\psi(x) = \Gamma(x)^{-1} d\Gamma(x)/dx \quad (2.10)$$

with $\Gamma(x)$ denoting the Gamma function (Kraskov *et al.*, 2004). In addition, l represents the number of nearest neighbors identified through data clustering, $\langle \cdot \rangle$ denotes the average over all observations in the data set, $n_{S_{X_1}}$ and $n_{S_{X_2}}$ are the numbers of samples in proximity to the nearest neighbors within two IC subspaces, and n is the number of samples in the benchmark or monitored data set. Hence, the multidimensional mutual information based dissimilarity index D_{MMI} can be defined as follows to evaluate the statistical dependency between the benchmark and monitored IC subspaces

$$D_{\text{MMI}} = \frac{I_1^2}{I_2^2} \cdot \frac{1}{\text{MMI}(S_{X_1}, S_{X_2})} \quad (2.11)$$

where I_1^2 and I_2^2 are the ICA based I^2 statistics for the benchmark and monitored data sets. The larger dissimilarity index value indicates the higher tendency of monitored operation to be abnormal because of the more distinct patterns of the monitored set with respect to the normal benchmark set.

2.3 ICA Mixture Model Based Dissimilarity Approach for Multimode Process Monitoring

2.3.1 ICA Mixture Model

Finite mixture model can be used to approximate a wide range of non-Gaussian probability density functions and has been widely applied to classification, regression and probability density estimation. If the data in each component within the mixture model are generated from a linear combination of independent and non-Gaussian sources, the underlying data generation mechanism can be characterized by ICA mixture model. In contrast to Gaussian mixture model, ICA mixture model allows modeling of different classes with locally non-Gaussian structure (Lee *et al.*, 2000).

Suppose that the data $X = [x(1), x(2), \dots, x(n)] \in \mathbb{R}^{m \times n}$ are generated from a multimode process. The joint probability density function of the observed data is formulated as

$$p(X|\Theta) = \prod_{t=1}^n p(x(t)|\Theta) \quad (2.12)$$

The probability density function of $x(t)$ can be then expressed as the following mixture model (Lee *et al.*, 2000):

$$p(x(t)|\Theta) = \sum_{k=1}^K p(x(t)|C_k, \theta_k) p(C_k) \quad (2.13)$$

where K is the number of non-Gaussian classes, C_k denotes the k -th component, $p(C_k)$ represents the corresponding prior probability, and $\Theta = (\theta_1, \theta_2, \dots, \theta_K)$ are the parameters of each density function $p(x(t)|C_k, \theta_k)$. The above mixture density

model is equivalent to a Gaussian mixture model when $p(x(t)|C_k, \theta_k)$ is multivariate Gaussian density function. If the component densities are non-Gaussian and can be described by the ICA model in Eq. 4.1, then the mixture density model becomes ICA mixture model.

To construct an ICA mixture model, the parameters for each class $\theta_k = \{A_k, b_k\}$ need to be estimated. With a set of benchmark data $X = [x(1), x(2), \dots, x(n)]$, the log-likelihood function can be expressed as

$$\log[p(X|\Theta)] = \sum_{t=1}^n \log[p(x(t)|\Theta)] \quad (2.14)$$

thus the parameter estimation problem can be further formulated as the following optimization problem

$$\hat{\Theta} = \arg \max_{\Theta} (\log[p(X|\Theta)]) \quad (2.15)$$

The iterative learning algorithm, which performs gradient ascent search on the log-likelihood function in Eq. 4.2, can be used to estimate the parameter values of the density functions (Lee *et al.*, 2000). For each measurement sample x_t , compute the log-likelihood function of the data for each class as follows

$$\log[p(x(t)|C_k, \theta_k)] = \log[P(s(t)_k)] - \log[|\det(A_k)|] \quad (2.16)$$

where $s(t)_k = A_k^{-1}(x(t) - b(t)_k)$ is implicitly modeled for the adaptation of A_k . Then the posterior probability of the t -th training sample within the k -th class is computed

as

$$p(C_k|x(t), \Theta) = \frac{p(x(t)|C_k, \theta_k)p(C_k)}{\sum_{k=1}^K p(x(t)|C_k, \theta_k)p(C_k)} \quad (2.17)$$

The gradient ascent strategy is used to adapt mixing matrix A_k and bias terms b_k for each class. Further, the extended information-maximization ICA learning rule is employed to approximate the gradient as

$$\Delta A_k = -p(C_k|x(t), \Theta)A_k[I - \Phi_k \tanh(s(t)_k)s(t)_k^T - s(t)_k s(t)_k^T] \quad (2.18)$$

$$b_k = \frac{\sum_{t=1}^n x(t)p(C_k|x(t), \Theta)}{\sum_{t=1}^n p(C_k|x(t), \Theta)} \quad (2.19)$$

where I is the identity matrix and Φ_k represents the m -dimensional diagonal matrix with the i -th diagonal entry $\phi_{k,i}$ for the k -th class as follows

$$\phi_{k,i} = \text{sign}(E\{\text{sech}^2(s(t)_{k,i})\}E\{s(t)_{k,i}^2\} - E\{[\tanh(s(t)_{k,i})]s(t)_{k,i}\}) \quad (2.20)$$

and $s(t)_{k,i}$ is the i -th element of the independent component $s(t)_k \in \mathbb{R}^m$ for the k -th class.

2.3.2 ICA Mixture Model Based Dissimilarity Method

For multimode processes, each subset of measurement data from the same operating condition is characterized by a local ICA model. Therefore, the entire data set from different operating conditions can be mapped into ICA mixture model, where the

number of components is equivalent to the number of operating modes throughout the process. The ICA dissimilarity index D_{MMI} is integrated with ICA mixture model to quantify the dissimilarity between the benchmark and monitored sets within the local ICA model corresponding to the current operating condition.

Consider the benchmark data set $X_b \in \mathbb{R}^{M \times N}$ from all different operating modes and the monitored set $X_m \in \mathbb{R}^{M \times R}$. Both sets consist of M process variables while different number of samples (N samples in the benchmark set and R samples in monitored set). For the k -th subset of benchmark data $X_b^{(k)} \in \mathbb{R}^{M \times N_k}$ with N_k samples from the k -th operating mode, a local ICA model can be built via the FastICA algorithm. Thus an ICA mixture model is constructed by the combination of the K local ICA models. For the benchmark samples from the k -th mode, the relationship between the independent components $S_b^{(k)}$ and the measurements $X_b^{(k)}$ is given by

$$X_b^{(k)} = A_b^{(k)} S_b^{(k)} + E_b^{(k)} \quad (2.21)$$

where $A_b^{(k)}$ and $E_b^{(k)}$ are the mixing and residual matrices for the k -th class in the benchmark set. $S_b^{(k)} = [s_b^{(k)}(1), s_b^{(k)}(2), \dots, s_b^{(k)}(N_k)] \in \mathbb{R}^{D_k \times N_k}$ are the independent components for the k -th mode, where D_k is the number of ICs in the k -th local ICA model. Further, the objective is to find a demixing matrix $W_b^{(k)}$ as follows

$$\hat{S}_b^{(k)} = W_b^{(k)} X_b^{(k)} \quad (2.22)$$

in order to make the rows of the reconstructed matrix $\hat{S}_b^{(k)}$ as independent of each other as possible. Whitening serves as the initial step to eliminate the cross-correlation among the random variables. At the n -th sampling instant, the transformation can

be expressed as

$$z_b^{(k)}(n) = Q_b^{(k)} x_b^{(k)}(n) \quad (2.23)$$

where $Q_b^{(k)} = \Lambda^{-1/2} U^T$ is the whitening matrix, and U and Λ are generated from the eigenvalue decomposition of the covariance matrix as

$$E(x_b^{(k)}(n) x_b^{(k)}(n)^T) = U \Lambda U^T \quad (2.24)$$

After the transformation we have

$$z_b^{(k)}(n) = Q_b^{(k)} x_b^{(k)}(n) = Q_b^{(k)} A_b^{(k)} s_b^{(k)}(n) = B_b^{(k)} s_b^{(k)}(n) \quad (2.25)$$

where $B_b^{(k)}$ is an orthogonal matrix. The i -th column vector $b_{b,i}^{(k)}$ is calculated iteratively so that the i -th independent component has the maximum non-Gaussianity. According to Eq. 2.25, $s_b^{(k)}(n)$ can be estimated as follows

$$\hat{s}_b^{(k)}(n) = B_b^{(k)T} Q_b^{(k)} x_b^{(k)}(n) \quad (2.26)$$

where the demixing matrix $W_b^{(k)} = B_b^{(k)T} Q_b^{(k)}$. The number of ICs, D_k , for the k -th class is determined by the L_2 norm of each row of $W_b^{(k)}$ under the assumption that the rows of $W_b^{(k)}$ with the highest norm have the largest effect on the variations of the ICs. Consequently, the ICA mixture model with K local ICA models corresponding to different operating modes in the benchmark set can be built with the IC subspaces $S_b^{(k)}$ extracted from each class. The I^2 statistic is further calculated from the ICA

mixture model for the systematic part of the process variation as follows

$$I_b^{(k)2}(n) = \hat{s}_b^{(k)}(n)^T \hat{s}_b^{(k)}(n) \quad (2.27)$$

In order to monitor process dynamics effectively, a sliding window with the size w is rolled over the monitored set as illustrated in Fig 4.1. Let $X_m(i) = [x(i), x(i+1), \dots, x(i+w-1)]$ be the i -th monitored data set. Then the next monitored set is $X_m(i+1) = [x(i+1), x(i+2), \dots, x(i+w)]$. Hence, a series of local ICA models can be built on the subsets of monitored data and the corresponding IC subspaces $S_m^{(i)}$ can be obtained. For each subset of monitored data $X_m^{(i)}$, the center point is first calculated as $x_c^{(i)} = \sum_{j=1}^{i+w-1} x(j)/w$ and then the corresponding operating mode is determined according to the maximal posterior probability of $x_c^{(i)}$ belonging to different classes in the ICA mixture model as follows

$$\hat{C}_k = \arg \max_{C_k} (p(C_k | x_c^{(i)}, \Theta_b)) \quad (2.28)$$

where $\hat{C}_k$ denotes the identified mode for $x_c^{(i)}$ and $p(C_k | x_c^{(i)}, \Theta_b)$ is the posterior probabilities of this sample belonging to different operating modes with $\Theta_b = (\theta_b^{(1)}, \theta_b^{(2)}, \dots, \theta_b^{(K)}) = (\{A_b^{(1)}, E_b^{(1)}\}, \{A_b^{(2)}, E_b^{(2)}\}, \dots, \{A_b^{(K)}, E_b^{(K)}\})$. It should be noted that the posterior probability of the n -th sample within the k -th class is computed as

$$p(C_k | x(n), \Theta_b) = \frac{p(x(n) | C_k, \theta_b^{(k)}) p(C_k)}{\sum_{k=1}^K p(x(n) | C_k, \theta_b^{(k)}) p(C_k)} \quad (2.29)$$

where the probability density function $p(x(n)|C_k, \theta_b^{(k)})$ for the k -th component is formulated as

$$p(x(n)|C_k, \theta_b^{(k)}) = \frac{p(s_b^{(k)}(n))}{|\det(A_b^{(k)})|} \quad (2.30)$$

Thus the log-likelihood of the n -th sample $x(n)$ belonging to the k -th class can be

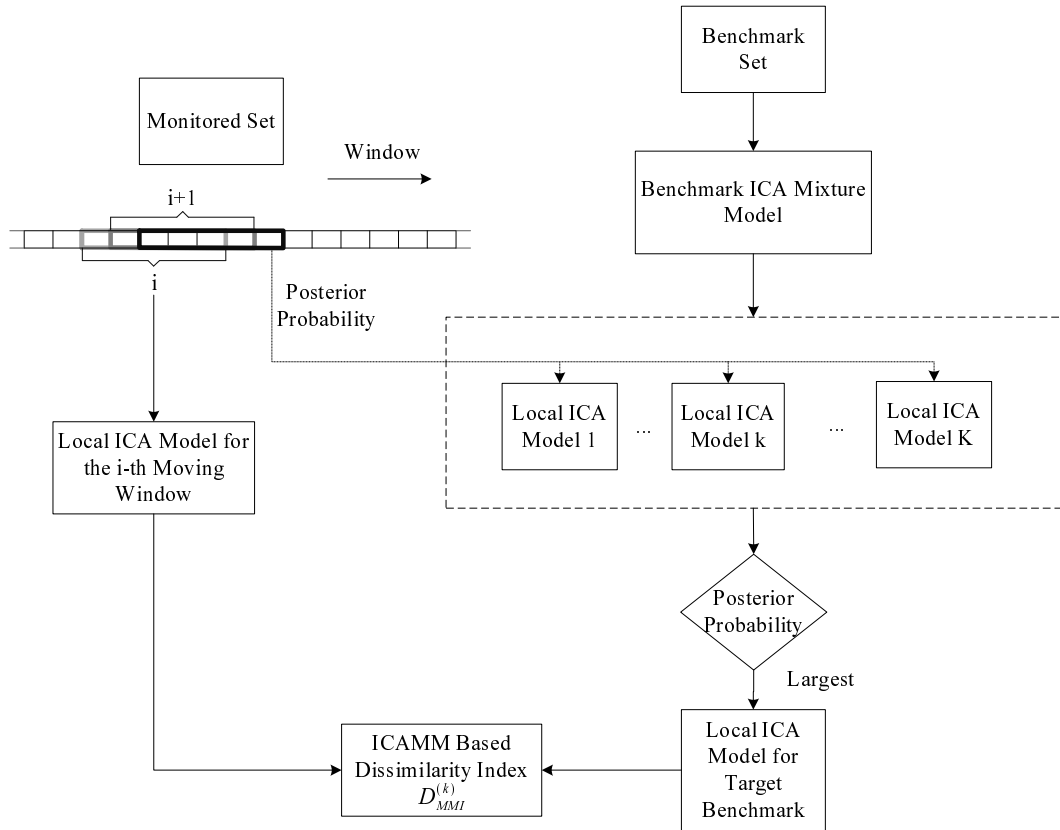


Figure 2.1: Illustration of moving window strategy in the ICA mixture model based dissimilarity method

expressed as

$$\log [p(x(n)|C_k, \theta_b^{(k)})] = \log [p(s_b^{(k)}(n))] - \log [|\det(A_b^{(k)})|] \quad (2.31)$$

where

$$\log [P(s_b^{(k)}(n))] = - \sum_{i=1}^{D_k} \{ \phi_i^{(k)} \log[\cosh(s_{b,i}^{(k)}(n))] - \frac{[s_{b,i}^{(k)}(n)]^2}{2} \} \quad (2.32)$$

The adaptation of the source density parameters is given as follows

$$\phi_i^{(k)} = \text{sign}[\text{kurt}(s_{b,i}^{(k)})]. \quad (2.33)$$

which is the sign function of the kurtosis of the i -th independent component $s_{b,i}^{(k)}$ for the k -th class. The distribution of $s_{b,i}^{(k)}$ is Gaussian when $\phi_i^{(k)}$ is zero while super-Gaussian and sub-Gaussian when $\phi_i^{(k)} = 1$ and $\phi_i^{(k)} = -1$, respectively (Lee *et al.*, 2000).

The number of classes, K , can be determined by maximizing the log-likelihood function. Meanwhile, the operating mode corresponding to the largest posterior probability for each sample, $\hat{C}_k$ is chosen and thus the ICA mixture model based dissimilarity index $D_{\text{MMI}}^{(k)}(i)$ can be defined between the monitored IC subspace $S_m(i)$ and the target benchmark IC subspace $S_b^{(k)}$ as follows

$$D_{\text{MMI}}^{(k)}(i) = \frac{I_m^2(i)}{I_b^{(k)2}} \cdot \frac{1}{\text{MMI}(S_b^{(k)}, S_m(i))} \quad (2.34)$$

where $I_m^2(i)$ and $I_b^{(k)2}$ are the ICA based I^2 statistics for the i -th monitored set and the target benchmark set corresponding to the k -th operating mode $\hat{C}_k$, and $\text{MMI}(S_b^{(k)}, S_m(i))$ is the multidimensional mutual information between the IC subspaces of the target benchmark set $S_b^{(k)}$ and the i -th monitored set $S_m(i)$.

With the ICA mixture model based dissimilarity index defined, the corresponding control limit for each operating mode can be estimated by kernel density estimation

(Bishop, 1995). In this study, the following Gaussian kernel function is selected

$$K(u) = \frac{1}{\sqrt{2\pi}} e^{(-\frac{1}{2}u^2)} \quad (2.35)$$

Then the control limit for the k -th class under the confidence level $(1 - \alpha) \times 100\%$ is estimated as

$$\int_{-\infty}^{D_{\text{MMI},\alpha}^{(k)}} \hat{f}_h(D_{\text{MMI}}^{(k)}) dD_{\text{MMI}}^{(k)} = 1 - \alpha \quad (2.36)$$

where $D_{\text{MMI},\alpha}^{(k)}$ is the estimated control limit value and

$$\hat{f}_h(D_{\text{MMI}}^{(k)}) = \frac{1}{nh} \sum_{i=1}^n K\left(\frac{D_{\text{MMI}}^{(k)} - D_{\text{MMI}}^{(k)}(i)}{h}\right) \quad (2.37)$$

Here h is the bandwidth of kernel function and is selected by least squares cross-validation strategy (Bowman, 1984). The process is considered to be normal if $D_{\text{MMI}}^{(k)} \leq D_{\text{MMI},\alpha}^{(k)}$ and the monitored set belongs to the k -th mode. Otherwise, the fault alarms will be triggered.

The detailed implementation procedure of the ICA mixture model based dissimilarity approach is summarized below and the corresponding schematic diagram is shown in Fig 4.2.

- i) Collect benchmark data X_b from normal process operation under different operating conditions;
- ii) Build ICA mixture model from benchmark data and estimate the model parameter set $\theta^{(k)} = \{A_b^{(k)}, E_b^{(k)}\}$;
- iii) Extract the IC subspaces $S_b^{(k)}$ for $1 \leq k \leq K$ from the ICA mixture model corresponding to the benchmark set;

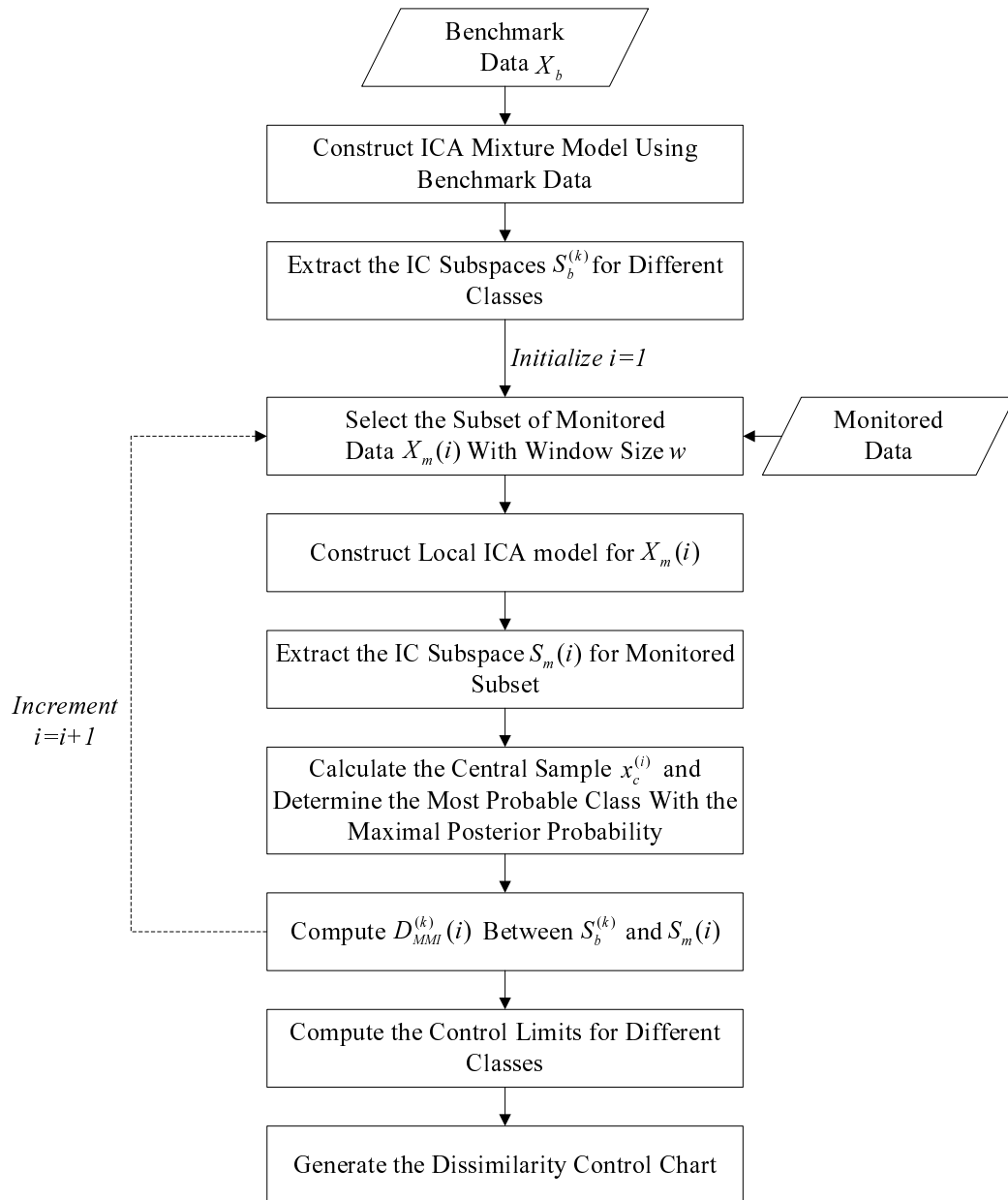


Figure 2.2: Flow chart of the proposed ICA mixture model based dissimilarity method

- iv) Set the initial iteration number as $i = 1$ and select the subset of the monitored data with the window size w as $X_m(i) = [x(i), x(i+1), \dots, x(i+w-1)]$;
- v) For the i th monitored window, use the current monitored data subset $X_m(i)$ to build a local ICA model and extract the IC subspace $S_m(i)$;
- vi) Calculate the center sample $x_c^{(i)}$ for the i th monitored window and further compute its posterior probabilities with respect to all classes $p(C_k|x_c^{(i)}, \Theta)(k = 1, 2, \dots, K)$ through Eq. 4.29;
- vii) Determine the most possible class for the monitored subset $X_m(i)$ with through the maximized posterior probability;
- viii) Compute the ICA mixture model based dissimilarity index $D_{\text{MMI}}^{(k)}(i)$ between the IC subspaces of the monitored subset $X_m(i)$ and the benchmark set for the class C_k ;
- ix) If $x(i+w-1)$ is not the last sampling point in the monitored set, set $i = i+1$ and return to step (6), otherwise continue;
- x) Compute the corresponding control limits for different classes in the estimated ICA mixture model;
- xi) Generate the control chart using the estimated $D_{\text{MMI}}^{(k)}$ index values and the corresponding control limits.

2.4 Application Example

2.4.1 Illustrative numerical example

A numerical example is used to illustrate the usage of the proposed ICA mixture model based dissimilarity approach for monitoring multimode process with non-Gaussianity in each mode. The process data $\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$ are generated from the following system

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 3 & 4 \\ 1 & 2 \\ 2 & 1 \end{bmatrix} \begin{bmatrix} t_1 \\ t_2 \end{bmatrix} + \begin{bmatrix} e_1 \\ e_2 \\ e_3 \end{bmatrix} \quad (2.38)$$

where $\begin{bmatrix} e_1 & e_2 & e_3 \end{bmatrix}^T$ are zero-mean Gaussian noise with standard deviations of $0.2I$ and $\begin{bmatrix} t_1 & t_2 \end{bmatrix}^T$ are non-Gaussian data generated from the following model

$$\begin{bmatrix} t_1 \\ t_2 \end{bmatrix} = \begin{bmatrix} -4s^3 + 3s^2 + 2s \\ 2s^3 + s^2 - 4s \end{bmatrix} \quad (2.39)$$

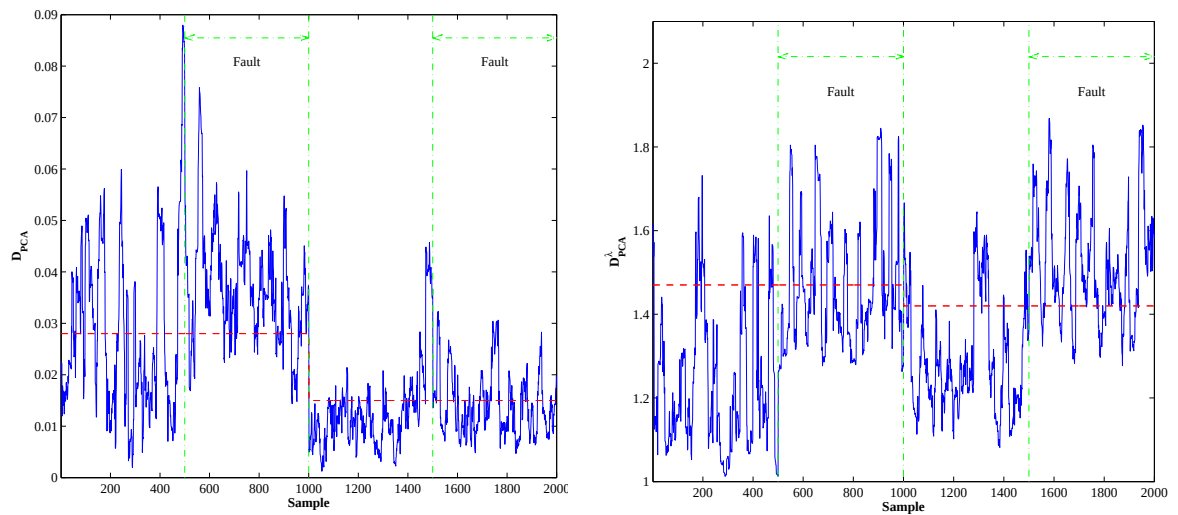
with s donating the Gaussian signal source. Two operating modes are simulated with different signal sources as follows

Mode 1: $s : N(0, 1)$

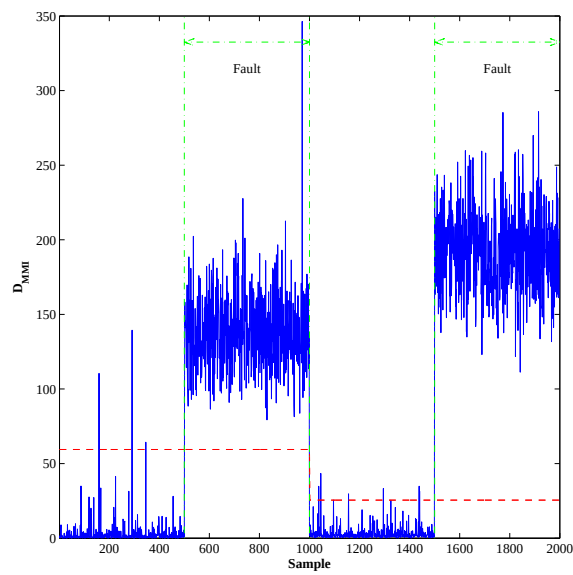
Mode 2: $s : N(-2, 0.8)$

The generated process data $\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$ are essentially non-Gaussian within each operating mode due to the system nonlinearity.

In the training period, 2000 normal samples are generated under each operating mode, and all the 4000 samples are used as the benchmark data to construct the ICA mixture model. Furthermore, one test case with both operating modes is designed to evaluate the performance of the proposed monitoring method. In this test case, the process begins with normal operation in mode 1 from the first until the 500-th sample and then a step error of $\begin{bmatrix} 0.082 & -0.041 & -0.041 \end{bmatrix}^T$ is added to $\begin{bmatrix} x_1 & x_2 & x_3 \end{bmatrix}^T$ from the 501-th sample and remains until the 1000-th sample. Subsequently, the process is shifted to mode 2 with 500 normal samples before the other step error of $\begin{bmatrix} 0.041 & 0.041 & -0.082 \end{bmatrix}^T$ occurs from the 1501-th sample through the end of the operation. The process monitoring results of the eigenvalue decomposition based and the modified angle based PCA mixture dissimilarity method as well as the proposed ICA mixture model based dissimilarity method are shown in Figs. 2.3a, 2.3b and 2.3c, respectively. The confidence level is set to 95% while the widow size is chosen as 25. It can be observed that the two PCA mixture dissimilarity indices are insensitive to the process faults and cannot distinguish clearly between the normal and faulty periods. In contrast, the ICA mixture model based dissimilarity method is able to identify the faulty operations across different operating modes as shown in Fig. 2.3c. The monitoring index D_{MMI} remains below the corresponding confidence limit for the vast majority of the first 500 normal samples in both modes. Furthermore, the index value stays above the corresponding control limits once the fault happens and captures most of the faulty samples. The results of this numerical example demonstrate that the proposed ICA mixture model based dissimilarity method is more effective than the PCA mixture dissimilarity approaches for multimode process monitoring especially when there are significant non-Gaussian features within each mode.



(a) Eigenvalue decomposition based PCA mixture dissimilarity (b) Modified angle based PCA mixture dissimilarity



(c) ICA mixture model based dissimilarity method

Figure 2.3: Monitoring results in the numerical example

2.4.2 Tennessee Eastman Chemical Process

In this section, the proposed multimode dissimilarity approach is applied to the performance monitoring of the Tennessee Eastman Chemical process and its results are compared to those of the conventional PCA mixture model based dissimilarity methods to demonstrate its validity and effectiveness. The flow diagram of the Tennessee Eastman Chemical process is shown in Fig. 4.4 (Downs and Vogel, 1993). There are five major unit operations in this process including a reactor, a product condenser, a vapor-liquid separator, a recycle compressor and a product stripper. Two products G and H along with a by-product F are produced through the chemical reactions with four reactants A , C , D , E and an inert B . The process involves 22 continuous measurement variables, 12 manipulated variables, and 19 composition measurements that are sampled infrequently. In our work, the 22 continuous measurement variables are selected for process performance monitoring purpose, as listed in Table 2.1. A sampling interval of 0.05h is used to collect the benchmark and monitored data. Moreover, the process may run at one of the six operating modes, as summarized in Table 2.2. Meanwhile, the pre-defined abnormal operation events are listed in Table 2.3. Since the process is essentially open-loop unstable, the decentralized control strategy is used for the stable closed-loop operation (Ricker, 1996).

During the training period, 1000 samples are collected under each of the six operating modes and total 6000 samples are obtained to form the benchmark set. In order to examine the performance of the proposed monitoring approach, three test cases with multiple operating modes and various types of process faults are designed, as shown in Table 2.4. Three different dissimilarity based monitoring methods are applied to all the above test cases and the sliding window size in this study is set to 25.

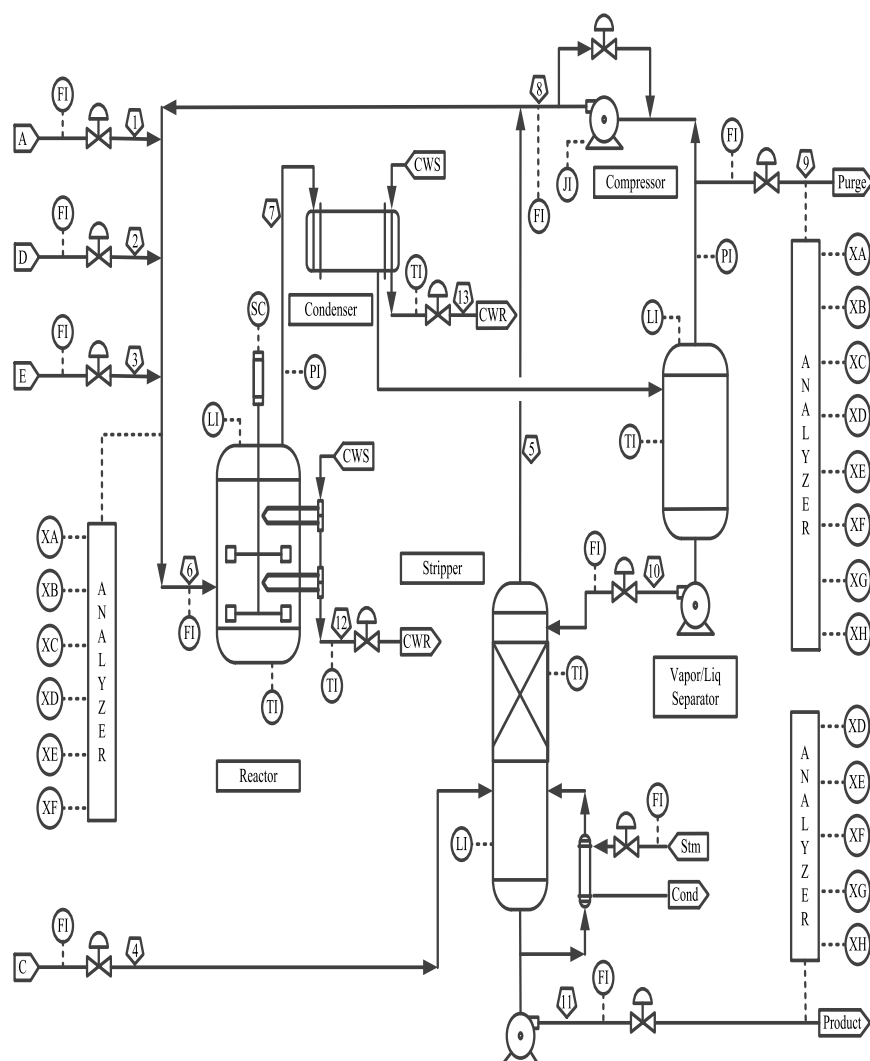
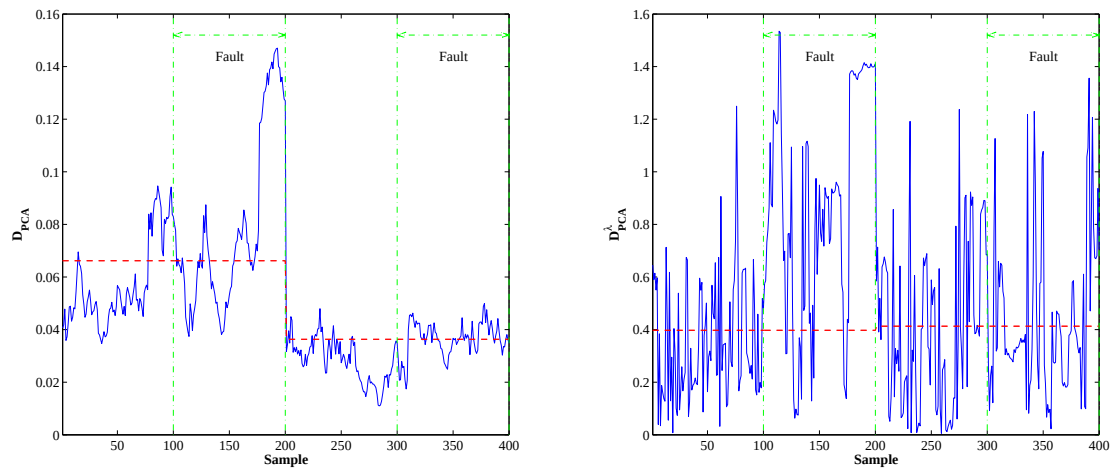
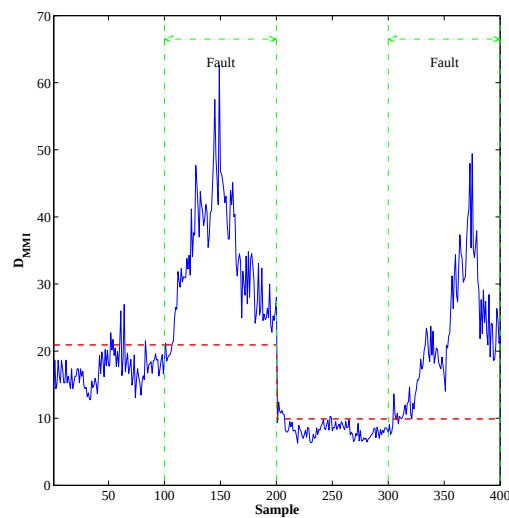


Figure 2.4: Process flow diagram of the Tennessee Eastman Chemical process



(a) Eigenvalue decomposition based PCA mixture dissimilarity method (b) Modified angle based PCA mixture dissimilarity method



(c) ICA mixture model based dissimilarity method

Figure 2.5: Monitoring results of the first test case of the Tennessee Eastman Chemical process

Table 2.1: Monitored variables in the Tennessee Eastman Chemical process

Variable No.	Variable description
1	A Feed (stream 1)
2	D Feed (stream 2)
3	E Feed (stream 3)
4	A and C Feed (stream 4)
5	Recycle Flow (stream 8)
6	Reactor Feed (stream 6)
7	Reactor Pressure
8	Reactor Level
9	Reactor Temperature
10	Purge Rate (stream 9)
11	Separator Temperature
12	Separator Level
13	Separator Pressure
14	Separator Underflow (stream 10)
15	Stripper Level
16	Stripper Pressure
17	Stripper Underflow (stream 11)
18	Stripper Temperature
19	Steam Flow
20	Compressor Work
21	Reactor Coolant Temperature
22	Condenser Coolant Temperature

In the first test case, the process begins with Mode 3 along with a step error in condenser cooling water temperature from the 101-st to the 200-th samples. Then the process is shifted to Mode 2 with 100 normal samples followed by a random variation in condenser cooling water inlet temperature for another 100 samples. The fault detection results of different kinds of mixture model dissimilarity methods are shown in Figs. 2.5a, 2.5b and 2.5c, respectively. It is obvious that PCA mixture dissimilarity indices D_{PCA} and D_{PCA}^{λ} miss a vast majority of the faulty samples and lead to very low sensitivity to process faults. The fault detection rates for D_{PCA} and

Table 2.2: Six operating modes in the Tennessee Eastman Chemical process

Operating mode	G/H Mass Ratio	Production Rate (Stream 11)
1	50/50	7038 kg/h G and 7038 kg/h H
2	10/90	1408 kg/h G and 12669 kg/h H
3	90/10	10000 kg/h G and 1111 kg/h H
4	50/50	Maximum
5	10/90	Maximum
6	90/10	Maximum

D_{PCA}^{λ} are as low as 56.5% and 60.9%, as shown in Table 2.5. The performance in terms of false alarms for these two PCA mixture dissimilarity methods also appear to be undesirable as the false alarm rates for D_{PCA} and D_{PCA}^{λ} are 20.202% and 39.4%, respectively. It can be readily observed from Figs. 2.5a and 2.5b that the abnormal operating events across different modes cannot be well isolated by the PCA mixture model based dissimilarity methods. In comparison, the monitoring results of the proposed ICA mixture model dissimilarity method is shown in Fig. 2.5c. Apparently the performance of fault detection is satisfactory as the fault detection rate reaches 93.6% while the false alarm rate is as low as 6.6%. Though there are very short delays in triggering fault alarms, the presented method can detect the process faults accurately. The significantly improved performance is due to the fact that the process non-Gaussianity is taken into account within each local mode of the ICA mixture model.

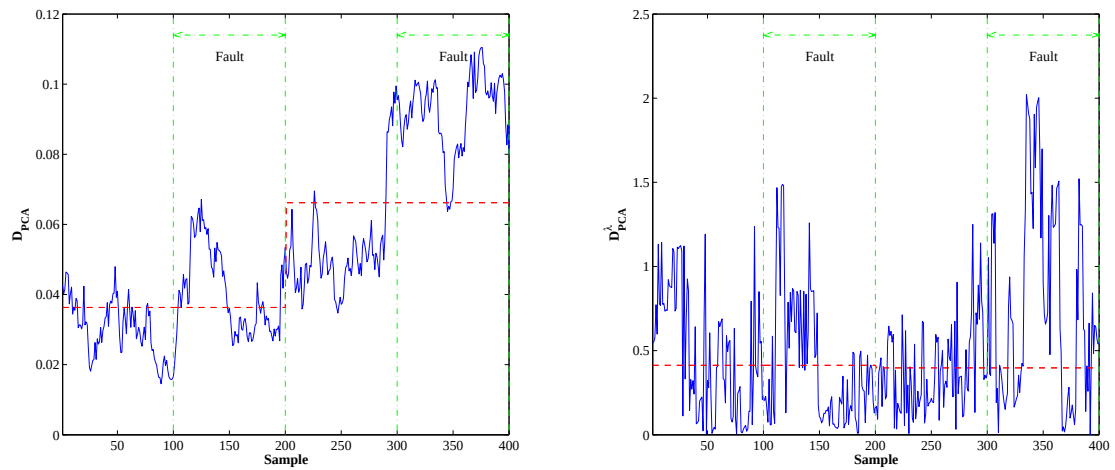
The second test case starts with the normal operation at Mode 2 for 100 samples followed by increased random variations in reactor cooling water temperature. After that, the process returns to the normal operation under Mode 3 and lasts 100 samples before a fault of increased random variations occurs in condenser cooling water inlet temperature from the 301-st through the 400-th samples. The monitoring results of

Table 2.3: Pre-defined faults in the Tennessee Eastman Chemical process

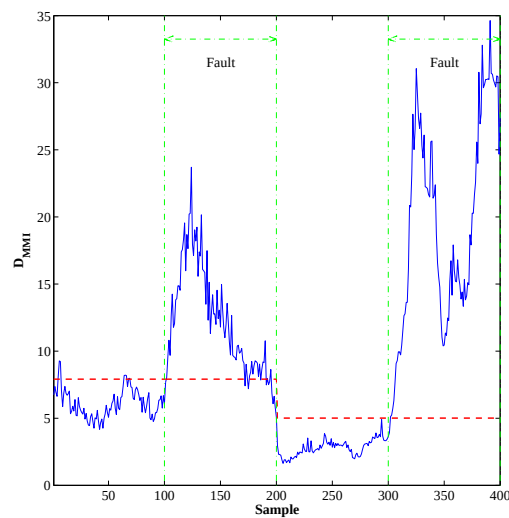
Fault No.	Description
1	Step in A/C feed ratio, B composition constant
2	Step in B composition, A/C ratio constant
3	Step in D feed temperature (stream 2)
4	Step in reactor cooling water inlet temperature
5	Step in condenser cooling water inlet temperature
6	A feed loss (step change in stream 1)
7	C header pressure loss (step change in stream 4)
8	Random variation in A+C feed composition (stream 4)
9	Random variation in D feed temperature (stream 2)
10	Random variation in C feed temperature (stream 4)
11	Random variation in reactor cooling water inlet temperature
12	Random variation in condenser cooling water inlet temperature
13	Slow drift in reaction kinetics
14	Sticking reactor cooling water valve
15	Sticking condenser cooling water valve

the PCA mixture dissimilarity methods are shown in Figs. 2.6a and 2.6b, respectively. It can be seen from both plots that significant portions of normal samples exceed the corresponding confidence limits with the false alarm rate of 19.2% and 44.9%, respectively. Meanwhile, the fault detection rates are only 74.8% and 52.5% with large numbers of faulty samples undetected. In contrast, the superiority of the ICA mixture model dissimilarity method over the other dissimilarity approaches is demonstrated in Fig. 2.6c. The D_{MMI} index shows a strong capability to distinguish between the normal and faulty samples across different modes with very short delays of fault detection. Despite the presence of different kinds of faults, the fault detection rate of the proposed method is as high as 92.6% while the lowest false alarm rate of 4.0% is achieved.

In the last test case, the process operation is changed between Modes 1 and 2.



(a) Eigenvalue decomposition based PCA mixture dissimilarity method (b) Modified angle based PCA mixture dissimilarity method



(c) ICA mixture model based dissimilarity method

Figure 2.6: Monitoring results of the second test case of the Tennessee Eastman Chemical process

Table 2.4: Three test cases in the Tennessee Eastman Chemical process

Case No.	Description
Case 1	Normal operation: Samples 1-100, Mode 3 Faulty operation: Samples 101-200, Mode 3 IDV5: Step change in condenser cooling water temperature Normal operation: Samples 201-300, Mode 2 Faulty operation: Samples 301-400, Mode 2 IDV12: Random variation in condenser cooling water inlet temperature
Case 2	Normal operation: Samples 1-100, Mode 2 Faulty operation: Samples 101-200, mode 2 IDV11: Random variation in reactor cooling water temperature Normal operation: Samples 201-300, Mode 3 Faulty operation: Samples 301-400, Mode 3 IDV12: Random variation in condenser cooling water inlet temperature
Case 3	Normal operation: Samples 1-100, Mode 1 Faulty operation: Samples 101-200, Mode 1 IDV12: Random variation in condenser cooling water inlet temperature Normal operation: Samples 201-300, Mode 2 Faulty operation: Samples 301-400, Mode 2 IDV13: Slow drift in reaction kinetics

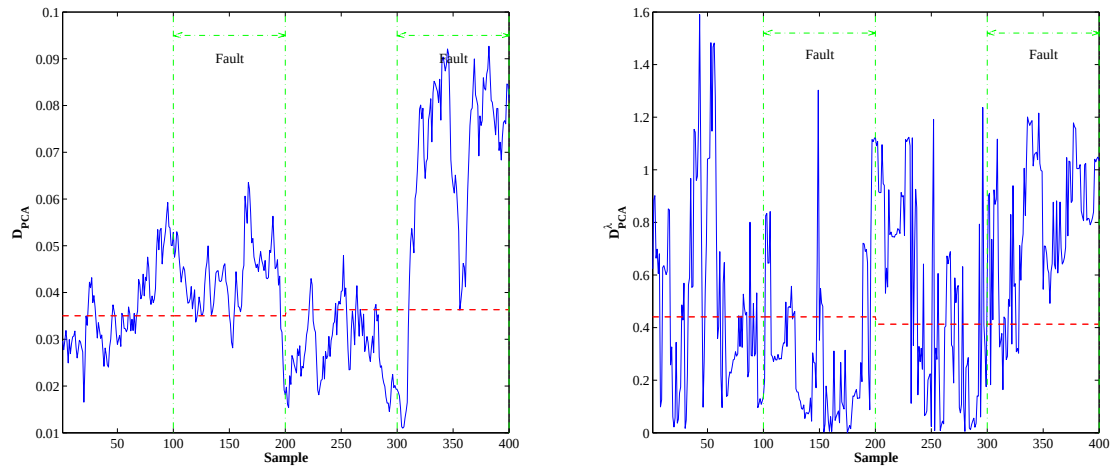
First a fault of increased random variations in condenser cooling water inlet temperature takes place from the 101-st until the 200-th samples. Then the second fault of slow drift in reaction kinetics occurs during the period from the 301-st to the 400-th samples. It is easily observed from Figs. 2.7a and 2.7b that both the D_{PCA} and D_{PCA}^{λ} indices perform poorly on detecting faulty measurements precisely and avoiding false alarms for normal samples. In the D_{PCA} plot, significant number of normal samples under Mode 1 jump above the corresponding control limit with false alarms triggered. Although it performs better in the second normal period, the overall false

Table 2.5: Comparison of fault detection results among different types of dissimilarity methods

Case No.	Monitoring method	Fault detection rate (%)	False alarm rate (%)
Numerical	D_{PCA}	58.6	30.7
	D_{PCA}^{λ}	72.2	23.9
	$D_{MMI}^{(k)}$	99.8	0.4
Case 1	D_{PCA}	53.5	20.2
	D_{PCA}^{λ}	60.9	39.4
	$D_{MMI}^{(k)}$	93.6	6.6
Case 2	D_{PCA}	74.8	19.2
	D_{PCA}^{λ}	52.5	44.9
	$D_{MMI}^{(k)}$	92.6	4.0
Case 3	D_{PCA}	88.6	31.3
	D_{PCA}^{λ}	57.9	51.5
	$D_{MMI}^{(k)}$	92.1	3.5

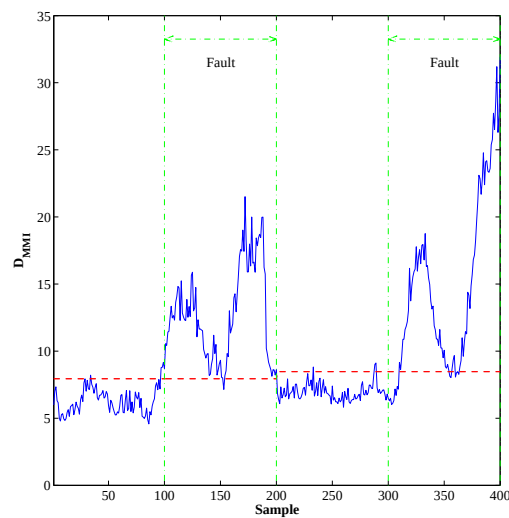
alarm rate of 31.3% is still unsatisfactory. Likewise, the D_{PCA}^{λ} index cannot distinguish the normal and faulty samples in Mode 1, resulting in the poor fault detection and false alarm rates of 57.9% and 51.5%, respectively. The changes of operating modes and different kinds of process faults, however, are accurately identified by the proposed ICA mixture model dissimilarity method. Only 3.5% of normal samples trigger false alarms while the fault detection rate is as high as 92.1%. Therefore, it is confirmed that the proposed dissimilarity method has significant superiority for monitoring multimode processes with non-Gaussianity in local operating modes.

The Matlab R2013a is used to run the simulation of the numerical example and the Tennessee Eastman Chemical process on an Intel Core2 Quad machine with 6 GB RAM. All the test cases demonstrate the validity and effectiveness of the proposed ICA mixture model dissimilarity method. The main reason of the superior performance compared with the PCA dissimilarity method is that the non-Gaussian



(a) Eigenvalue decomposition based PCA mixture dissimilarity method

(b) Modified angle based PCA mixture dissimilarity method



(c) ICA mixture model based dissimilarity method

Figure 2.7: Monitoring results of the third test case of the Tennessee Eastman Chemical process

features can be well characterized in each mode by determining the higher-order statistics. The statistical dependency between the IC subspaces are determined and the multimode process fault can be detected with higher accuracy. Thus the proposed ICA mixture model dissimilarity method provides a reliable and effective way for monitoring the multimode process with non-Gaussian features in each operating mode.

2.5 Conclusions

In this article, an ICA mixture model based non-Gaussian dissimilarity method is proposed for monitoring the performance of multimode processes with local non-Gaussianity. An ICA mixture model is first built from benchmark data to characterize the multimode operation and non-Gaussian process features. With a sliding window along the monitored set, the local class with the maximum Bayesian posterior probability for each monitored subset is identified as the operating mode. Then the statistical independency between the IC subspaces of the benchmark set and the monitored subset corresponding to the local operating mode are estimated as the dissimilarity factor to evaluate the likelihood of the monitored operation to be abnormal.

The presented method is applied to three test cases in the Tennessee Eastman Chemical process and the monitoring results are compared to those of the PCA mixture model dissimilarity methods. It is shown that the new ICA mixture model dissimilarity method has strong capability of detecting process faults while mitigating false alarms for monitoring the performance of multimode non-Gaussian processes. Future research may focus on extending the ICA mixture model dissimilarity method for fault diagnosis to isolate the root-cause variables.

Bibliography

- Albazzaz, H. and Wang, X. Z. (2004). Statistical process control charts for batch operations based on independent component analysis. *Ind. Eng. Chem. Res.*, **43**, 6731–6741.
- AlGhazzawi, A. and Lennox, B. (2008). Monitoring a complex refining process using multivariate statistics. *Control Eng. Pract.*, **16**, 294 – 307.
- Bishop, C. M. (1995). *Neural Networks for Pattern Recognition*. Oxford University Press, Oxford, UK.
- Bowman, A. (1984). An alternative method of cross-validation for the smoothing of density estimates. *Biometrika*, **71**(2), 353–360.
- Chen, J. and Liu, J. (1999). Mixture principal component analysis models for process monitoring. *Ind. Eng. Chem. Res.*, **38**, 1478–1488.
- Chiang, L. H., Russell, E. L., and Braatz, R. D. (2001). *Fault Detection and Diagnosis in Industrial Systems*. Advanced Textbooks in Control and Signal Processing. Springer-Verlag, London, Great Britain.
- Chiang, L. H., Kotanchek, M. E., and Kordon, A. K. (2004). Fault diagnosis based on Fisher discriminant analysis and support vector machines. *Comput. Chem. Eng.*, **28**, 1389–1401.
- Choi, S., Park, J., and Lee, I.-B. (2004). Process monitoring using a Gaussian mixture model via principal component analysis and discriminant analysis. *Comput. Chem. Eng.*, **28**, 1377–1387.

- Choi, S. W., Martin, E. B., Morris, A. J., and Lee, I.-B. (2006). Adaptive multivariate statistical process control for monitoring time-varying processes. *Ind. Eng. Chem. Res.*, **45**, 3108–3118.
- Downs, J. J. and Vogel, E. F. (1993). A plant-wide industrial process control problem. *Comput. Chem. Eng.*, **17**, 245–255.
- Hyvärinen, A. and Oja, E. (2000). Independent component analysis: algorithms and applications. *Neural Networks*, **13**, 411–430.
- Kaneko, H., Arakawa, M., and Funatsu, K. (2008). Development of a new regression analysis method using independent component analysis. *J. Chem. Inf. Model.*, **48**(3), 534–541.
- Kano, M., Hasebe, S., Hashimoto, I., and Ohno, H. (2002). Statistical process monitoring based on dissimilarity of process data. *AIChE J.*, **48**, 1231–1240.
- Kosanovich, K. A., Dahl, K. S., and Piovoso, M. J. (1996). Improved process understanding using multiway principal component analysis. *Ind. Eng. Chem. Res.*, **35**, 138–146.
- Kraskov, A., Stögbauer, H., and Grassberger, P. (2004). Estimating mutual information. *Phys. Rev. E.*, **69**, 066138.
- Ku, W., Storer, R., and Georgakis, C. (1995). Disturbance detection and isolation by dynamic principal component analysis. *Chemometr. Intell. Lab.*, **30**, 179–196.
- Lee, J., Kang, B., and Kang, S. (2011). Integrating independent component analysis and local outlier factor for plant-wide process monitoring. *J. Proc. Cont.*, **21**, 1011–1021.

- Lee, J.-M., Yoo, C., Choi, S., Vanrolleghem, P., and Lee, I.-B. (2004a). Nonlinear process monitoring using kernel principal component analysis. *Chem. Eng. Sci.*, **59**, 223–234.
- Lee, J.-M., Yoo, C., and Lee, I.-B. (2004b). Statistical monitoring of dynamic processes based on dynamic independent component analysis. *Chem. Eng. Sci.*, **59**, 2995–3006.
- Lee, T.-W., Lewicki, M., and Sejnowski, T. (2000). ICA mixture models for unsupervised classification of non-Gaussian classes and automatic context switching in blind signal separation. *IEEE Trans. Pattern Anal.*, **22**, 1078–1089.
- Mahadevan, S. and Shah, S. (2009). Fault detection and diagnosis in process data using one-class support vector machines. *J. Proc. Cont.*, **19**, 1627–1639.
- Martin, E. B. and Morris, A. J. (1996). Non-parametric confidence bounds for process performance monitoring charts. *J. Proc. Cont.*, **6**, 349–358.
- Miletic, I., Quinn, S., Dudzic, M., Vaculic, V., and Champagne, M. (2004). An industrial perspective on implementing on-line applications of multivariate statistics. *J. Proc. Cont.*, **14**, 821–836.
- Nomikos, P. and MacGregor, J. F. (1994). Monitoring batch processes using multiway principal component analysis. *AIChE J.*, **40**, 1361–1375.
- Qin, S. J. (2003). Statistical process monitoring: Basics and beyond. *J. Chemometr.*, **17**, 480–502.
- Qin, S. J. and Yu, J. (2007). Recent developments in multivariable controller performance monitoring. *J. Proc. Cont.*, **17**, 221–227.

- Raich, A. and Çinar, A. (1996). Statistical process monitoring and disturbance diagnosis in multivariable continuous processes. *AIChE J.*, **42**, 995–1009.
- Rashid, M. and Yu, J. (2012a). Hidden Markov model based adaptive independent component analysis approach for complex chemical process monitoring and fault detection. *Ind. Eng. Chem. Res.*, **51**, 5506–5514.
- Rashid, M. and Yu, J. (2012b). A new dissimilarity method integrating multidimensional mutual information and independent component analysis for non-Gaussian dynamic process monitoring. *Chemometr. Intell. Lab.*, **115**, 44–58.
- Ricker, N. L. (1996). Decentralized control of the Tennessee Eastman challenge process. *J. Proc. Cont.*, **6**, 205–221.
- Singhal, A. and Seborg, D. E. (2002a). Pattern matching in historical batch data using PCA. *IEEE Contr. Sys. Mag.*, **22**, 53–63.
- Singhal, A. and Seborg, D. E. (2002b). Pattern matching in multivariate time series databases using a moving-window approach. *Ind. Eng. Chem. Res.*, **41**, 3822–3838.
- Singhal, A. and Seborg, D. E. (2005). Effect of data compression on pattern matching in historical data. *Ind. Eng. Chem. Res.*, **44**, 3203–3212.
- Singhal, A. and Seborg, D. E. (2006). Evaluation of a pattern matching method for the Tennessee Eastman challenge process. *J. Proc. Cont.*, **16**, 601–613.
- Treasure, R., Kruger, U., and Cooper, J. (2004). Dynamic multivariate statistical process control using subspace identification. *J. Proc. Cont.*, **14**, 279–292.
- Venkatasubramanian, V., Rengaswamy, R., Yin, K., and Kavuri, S. N. (2003). A review of process fault detection and diagnosis: Part I: Quantitative model-based methods. *Comput. Chem. Eng.*, **27**, 313–326.

- Yu, J. (2012a). A Bayesian inference based two-stage support vector regression framework for soft sensor development in batch bioprocesses. *Comput. Chem. Eng.*, **41**, 134–144.
- Yu, J. (2012b). A nonlinear kernel Gaussian mixture model based inferential monitoring approach for fault detection and diagnosis of chemical processes. *Chem. Eng. Sci.*, **68**, 506–519.
- Yu, J. (2012c). A particle filter driven dynamic gaussian mixture model approach for complex process monitoring and fault diagnosis. *J. of Process. Control*, **22**, 778–788.
- Yu, J. (2013). A support vector clustering-based probabilistic method for unsupervised fault detection and classification of complex chemical processes using unlabeled data. *AIChE J.*, **59**, 407–419.
- Yu, J. and Qin, S. J. (2008). Multimode process monitoring with Bayesian inference-based finite Gaussian mixture models. *AIChE J.*, **54**, 1811–1829.
- Yu, J. and Qin, S. J. (2009a). MIMO control performance monitoring using left/right diagonal interactors. *J. of Process. Control*, **19**, 1267–1276.
- Yu, J. and Qin, S. J. (2009b). Multiway Gaussian mixture model based multiphase batch process monitoring. *Ind. Eng. Chem. Res.*, **48**, 8585–8594.
- Yu, J. and Qin, S. J. (2009c). Variance component analysis based fault diagnosis of multi-layer overlay lithography processes. *IIE Trans.*, **41**, 764–775.
- Yu, J. and Rashid, M. (2013). A novel dynamic bayesian network-based networked process monitoring approach for fault detection, propagation identification, and root cause diagnosis. *AIChE J.*, **59**, 2348–2365.

Zhao, S. J., Zhang, J., and Xu, Y. M. (2004). Monitoring of processes with multiple operating modes through multiple principle component analysis models. *Ind. Eng. Chem. Res.*, **43**, 7025–7035.

Chapter 3

Multivariate Video Analysis and Gaussian Process Regression Model Based Soft Sensor for Online Estimation and Prediction of Nickel Pellet Size Distributions

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Contributions:

Jingyan Chen developed the two video analysis methods in this chapter in consultation with Dr. Jie Yu and Dr. Yale Zhang. All the images and videos of nickel pellets are provided by Dr. Yale Zhang and the video analysis are performed by Jingyan Chen. The paper is written by Jingyan Chen and edited by Dr. Jie Yu and Dr. Yale Zhang.

3.1 Introduction

Particle size distribution is a crucially important quality variable in different industrial operations including mining, materials and pharmaceutical processes. Specifically in mining industry, accurate pellet size measurement and prediction can substantially improve product quality, production yield and energy efficiency. Mechanical sieving serves as one of the traditional pellet sizing methods, in which pellets are passed through the grids of mesh in order to determine the corresponding size distributions (Koh *et al.*, 2009). However, the intrusive test requires representative samples manually taken from the pellet decomposers and such off-line analysis is not suitable for automatic control and real-time optimization of pellet production processes.

Predictive model based soft sensors have attracted increasing attention from academia and industry in the past decades (Kano and Nakagawa, 2008; Kadlec *et al.*, 2011; Yu, 2012a; Yu and Qin, 2008, 2009). Soft sensors usually make use of available process measurement data or prior knowledge on process mechanism to build predictive models for estimating key product quality variables that cannot be easily measured by physical hardware in a real-time fashion (Lin *et al.*, 2007; Kadlec *et al.*, 2009; Yu, 2012c). There are two types of soft sensors, namely mechanistic model based and process data driven soft sensors. Traditional model-based soft sensors are mainly based on first-principle process models along with extended Kalman filter or adaptive observer techniques (Doyle III, 1998; Assis and Filho, 2000). However, the model development requires in-depth process knowledge on physical and chemical mechanisms and the modeling effort can be quite heavy. Alternatively, data-driven soft sensors rely on process data and thus can alleviate the mechanistic model development effort and knowledge requirement. Different kinds of data-driven soft sensor methods have been developed, including principal component analysis (PCA), partial

least squares (PLS), artificial neural networks (ANN), support vector machine (SVM) and Gaussian process regression (GPR) (Hoskins and Himmelblau, 1988; Kresta *et al.*, 1994; Yan *et al.*, 2004; Yu, 2012b,e; Yu *et al.*, 2013). Though PCA and PLS based soft sensors can deal with the variable con-linearity and identify the statistical models within lower-dimensional latent subspace, they are essentially linear models and thus may not account for significant process nonlinearity. Alternatively, ANN, SVM and GPR approaches can be adopted to construct data-driven soft sensors for nonlinear processes (Qin and McAvoy, 1992; Ruiz *et al.*, 2000; Napoli and Xibilia, 2011; Rashid and Yu, 2012; Yu, 2012d,e). Soft sensor concept and methods are definitely attractive for measuring pellet size distributions in an on-line fashion instead of off-line lab analysis. With reliable soft sensors for online size measurement, model predictive control and real-time optimization of particle processes become possible. A soft sensor approach by integrating ANN and PCA is developed to dynamically estimate the particle size distributions of grinding circuits, where on-line adaption of neural network model is achieved to deal with the time varying nature of grinding circuits and meanwhile the structure of neural network is simplified through PCA strategy (Du *et al.*, 1997). More recently, a soft sensor approach relying on the parameter-constrained identification algorithm for on-line particle size estimation in wet grinding circuits is developed by taking into account prior process knowledge (Sbarbaro *et al.*, 2008). In addition, a neural network based soft sensor is designed to predict the size distributions of disarranged ore particles by utilizing particle images and their uniformity (Ko and Shang, 2011).

Recently, multivariate image analysis techniques have been widely explored for soft sensor based pellet size measurement and show significant advantages over traditional mechanical sieving approach that is labor and time intensive. The main purpose of image analysis is to extract useful measurement information from digitized images

by analyzing their pixel arrays. Depending on the image features acquired, different methods are further developed for analyzing and measuring various types of parameters such as particle counts, shape characteristics, area fractions, and spatial and size distributions (MacGregor *et al.*, 2005; Torabi *et al.*, 2005). Multivariate image analysis approaches typically involve latent subspace projections of images and reduce dimensionality of data matrices, which are different from the filtering and edge detection steps of regular image processing (Bharati and MacGregor, 1998; Prats-Montalbán *et al.*, 2011). Multivariate images are then decomposed into orthogonal components through transformation into a number of latent variables that retain orthogonal components through transformation into a number of latent variables that retain most of image information (Yu and MacGregor, 2004). For the purpose of isolating pellets from background images, the multivariate PCA model of blank background is built and the pellets are identified by comparing the background model so as to estimate the pellet size distributions (Sarkar *et al.*, 2009). Moreover, image segmentation based on multi-flash imaging is introduced to capture the geometric edges around particles from shadow information (Koh *et al.*, 2009). For quantitative prediction purpose, PLS model is also built from histogram features within latent-variable score plots in order to predict the coating concentration of snack products (Yu and MacGregor, 2003). Likewise, a method based on PLS model and angle measuring technique is employed to predict the particle size distributions of natural sands (Dahl and Esbensen, 2007). Moreover, the fiber diameter distributions in nano-fibers are predicted by utilizing wavelet transformation and grey-level co-occurrence matrices (Facco *et al.*, 2010). In addition to active academic research, a commercial system termed as WipFrag is developed to estimate the pellet size distributions in an on-line fashion, where size measurements are obtained by using thresholding, gradient operators, and morphological technique (Maerz, 1999; Koh *et al.*, 2009). Though image

analysis based pellet sizing methods can acquire size distributions non-intrusively, the high precision of estimation and prediction may not be guaranteed due to some limiting factors such as the overlapping effects among different sizes of pellets and the undetected areas caused by the specific positions of camera systems.

Image analysis based soft sensor approaches have been intensively investigated for particle size distribution measurement within emulsion and suspension polymerization systems of industrial crystallization processes. For instance, the light scattering technique focuses a laser beam through a probe tip and then collects the scattered laser light to obtain the crystal size information (Braatz and Hasebe, 2002; Monnier *et al.*, 1996; Tähti *et al.*, 1999). Nevertheless, this method is more appropriate for determining the suspension size distributions under low volume fractions. Alternatively, the laser backscattering approach is explored to characterize the particle size distributions in suspension polymerization reactors with high particle densities but a large number of calibration experiments are required (Togkalidou *et al.*, 2001). Meanwhile, inverse modeling method is integrated with laser backscattering approach to determine polymeric bead size distributions under the assumption that the backscattering light is perfect at different angles (Hukkanen and Braatz, 2003; Fujiwara *et al.*, 2005). Alternative effort has also been attempted to estimate particle shape and size distributions by wavelet transform and multi-scale segmentation based image analysis methods (Chen and Wang, 2005; Calderon De Anda *et al.*, 2005b,a). In order to handle high particle concentrations, illumination through reflected light is required in the above techniques, which may lead to poorly identified particle boundaries. Furthermore, model-based object recognition algorithm is applied to identify crystal objects with a wide range of sizes and shapes by matching raw image features with pre-defined models (Larsen *et al.*, 2006, 2007). However, the overlapping effect in still images given high particle concentrations still poses a significant challenge towards

the precise estimation of size distributions.

Aimed at eliminating the particle overlapping effect that cannot be easily handled by conventional image analysis based methods, two video analysis based approaches are proposed in this study by making use of the videos of free-falling pellets for estimating their size distributions without any intrusive tests. In the first video analysis approach, the edges of the free-falling tracks in different video frames are captured and thus the pellet diameters are equivalent to the widths of the corresponding free-falling tracks. For the second video analysis method, the filtered gray-scale video frames are scanned row by row so as to obtain the filtered gray-scale curves. Then Gaussian process regression (GPR) models are constructed for decomposing and fitting different sub-curves in order to estimate and predict the diameters of various pellets along the horizontal direction. Furthermore, a counting rule for pellet size distribution is developed to get rid of the overlapping effect along the vertical direction of free-falling pellets. The performance of these two video analysis based pellet sizing methods is demonstrated and compared through the lab-scale video clips of free-falling nickel pellets. With the precise measurement of pellet size distributions, the amount of nickel seeds added to the decomposer can be optimally controlled so as to avoid undesirable product quality fluctuations as well as improve production unit availability.

The remainder of this paper is organized as follows. The conventional image analysis based pellet sizing method and its challenges are briefly described in Section 2. Then the two video analysis based pellet sizing methods along with the corresponding illustrative examples of two test videos are shown in Section 3. In Section 4, the measurement results of pellet size distributions from these two video analysis based methods are presented and compared. Finally, the conclusions and future work are discussed in Section 5.

3.2 Image Analysis Based Pellet Sizing Method

Image analysis based pellet sizing techniques have been widely explored for on-line measurement and basically consist of image acquisition, image preprocessing, feature extraction and size estimation steps. High resolution images are first captured from a particular location within pellet processes and then digitized into pixel images in order to extract useful geometric features for estimating pellet size distributions. The success of image analysis based pellet sizing method relies on the quality of images as well as the effectiveness of image analysis. Traditional image analysis based pellet sizing methods require efficient edge detection of different pellets in the preprocessed and filtered images. First the image of well mixed nickel pellets in a bin is taken. Then different layers of filters are applied to the image so as to extract significant features and identify pellet edges. After edge detection, pellet diameters can be identified from the local maximum distances and thus pellet size distributions may be estimated by incorporating all pellet diameters in the images.

In order to illustrate the conventional image analysis based pellet sizing method, the image of nickel pellet samples is analyzed to obtain pellet size distribution. The original image, its pellet edge detection results, and the corresponding pellet size estimation results are depicted in Fig. 4.1 (a), (b), and (c), respectively. Moreover, the estimated pellet size distribution and cumulative distribution compared with the actual ones are shown in Fig. 4.1 (d). The significant inconsistency between the actual and estimated pellet size distributions implies that the conventional image analysis based pellet sizing method may not be accurate and reliable. The main reason of the poor prediction results lies in the overlapping effect of different pellets in still images. Basically those small pellets tend to move onto lower layers and thus are hidden behind the large pellets in upper layers. Consequently, the overlapped small

pellets can hardly be detected and identified from the edge detection strategy. It is therefore desirable to develop new approaches in order to eliminate the overlapping effect of pellets and obtain size distribution prediction results with higher accuracy.

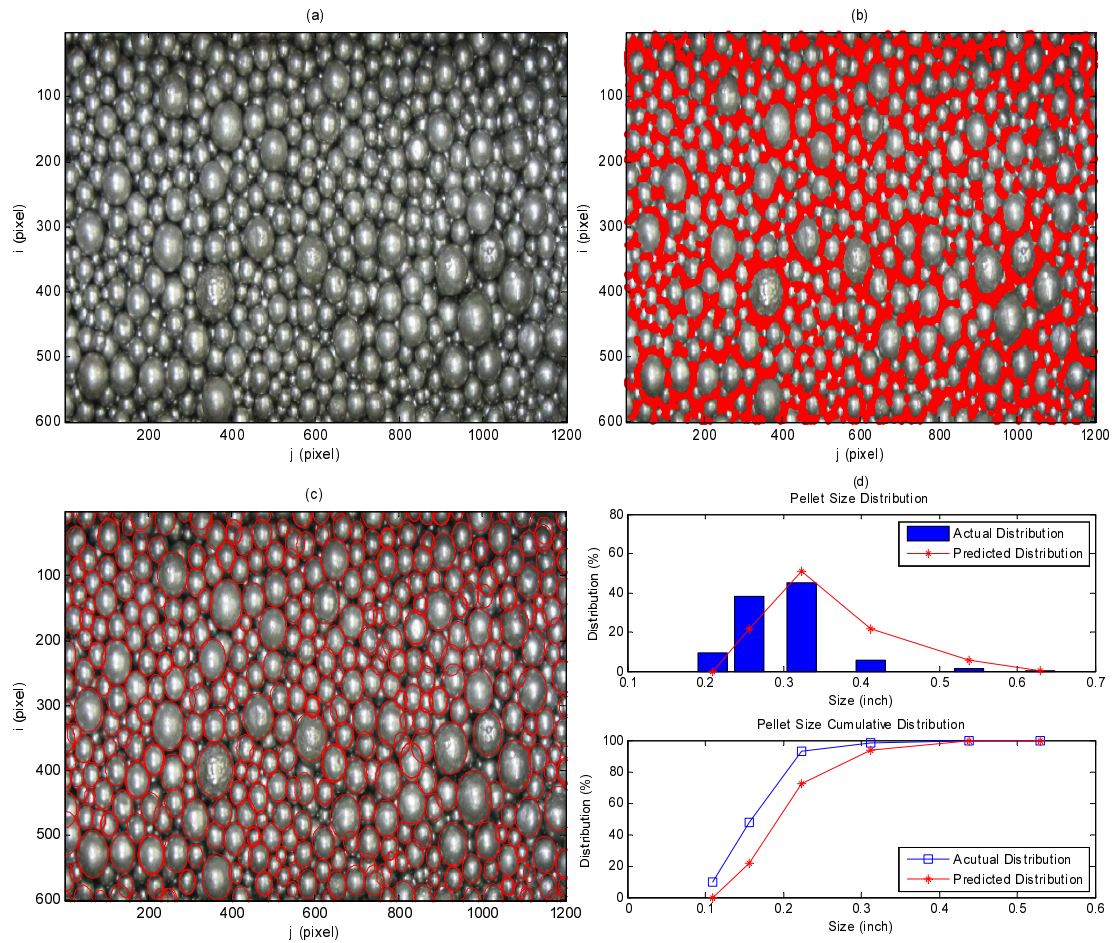


Figure 3.1: Illustrative example of image analysis based pellet sizing method: (a) original image; (b) pellet edge detection results; (c) pellet identification results; and (d) pellet size distribution and cumulative distribution

3.3 Video Analysis Based Pellet Sizing Soft Sensor Methods

Due to the limitation of overlapping effect in the conventional image analysis based pellet sizing method, two kinds of video analysis based pellet sizing approaches are developed to estimate the nickel pellet size distributions in our study. The videos of free-falling pellets are taken with proper lighting conditions. Then the free-falling tracks of nickel pellets in different video frames are utilized for measuring the pellet diameters. In the first video analysis method, the Sobel edge detection strategy is employed in the black and white binary video frames in order to capture the features on pellet diameters and further estimate the size distributions. In the second video analysis approach, the filtered gray-scale frames are scanned row by row so that the diameters of different pellets can be obtained from the filtered gray-scale curves. Then Gaussian process regression models are developed to decompose the gray-scale curves and predict the pellet diameters along the horizontal direction. Further, a counting rule is designed to eliminate the overlapping effect of pellets along the vertical direction. It is assumed that there are total P frames in the video and all the pellets take the time of n video frames to fall from the top to the bottom of the video region. As long as the pellet diameters in every n consecutive frames are measured, the size distribution of all the pellets in the video can be obtained. In addition, the position and lighting of video camera are fixed for all the video to ensure that the ratio between the number of pixels in the video frames and the number of inches in geometric size remains the same.

3.3.1 Pre-processing of Video Frames

In order to extract useful geometric features on pellet sizes from different video frames, preprocessing procedure is designed to remove the color gradient and the background illumination. Consider the RGB (red-green-blue) color image $I_1(i, j)$ in the p -th video frame, where $I_1(i, j)$ denotes the RGB value for the i -th pixel row and the j -th pixel column. Since the color is not the main feature for estimating pellet sizes, the RGB color image $I_1(i, j)$ is converted to the gray-scale image $I_2(i, j)$ by performing a weighted sum of the R, G, and B components of the corresponding pixel row and column as follows

$$I_2(i, j) = 0.2989R(i, j) + 0.5870G(i, j) + 0.1140B(i, j) \quad (3.1)$$

where the coefficients represent human perception of red, green and blue colors and are used in standard color video systems (Čadík, 2008). In order to remove the non-uniform background from the gray-scale image $I_2(i, j)$, the background illumination $I_3(i, j)$ is estimated by conducting morphological opening on $I_2(i, j)$ as

$$I_3 = I_2 \circ b = (I_2 \ominus b) \oplus b \quad (3.2)$$

where b is the disk-shaped structuring element with the corresponding size less than that of the smallest free-falling track while the morphological opening operation $\circ$ is equivalent to an erosion $\ominus$ followed by a dilation $\oplus$. The erosion and dilation operations are defined as follows (Lillesand *et al.*, 2008; Zhou *et al.*, 2009)

$$f(i, j) = [I_2 \ominus b](i, j) = \min_{(s, t) \in b} \{I_2(i + s, j + t)\} \quad (3.3)$$

and

$$[f \oplus b](i, j) = \max_{(s,t) \in b} \{f(i-s, j-t)\} \quad (3.4)$$

Thus the filtered gray-scale image $I_4(i, j)$ with uniform background can be obtained as

$$I_4(i, j) = I_2(i, j) - I_3(i, j) \quad (3.5)$$

The gray-scale value is zero in the background part of $I_4(i, j)$ since the background illumination is removed.

3.3.2 The First Video Analysis Based Pellet Sizing Method

The first video analysis based pellet sizing method is conducted by detecting the edges of free-falling tracks and the width of each track equals the diameter of the corresponding free-falling pellet. The illustrative procedures of this method is shown in Fig. 4.2. The black and white binary image $I_5(i, j)$ is first obtained by thresholding the filtered gray-scale frame $I_4(i, j)$ as follows

$$I_5(i, j) = \begin{cases} 1(white), & I_4(i, j) \geq L \\ 0(black), & I_4(i, j) < L \end{cases} \quad (3.6)$$

where L is the normalized global threshold that can be obtained from Otsu's method by minimizing the intra-class variance of the black and white pixels (Otsu, 1975). The Sobel operation for approximating the gradient of binary function at each image point is then applied to detect the geometric edges of the free-falling tracks (Parker, 2010; Maaß *et al.*, 2012). Assume that $G_i(i, j)$ and $G_j(i, j)$ are the images containing

the approximate horizontal and vertical derivatives at each point

$$G_i(i, j) = \begin{bmatrix} 1 & 0 & -1 \\ 2 & 0 & -2 \\ 1 & 0 & -1 \end{bmatrix} * I_5(i, j) \quad (3.7)$$

$$G_j(i, j) = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 0 & 0 \\ -1 & -2 & -1 \end{bmatrix} * I_5(i, j) \quad (3.8)$$

where the operator $*$ denotes the 2-dimensional convolution operation. Thus the gradient magnitude $G(i, j)$ and direction $\Theta(i, j)$ at the image point (i, j) can be expressed as

$$G(i, j) = \sqrt{G_i^2(i, j) + G_j^2(i, j)} \quad (3.9)$$

and

$$\Theta(i, j) = \arctan \left(\frac{G_j(i, j)}{G_i(i, j)} \right) \quad (3.10)$$

Consequently, the edges can be identified at those points where the gradient of I_5 is maximized

$$(i^E, j^E) = \arg \max_{(i, j)} G(i, j) \quad (3.11)$$

where (i^E, j^E) represents the identified edge point. Once the pellet diameters in n consecutive video frames are obtained, the pellet size distributions can then be

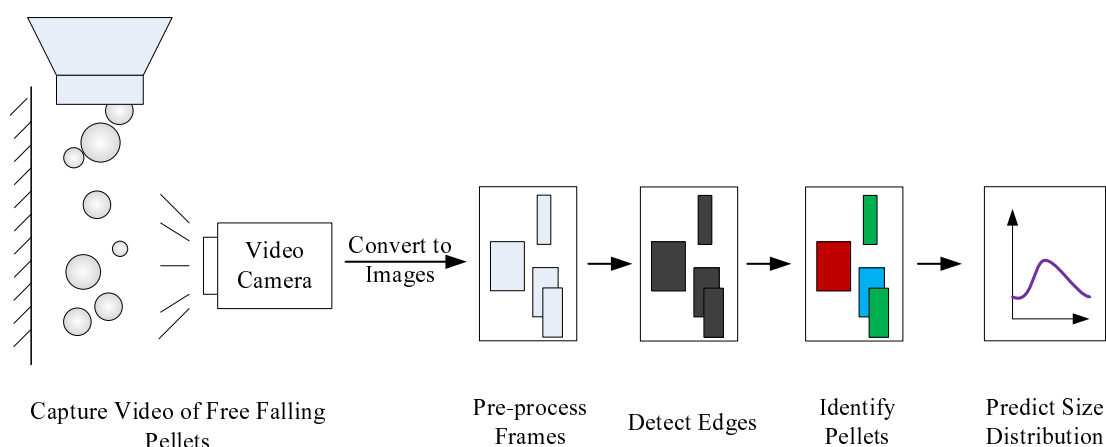


Figure 3.2: Illustrative procedure of the first video analysis based pellet sizing method

estimated.

An Illustrative Example

The first video analysis based pellet sizing method is applied to two lab-scale test videos of free-falling nickel pellets. The initial velocity of free-falling motion of pellets is assumed to be zero and the frame rate of the test videos is 29 frames per second. There are total 850 and 1160 frames in the first and the second test videos respectively and every 10 consecutive video frames are extracted for analysis. One of the frames in the first test video is used as an illustrative example to explain the major steps of the first video analysis method, as shown in Fig. 4.4. The RGB color image in Fig. 4.4 (a) is first converted to the filtered gray-scale image in Fig. 4.4 (b) by removing the color gradient and the background illumination. Then the filtered gray-scale image is transformed into the binary black and white image as shown in Fig. 4.4 (c) and the Sobel operation is employed to capture the geometric edges of free-falling tracks as highlighted by red contours in Fig. 4.4 (d). Thus the width of each identified

free-falling track equals the diameter of the corresponding nickel pellet and total 85 and 116 frames in the first and second test videos are processed. The estimated

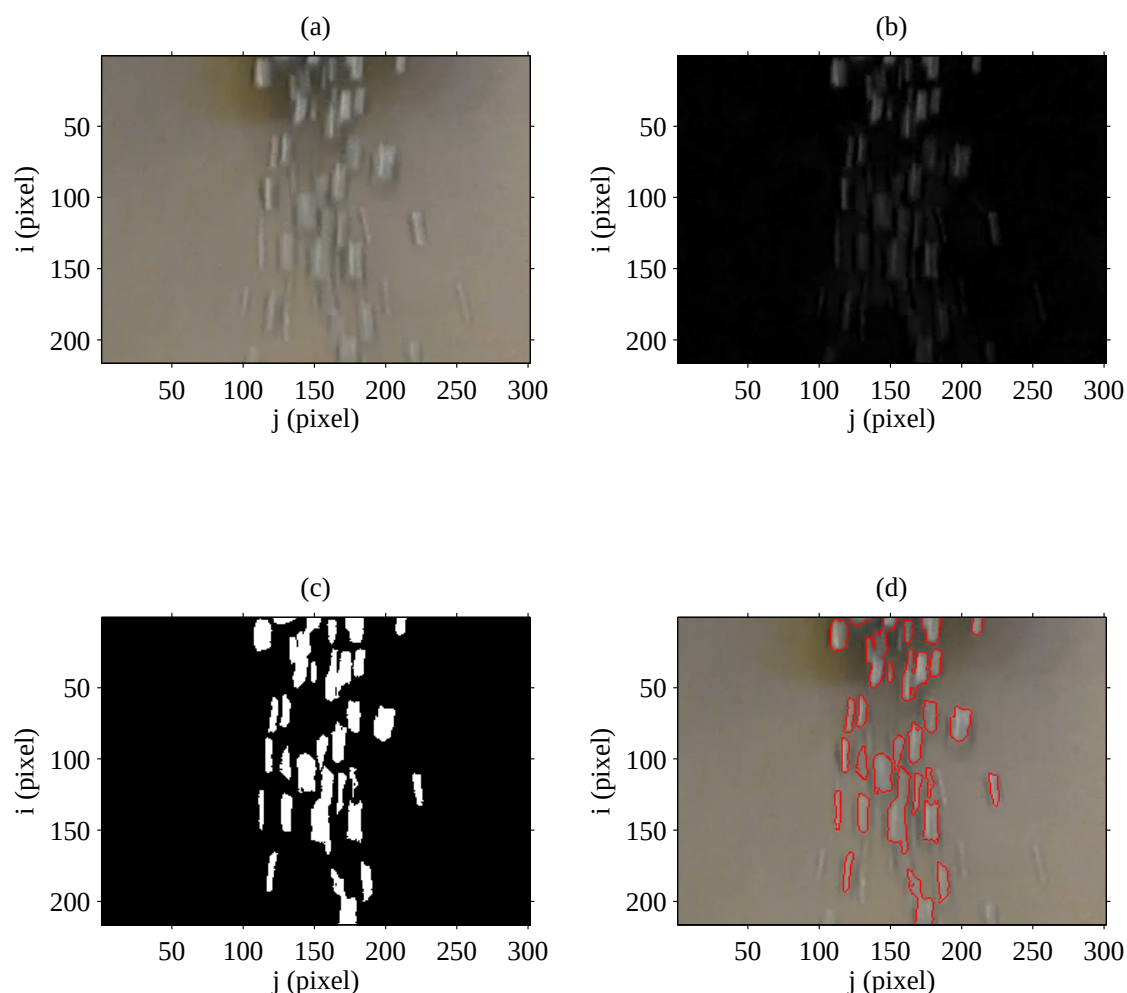


Figure 3.3: Illustrative example of the first video analysis based pellet sizing method: (a) original image; (b) filtered gray-scale image; (c) black and white image; and (d) edge detection results

size distributions and cumulative distributions are compared with the actual ones that are obtained by lab-scale mechanical sieving. The comparison results for the two test videos are shown in Figs. 4.5 and 4.6. It is obvious that the first video analysis method performs better than the conventional image analysis based pellet

sizing method in terms of size distribution prediction accuracy. Nevertheless, there are still some challenges in the first video analysis approach that may cause some unreliable estimation results. Specifically, some small pellets with relatively narrow free-falling tracks that are labeled as “1” in Fig. 4.7 cannot be identified by the Sobel edge detection method. Moreover, large number of pellets can still result in overlapping effect along the horizontal and vertical directions. The overlapped pellets labeled as “2” and “3” in Fig. 4.7 may be incorrectly captured as a single pellet and thus can lead to biased estimation of pellet size distributions.

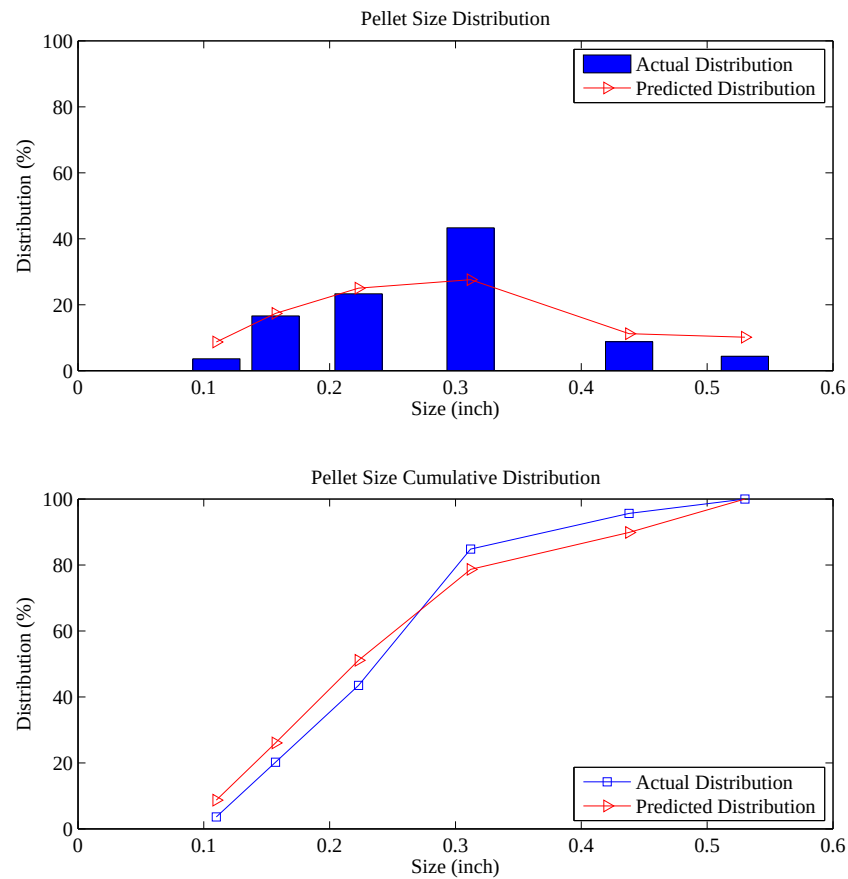


Figure 3.4: Pellet size distribution and cumulative distribution of the first video analysis based pellet sizing method for the first test video

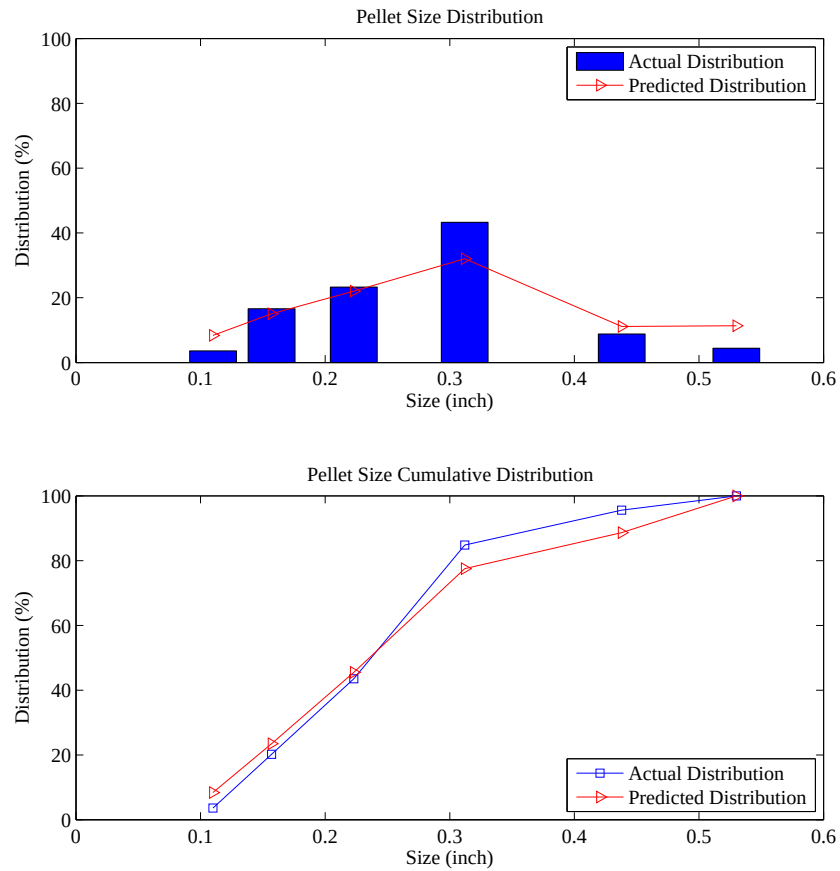


Figure 3.5: Pellet size distribution and cumulative distribution of the first video analysis based pellet sizing method for the second test video

3.3.3 The Second Video Analysis Based Pellet Sizing Method

Instead of detecting the geometric edges of the free-falling tracks in the converted black and white video frames, the second video analysis method as illustrated in Fig. 3.7 is designed to scan the filtered gray-scale image $I_4(i, j)$ row by row along the vertical direction. Since the background illumination is removed, the values of $I_4(i, j)$ are zero under uniform background. As such, if there is a free-falling pellet in the filtered gray-scale frame, the gray-scale values will be non-zero. For each pixel row

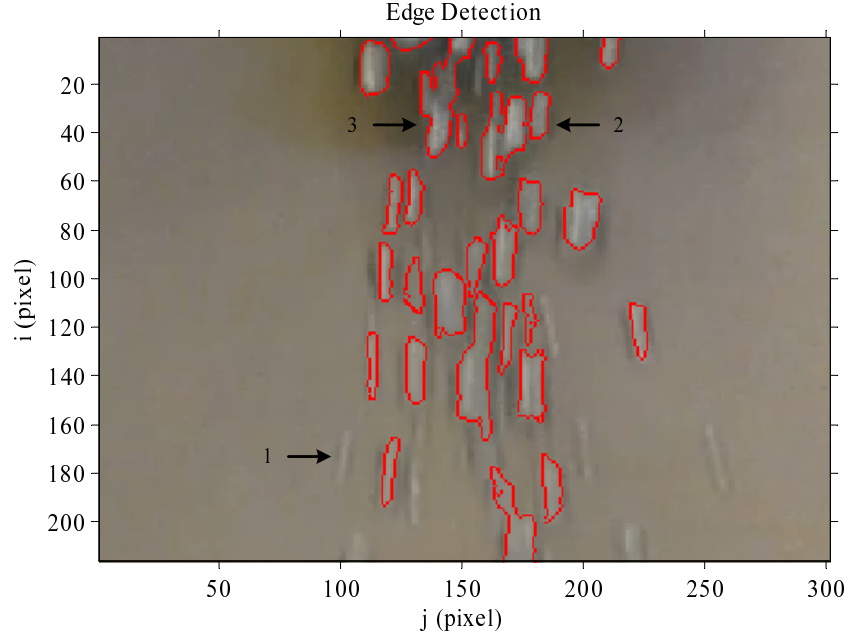


Figure 3.6: Illustration of the challenges for the first video analysis based pellet sizing method

in the filtered gray-scale image $I_4(i, j)$, a filtered gray-scale curve with a single peak indicates one pellet passing through that row and the width of the curve equals the diameter of the corresponding pellet. In addition, the gray-scale value tends to be larger in the central area and gradually decreases to zero on pellet edges because it is always brighter in the middle of the pellets.

The second video analysis based pellet sizing method is illustrated in Fig. 3.8, where the three dashed lines stand for the illustrative rows in the filtered gray-scale frame and the corresponding filtered gray-scale curves are shown in each row. Given that there is one pellet with the diameter d_1 passing through the first illustrative row, there is a corresponding filtered gray-scale curve with width d_1 along that pixel row. For the second illustrative row, the four overlapped pellets in the horizontal direction lead to a curve with four sub-curves and the GPR model can be further built to

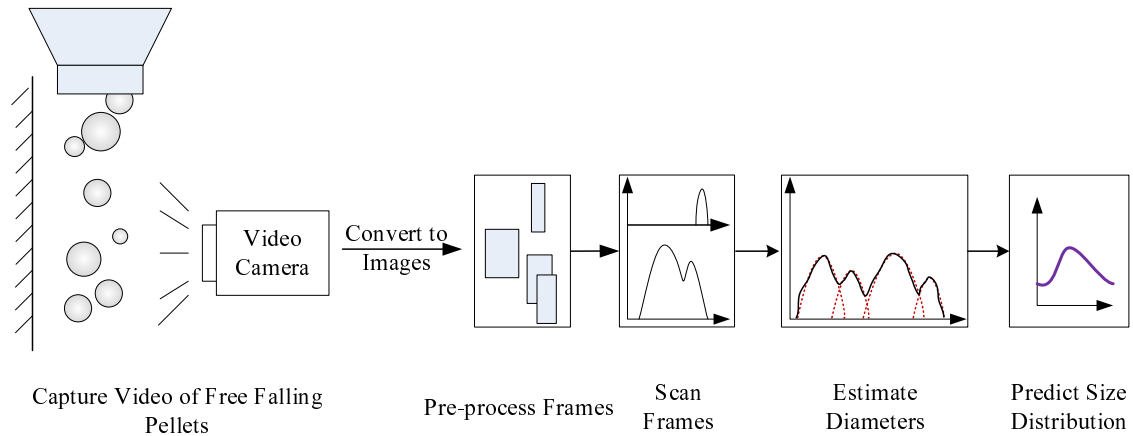


Figure 3.7: Illustration of the second video analysis based pellet sizing method

estimate the diameter of each pellet. There is also a small pellet with diameter d_2 passing through the second and the third illustrative rows, which results in the filtered gray-scale curve with the identical width d_2 in both the second and the third rows. The small pellets with relatively narrow free-falling tracks may not be accurately captured by the first video analysis method can be detected and identified in the second video analysis approach.

If the pellets are overlapped along the horizontal direction, the filtered gray-scale curve includes multiple sub-curves and the number of the sub-curves is equal to the number of the overlapped pellets. Because of the overlapping effects of pellets, the filtered gray-scale sub-curves need to be decomposed and then the diameters of the overlapped pellets can be estimated from the widths of the decomposed sub-curves. In the second video analysis method, GPR model is constructed to decompose the filtered gray-scale curve into sub-curves and further estimate the diameters of the overlapped pellets. Suppose that there are S peaks in the filtered gray-scale curve and thus S sub-curves need to be decomposed by GPR models to estimate the diameters

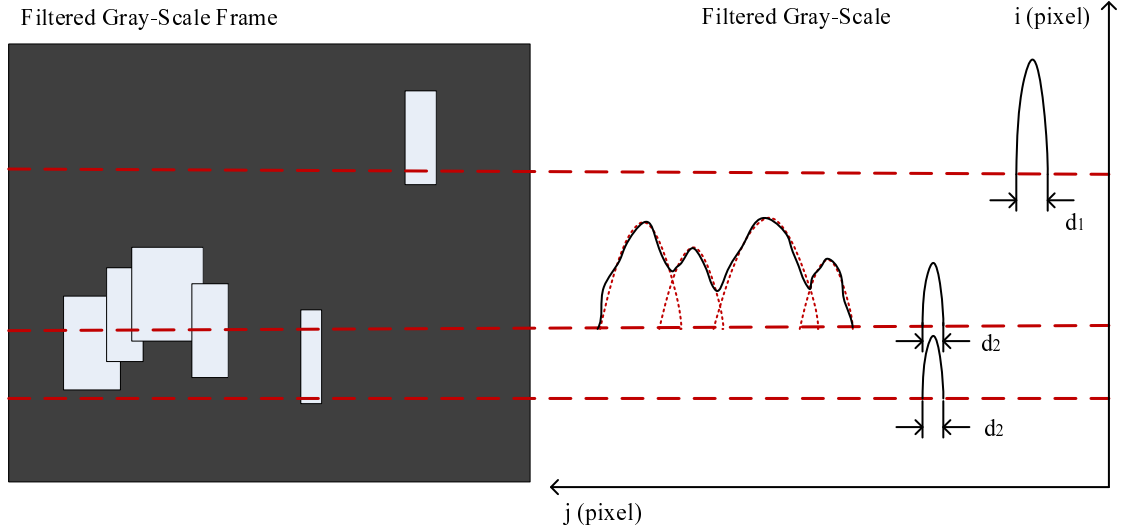


Figure 3.8: Illustration of the proposed pixel row based scanning of the filtered gray-scale frame in the second video analysis based pellet sizing method

of S overlapped pellets. Firstly, the filtered gray-scale curve is split into S sub-curves by the $S - 1$ local minimum points. For the s -th sub-curve, the samples in j -axis and the corresponding filtered gray-scale values are assumed to be $J_s = \{j_1, j_2, \dots, j_{n_s}\}$ and $F_s = \{f_s(j_1), f_s(j_2), \dots, f_s(j_{n_s})\}$, where n_s represents the number of gray-scale samples within the s -th sub-curve while f_s denotes the corresponding filtered gray-scale value. Thus the training data for GPR model of the s -th sub-curve is expressed as

$$D_s = \{j_i, f_s(j_i) \mid i = 1, \dots, n_s\} = \{J_s, F_s\} \quad (3.12)$$

The mean function of the Gaussian process is assumed to be zero while the squared

exponential function is chosen as the covariance function

$$k(j_m, j_n) = \sigma_f^2 \exp\left[-\frac{(j_m - j_n)^2}{2l^2}\right] \quad (3.13)$$

where σ_f and l are the maximum allowable covariance and Gaussian kernel width (Rasmussen and Williams, 2006). Then the GPR model is used to predict and extend the s -th filtered gray-scale sub-curve to the j -axis in order to further obtain the diameter of the s -th overlapped pellet. Given the predicted inputs $J_{s*} = \{j_{1*}, j_{2*}, \dots, j_{n_{s*}}\}$ with n_{s*} representing the width of the s -th sub-curve extended to the j -axis, the joint distribution of the training samples F_s and the predicted outputs F_{s*} for the s -th sub-curve is given by

$$\begin{bmatrix} F_s \\ F_{s*} \end{bmatrix} \sim \mathcal{N}(0, \begin{bmatrix} K_s & K_{s*}^T \\ K_{s*} & K_{s**} \end{bmatrix}) \quad (3.14)$$

where K_{s*} denotes the covariance matrix evaluated between all pairs of training and predicted samples given by

$$K_{s*} = \begin{bmatrix} k(j_{1*}, j_1) & k(j_{1*}, j_2) & \cdots & k(j_{1*}, j_{n_s}) \\ k(j_{2*}, j_1) & k(j_{2*}, j_2) & \cdots & k(j_{2*}, j_{n_s}) \\ \vdots & \vdots & \ddots & \vdots \\ k(j_{n_{s*}}, j_1) & k(j_{n_{s*}}, j_2) & \cdots & k(j_{n_{s*}}, j_{n_s}) \end{bmatrix} \quad (3.15)$$

Meanwhile, K_s and K_{s**} are the covariance matrices within the training and predicted samples respectively and they can be defined in the same way as the above covariance matrix K_{s*} (Stein, 1999). In addition, the conditional probability density function

$p(F_{s*} | F_s)$ follows a Gaussian distribution as

$$p(F_{s*} | F_s) \sim \mathcal{N}(K_{s*}K_s^{-1}F_s, K_{s**} - K_{s*}K_s^{-1}K_{s*}^T) \quad (3.16)$$

Thus the best prediction of F_{s*} is the following mean estimation

$$\bar{F}_{s*} = K_{s*}K_s^{-1}F_s \quad (3.17)$$

and the uncertainty of the prediction can be quantified by its covariance as follows

$$\text{var}(F_{s*}) = K_{s**} - K_{s*}K_s^{-1}K_{s*}^T \quad (3.18)$$

Moreover, in order to estimate the model parameters $\theta_s = \{\sigma_f, l\}$, the multivariate optimization problem can be formulated as

$$\theta_s^* = \arg \max_{\theta_s} \log p(F_s | J_s, \theta_s) \quad (3.19)$$

where

$$\log p(F_s | J_s, \theta_s) = -\frac{1}{2}F_s^T K_s^{-1}F_s - \frac{1}{2} \log |K_s| - \frac{n_s}{2} \log(2\pi) \quad (3.20)$$

Thus the diameter of the s -th overlapped pellet equals the distance between the two j -axis intersections of the predicted outputs $\bar{F}_{s*}$ in the s -th GPR model. Consequently, all the diameters of overlapped pellets can be obtained in this way and the overlapping effect along the horizontal direction is thus addressed.

The filtered gray-scale images of every n consecutive frames are scanned row by row and all the widths of the filtered gray-scale curves and sub-curves are estimated and counted. Since the video only records a short interval of free-falling motion, the lengths of free-falling tracks are assumed to be identical for all the pellets in the video

and expressed as w pixels. If there is no overlap in the vertical direction, one pellet should be scanned for w times because the filtered gray-scale frame is scanned row by row. Nevertheless, if there is any overlap in the vertical direction, the overlapped pellets would be scanned less than w times and the diameters of the overlapped pellets are counted less than w times accordingly. In order to obtain the precise prediction of pellet size distributions, the number of the pellets in the video frames needs to be counted reliably.

A counting rule is designed in this work to get accurate estimation of pellet size distributions. Assumed that any particular diameter d is counted for $N(d)$ times. Then the total number of the pellets with the diameter d is expressed as $M(d)$ below

$$M(d) = \text{ceil} \left(\frac{N(d)}{w} \right) \quad (3.21)$$

where the function $\text{ceil}(\cdot)$ is defined to round up a numerical value to the nearest integer. If there is no overlap in the vertical direction for the pellets with the diameter d , Eq. (4.1) can be simplified as

$$M(d) = \frac{N(d)}{w} \quad (3.22)$$

Thus the overlapping effect along the vertical direction can be avoided effectively by using Eq. (4.1). With the above counting rule, the predicted pellet size distributions in the second video analysis method can be closer to the actual ones as opposed to the first video analysis method. The schematic diagrams of the two video analysis based pellet sizing methods are shown in Fig. 3.9.

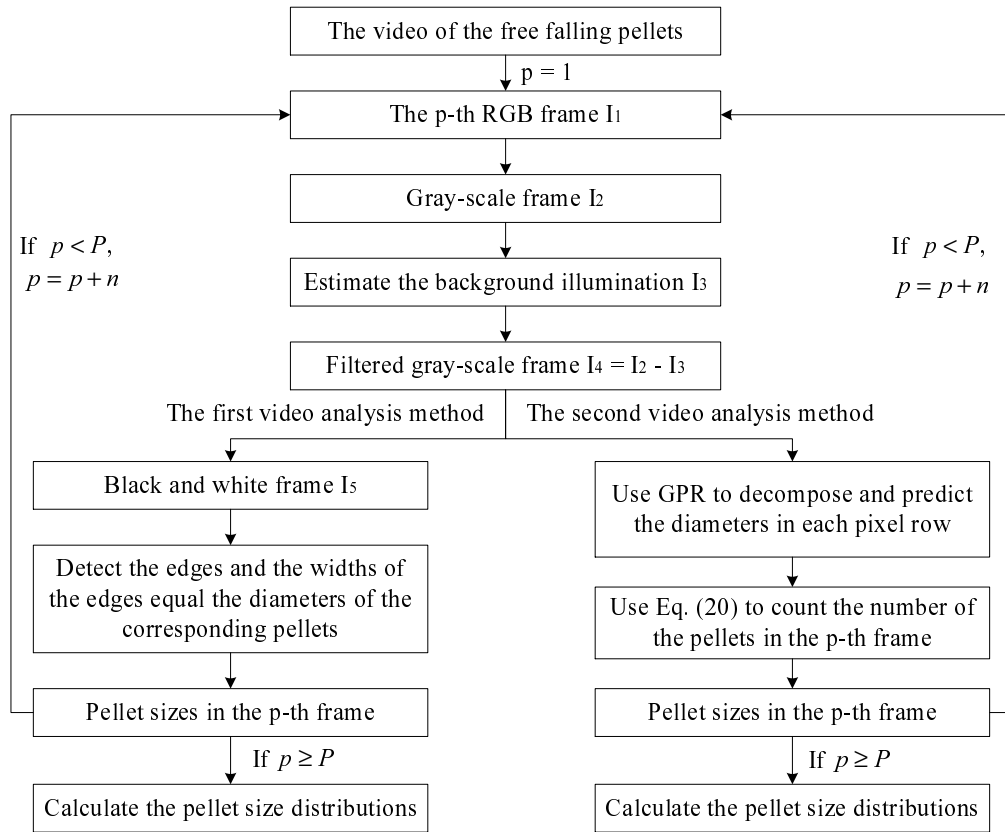


Figure 3.9: Schematic diagram of the two proposed video analysis based pellet sizing methods

An Illustrative Example

The two lab-scale test videos used in the first video analysis method are also used to examine the performance of the second video analysis method and one frame in the first test video is chosen as an illustrative example. The filtered gray-scale frame is shown in Fig. 3.10(a) with the dashed line indicating the 41-th pixel row and the filtered gray-scale curves for the 41-th row are depicted in Fig. 3.10(b). It can be seen from Fig. 3.10(b) that there are two filtered gray-scale curves with multiple sub-curves. The two sub-curves within the first gray-scale curve indicate that there

are two overlapped pellets along the horizontal direction and the decomposed and estimated sub-curves from GPR models are shown in Fig. 3.11(a) along with the corresponding 95% confidence intervals. The diameters of the two overlapped pellets can be obtained from the geometric distance between the two intersections in the j -axis of each estimated sub-curve. In addition, the three predicted sub-curves in the second gray-scale curve are shown in Fig. 3.11(b) and the diameters of these three overlapped pellets can be estimated from the corresponding intersections. The average length of the free-falling tracks used in the counting rule is $w = 30$ pixels in both test videos. After total 85 and 116 frames in the first and the second test videos are scanned row by row, the pellet size distributions can be estimated and the prediction results are shown in Figs. 3.12 and 3.13 for the first and the second test videos, respectively.

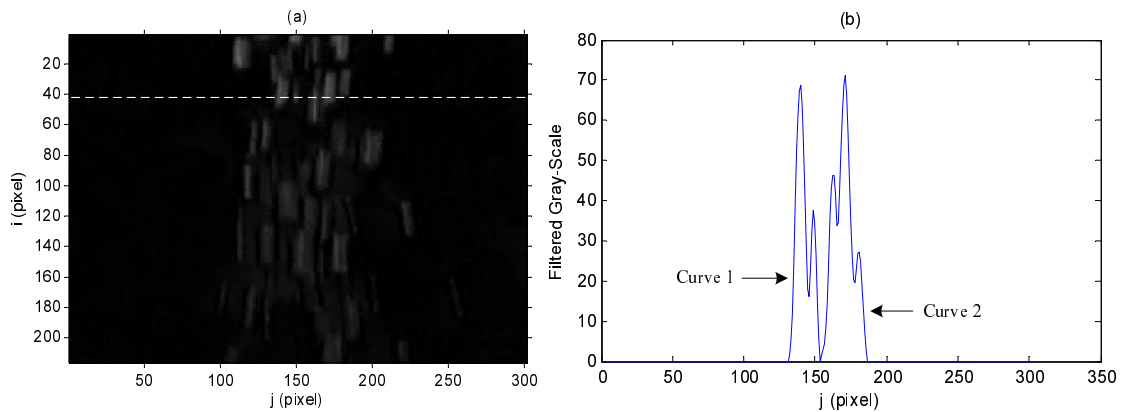


Figure 3.10: Illustrative example of the second video analysis based pellet sizing method: (a) filtered gray-scale frame with the 41-th pixel row marked; (b) the scanning result of the 41-th row

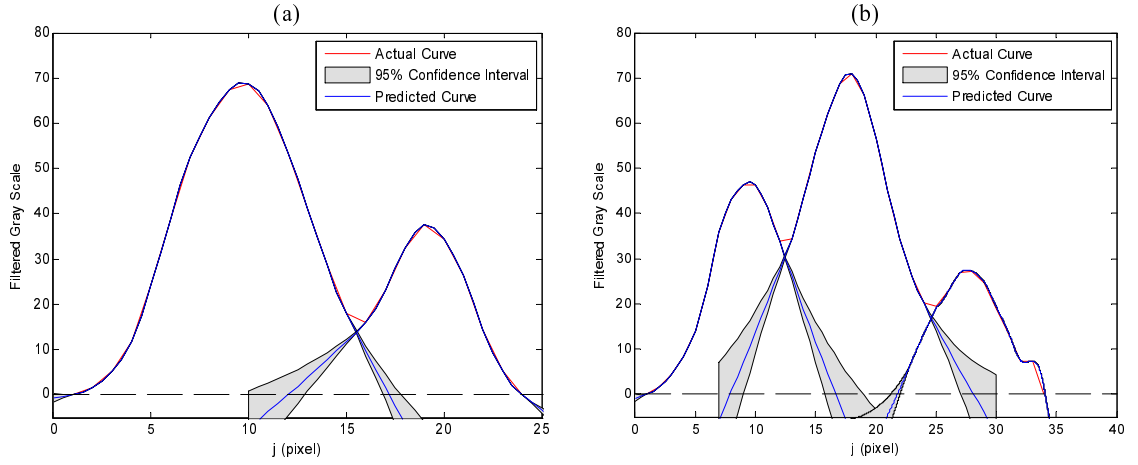


Figure 3.11: Predicted sub-curves and the corresponding confidence intervals of the Gaussian process regression models for the 41-th pixel row: (a) Curve 1 with two sub-curves; (b) Curve 2 with three sub-curves

3.4 Comparison of Pellet Size Distribution Prediction Results

In order to compare the estimation accuracy and performance of the two video analysis based pellet sizing soft sensor methods, the following mean absolute percentage error(MAPE) index is used

$$MAPE = \frac{100\%}{N} \sum_{i=1}^N \left| \frac{Y_i - \hat{Y}_i}{Y_i} \right| \quad (3.23)$$

where Y_i and $\hat{Y}_i$ are the actual and predicted percentages of the i -th bin of pellet size measurements and N is the total number of bins corresponding to different size intervals. The prediction results of pellet size distributions using the two video analysis methods for the two different test videos are compared in Table 3.1. It can be readily

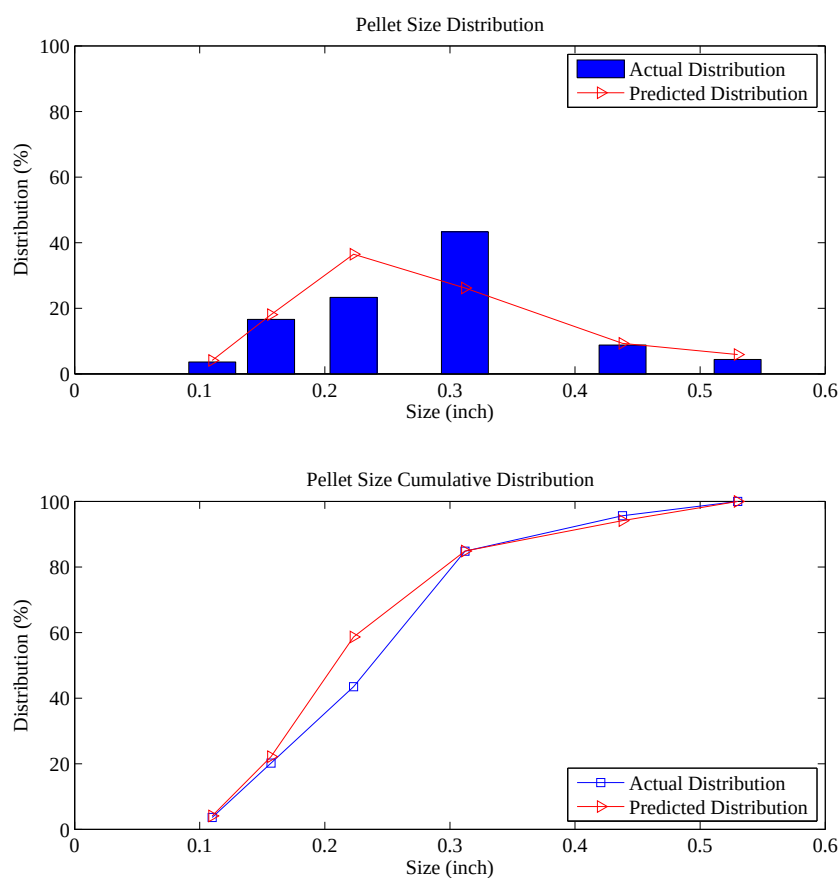


Figure 3.12: Pellet size distribution and cumulative distribution of the second video analysis based pellet sizing method for the first test video

seen that the second video analysis method shows improved accuracy of estimating pellet size distributions as opposed to the first video analysis method for both test videos. The smaller MAPE values of the second video analysis method are mainly due to its enhanced ability of eliminating the pellet overlapping effects along the horizontal and vertical directions.

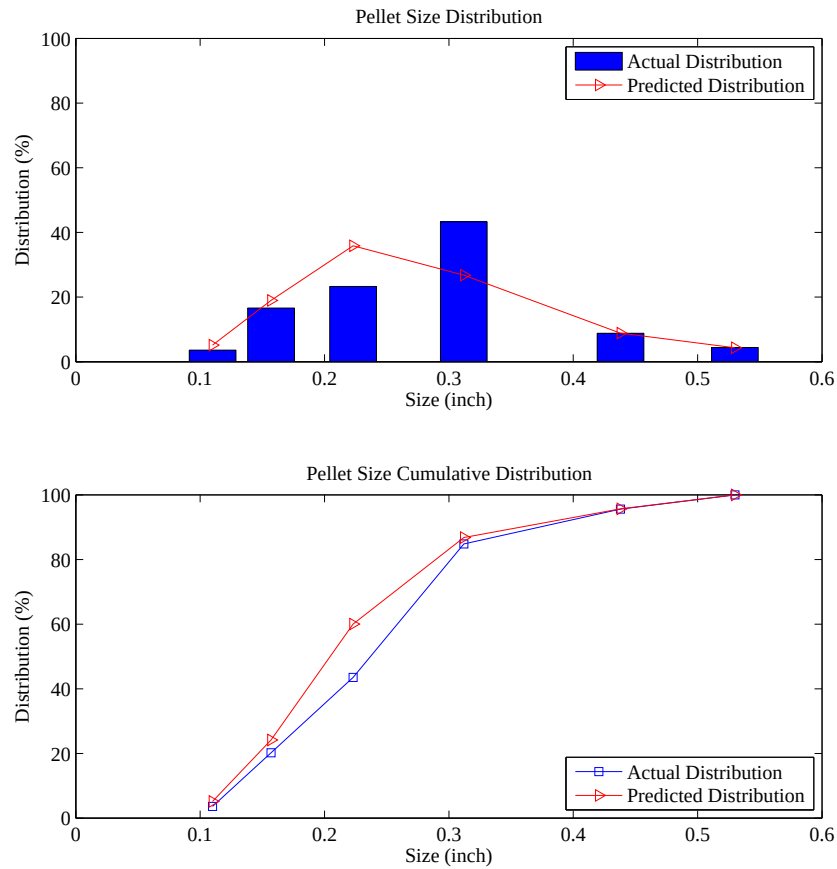


Figure 3.13: Pellet size distribution and cumulative distribution of the second video analysis based pellet sizing method for the second test video

3.5 Conclusions

In this paper, two video analysis based pellet sizing soft sensor methods are proposed to estimate and predict the size distributions of nickel pellets. These two approaches make use of the dynamic video frames to predict the pellet size distributions without any intrusive tests and show superiorities over the conventional image analysis based pellet sizing method. In the first video analysis approach, the diameters of free-falling pellets are identified by detecting the geometric edges of free-falling tracks in different

Table 3.1: Comparison of the MAPE values of predicted pellet size distributions between the two video analysis based pellet sizing methods for two test videos

	Video Analysis Method 1		Video Analysis Method 2	
Test Video No.	1	2	1	2
MAPE	33.46%	28.25%	9.98%	17.22%

video frames. For the second video analysis method, the filtered gray-scale frames are scanned row by row to extract the features for pellet diameters. In order to remove the overlapping effects along the horizontal and vertical directions, GPR models and a counting rule are developed for decomposing gray-scale sub-curves and estimating the pellet diameters with high accuracy.

These two video analysis based pellet sizing methods are applied to two test videos for measuring nickel pellet size distributions. It is shown that the second video analysis approach performs better than the first video analysis method in terms of smaller MAPE values by avoiding the overlapping effects. It should be pointed out that the developed video analysis based pellet sizing methods can be extended to other application as well. The only required assumption of the proposed methods is that the pellets or any other particles need to be free-falling with the identical initial speed. As long as the clear free-falling tracks are captured in the video frames, both proposed methods should be applicable. Future research may focus on further improving the soft sensor prediction accuracy of pellet size distributions and extending the video analysis based soft sensors towards different industrial applications.

Bibliography

- Assis, A. and Filho, R. (2000). Soft sensors development for on-line bioreactor state estimation. *Comput. Chem. Eng.*, **24**(2), 1099–1103.
- Bharati, M. and MacGregor, J. (1998). Multivariate image analysis for real-time process monitoring and control. *Ind. Eng. Chem. Res.*, **37**(12), 4715–4724.
- Braatz, R. and Hasebe, S. (2002). Particle size and shape control in crystallization processes. In *AIChE Symposium Series*, pages 307–327, New York, NY, USA.
- Čadík, M. (2008). Perceptual evaluation of color-to-grayscale image conversions. *Comput. Graph. Forum*, **27**(7), 1745–1754.
- Calderon De Anda, J., Wang, X., Lai, X., and Roberts, K. (2005a). Classifying organic crystals via in-process image analysis and the use of monitoring charts to follow polymorphic and morphological changes. *J. Proc. Cont.*, **15**(7), 785–797.
- Calderon De Anda, J., Wang, X., and Roberts, K. (2005b). Multi-scale segmentation image analysis for the in-process monitoring of particle shape with batch crystallisers. *Chem. Eng. Sci.*, **60**(4), 1053–1065.
- Chen, J. and Wang, X. (2005). A wavelet method for analysis of droplet and particle images for monitoring heterogeneous processes. *Chem. Eng. Comm.*, **192**(4), 499–515.
- Dahl, C. and Esbensen, K. (2007). Image analytical determination of particle size distribution characteristics of natural and industrial bulk aggregates. *Chemometrics Intell. Lab. Syst.*, **89**(1), 9–25.

- Doyle III, F. (1998). Nonlinear inferential control for process applications. *J. Proc. Cont.*, **8**(5), 339–353.
- Du, Y.-G., del Villar, R., and Thibault, J. (1997). Neural net-based softsensor for dynamic particle size estimation in grinding circuits. *Int. J. Miner. Proc.*, **52**(2), 121–135.
- Facco, P., Tomba, E., Roso, M., Modesti, M., Bezzo, F., and Barolo, M. (2010). Automatic characterization of nanofiber assemblies by image texture analysis. *Chemo-metrics Intell. Lab. Syst.*, **103**(1), 66–75.
- Fujiwara, M., Nagy, Z., Chew, J., and Braatz, R. (2005). First-principles and direct design approaches for the control of pharmaceutical crystallization. *J. Proc. Cont.*, **15**(5), 493–504.
- Hoskins, J. and Himmelblau, D. (1988). Artificial neural network models of knowledge representation in chemical engineering. *Comput. Chem. Eng.*, **12**(9), 881–890.
- Hukkanen, E. and Braatz, R. (2003). Measurement of particle size distribution in suspension polymerization using in situ laser backscattering. *Sensor Actuat. B-Chem.*, **96**(1), 451–459.
- Kadlec, P., Gabrys, B., and Strandt, S. (2009). Data-driven soft sensors in the process industry. *Comput. Chem. Eng.*, **33**(4), 795–814.
- Kadlec, P., Grbić, R., and Gabrys, B. (2011). Review of adaptation mechanisms for data-driven soft sensors. *Comput. Chem. Eng.*, **35**(1), 1–24.
- Kano, M. and Nakagawa, Y. (2008). Data-based process monitoring, process control, and quality improvement: Recent developments and applications in steel industry. *Comput. Chem. Eng.*, **32**(1), 12–24.

- Ko, Y.-D. and Shang, H. (2011). A neural network-based soft sensor for particle size distribution using image analysis. *Powder Technol.*, **212**(2), 359–366.
- Koh, T., Miles, N., Morgan, S., and Hayes-Gill, B. (2009). Improving particle size measurement using multi-flash imaging. *Miner. Eng.*, **22**(6), 537–543.
- Kresta, J., Marlin, T., and MacGregor, J. (1994). Development of inferential process models using PLS. *Comput. Chem. Eng.*, **18**(7), 597–611.
- Larsen, P., Rawlings, J., and Ferrier, N. (2006). An algorithm for analyzing noisy, in situ images of high-aspect-ratio crystals to monitor particle size distribution. *Chem. Eng. Sci.*, **61**(56), 52365248.
- Larsen, P., Rawlings, J., and Ferrier, N. (2007). Model-based object recognition to measure crystal size and shape distributions from in situ video images. *Chem. Eng. Sci.*, **62**(5), 1430–1441.
- Lillesand, T., Kiefer, R., and Chipman, J. (2008). *Remote sensing and image interpretation*. John Wiley & Sons, New York, NY, USA, 6th edition.
- Lin, B., Recke, B., Knudsen, J., and Jørgensen, S. (2007). A systematic approach for soft sensor development. *Comput. Chem. Eng.*, **31**(5), 419–425.
- Maaß, S., Rojahn, J., Hänsch, R., and Kraume, M. (2012). Automated drop detection using image analysis for online particle size monitoring in multiphase systems. *Comput. Chem. Eng.*, **45**, 27–37.
- MacGregor, J., Yu, H., Muñoz, S., and Flores-Cerrillo, J. (2005). Data-based latent variable methods for process analysis, monitoring and control. *Comput. Chem. Eng.*, **29**(6), 1217–1223.

- Maerz, N. (1999). Online fragmentation analysis: Achievements in the mining industry. In *Proceedings of the 7th Annual International Center for Aggregates Research (ICAR) Symposium*, Austin, TX, USA.
- Monnier, O., Klein, J.-P., Ratsimba, B., and Hoff, C. (1996). Particle size determination by laser reflection: methodology and problems. *Part. Part. Syst. Charact.*, **13**(1), 10–17.
- Napoli, G. and Xibilia, M. (2011). Soft sensor design for a Topping process in the case of small datasets. *Comput. Chem. Eng.*, **35**(11), 2447–2456.
- Otsu, N. (1975). A threshold selection method from gray-level histograms. *Automatica*, **11**(285–296), 23–27.
- Parker, J. (2010). *Algorithms for image processing and computer vision*. Wiley Publishing, Inc., Indianapolis, IN, USA, 2nd edition.
- Prats-Montalbán, J., J.A., D., and Ferrer, A. (2011). Multivariate image analysis: A review with applications. *Chemometrics Intell. Lab. Syst.*, **107**(1), 1–23.
- Qin, S. and McAvoy, T. (1992). Nonlinear PLS modeling using neural networks. *Comput. Chem. Eng.*, **16**(4), 379–391.
- Rashid, M. and Yu, J. (2012). Hidden Markov model based adaptive independent component analysis approach for complex chemical process monitoring and fault detection. *Ind. Eng. Chem. Res.*, **51**, 5506–5514.
- Rasmussen, C. and Williams, C. (2006). *Gaussian processes for machine learning*. MIT Press, Cambridge, MA, USA.

- Ruiz, D., Nougues, J., Calderon, Z., Espuña, A., and Puigjaner, L. (2000). Neural network based framework for fault diagnosis in batch chemical plants. *Comput. Chem. Eng.*, **24**(2), 777–784.
- Sarkar, D., Doan, X.-T., Ying, Z., and Srinivasan, R. (2009). In situ particle size estimation for crystallization processes by multivariate image analysis. *Chem. Eng. Sci.*, **64**(1), 9–19.
- Sbarbaro, D., Ascencio, P., Espinoza, P., Mujica, F., and Cortes, G. (2008). Adaptive soft-sensors for on-line particle size estimation in wet grinding circuits. *Cont. Eng. Pract.*, **16**(2), 171–178.
- Stein, M. (1999). *Interpolation of spatial data: Some theory for kriging*. Springer Verlag, New York, NY, USA.
- Tähti, T., Louhi-Kultanen, M., and Palosaari, S. (1999). On-line measurement of crystal size distribution during batch crystallization. In *Proceedings of the 14th International Symposium Industrial Crystallization*, Cambridge, UK.
- Togkalidou, T., Braatz, R., Johnson, B., Davidson, O., and Andrews, A. (2001). Experimental design and inferential modeling in pharmaceutical crystallization. *AIChE J.*, **47**(1), 160–168.
- Torabi, K., Sayad, S., and Balke, S. (2005). On-line adaptive Bayesian classification for in-line particle image monitoring in polymer film manufacturing. *Comput. Chem. Eng.*, **30**(1), 18–27.
- Yan, W., Shao, H., and Wang, X. (2004). Soft sensing modeling based on support vector machine and Bayesian model selection. *Comput. Chem. Eng.*, **28**(8), 1489–1498.

- Yu, H. and MacGregor, J. (2003). Multivariate image analysis and regression for prediction of coating content and distribution in the production of snack foods. *Chemometrics Intell. Lab. Syst.*, **67**(2), 125–144.
- Yu, H. and MacGregor, J. (2004). Monitoring flames in an industrial boiler using multivariate image analysis. *AIChE J.*, **50**(7), 1474–1483.
- Yu, J. (2012a). A Bayesian inference based two-stage support vector regression framework for soft sensor development in batch bioprocesses. *Comput. Chem. Eng.*, **41**, 134–144.
- Yu, J. (2012b). A Bayesian inference based two-stage support vector regression framework for soft sensor development in batch bioprocesses. *Comput. Chem. Eng.*, **41**, 134–144.
- Yu, J. (2012c). Multiway Gaussian mixture model based adaptive kernel partial least squares regression method for soft sensor estimation and reliable quality prediction of nonlinear multiphase batch processes. *Ind. Eng. Chem. Res.*, **51**(40), 13227–13237.
- Yu, J. (2012d). A nonlinear kernel gaussian mixture model based inferential monitoring approach for fault detection and diagnosis of chemical processes. *Chemical Engineering Science*, **68**, 506–519.
- Yu, J. (2012e). Online quality prediction of nonlinear and non-gaussian chemical processes with shifting dynamics using finite mixture model based gaussian process regression approach. *Chemical Engineering Science*, **82**, 22–30.
- Yu, J. and Qin, S. J. (2008). Multimode process monitoring with bayesian inference-based finite gaussian mixture models. *AIChE Journal*, **54**, 1811–1829.

- Yu, J. and Qin, S. J. (2009). Multiway gaussian mixture model based multiphase batch process monitoring. *Industrial & Engineering Chemistry Research*, **48**, 8585–8594.
- Yu, J., Chen, K., and Rashid, M. M. (2013). A bayesian model averaging based multi-kernel gaussian process regression framework for nonlinear state estimation and quality prediction of multiphase batch processes with transient dynamics and uncertainty. *Chemical Engineering Science*, **93**, 96–109.
- Zhou, Y., Srinivasan, R., and Lakshminarayanan, S. (2009). Critical evaluation of image processing approaches for real-time crystal size measurements. *Comput. Chem. Eng.*, **33**(5), 1022–1035.

Chapter 4

Closed-Loop Subspace Projection Based State-Space Model-Plant Mismatch Detection and Isolation for MIMO MPC Performance Monitoring and Diagnosis

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4.1 Introduction

Effective control performance monitoring and diagnosis can determine whether specified performance targets are met and help ensure the plant-wide operation efficiency, quality and safety (Jelali, 2006; Qin and Yu, 2007). Control systems are assessed against certain performance benchmarks that are typically estimated from either process models or routine operating data. As model predictive control (MPC) system has become the most popular advanced process control (APC) strategy, some effort has been attempted specifically on MPC performance monitoring and diagnosis (Morari and Lee, 1999; Qin and Badgwell, 2003; Jelali, 2006). For MPC performance assessment, a method based on similarity factors and pattern recognition is developed to evaluate the condition of MPC controllers (Loquasto III and Seborg, 2003). Moreover, the actual key performance index (KPI) is compared with the designed KPI through the design case based MPC performance monitoring (Patwardhan and Shah, 2002). This method is improved by taking into account the ratio of historical and achieved performance of closed-loop MPC system (Schäfer and Cinar, 2004). Nevertheless, the MPC performance benchmarks rely on process model in setting objective function and thus may be biased due to potential model-plant mismatch.

MPC performance monitoring is a challenging task because its performance degradation can be caused by various factors such as significant model-plant mismatch, poor controller tuning, improper control structure design, sensor and actuator faults, constraint changes, and inappropriate targets from the upper-level optimization systems (Sun *et al.*, 2013). Among the above factors causing poor MPC performance, the model-plant mismatch is a critical issue because unreliable plant models may result in poor system output predictions and further affect the optimized system input sequence. Not only the improper step tests and model identification can lead

to significant model-plant mismatches, but also the plant nonlinearities and shifted dynamics may result in biased plant models in certain operating regions. Since MIMO model re-identification requires intrusive step tests and may disturb the normal plant operation, it is highly desirable to detect significant model-plant mismatches and further diagnose the mismatched input-output model channels in order to reduce model re-identification effort substantially.

Model-plant mismatch detection of MIMO MPC systems has attracted increasing attention from academia and industry. A partial correlations analysis strategy between manipulated variables and model output residuals is developed for model-plant mismatch diagnosis by using closed-loop operating data in the presence of unmeasured disturbances (Badwe *et al.*, 2009). Alternately, a stepwise method is proposed for model mismatch detection by utilizing the indirect variable selection (Kano *et al.*, 2010). Meanwhile, a subspace approach is developed for model-plant mismatch detection by estimating the Markov vector of each sub-model and then the mismatched channels are captured according to the area index (Wang *et al.*, 2012). More recently, a model quality index is proposed for model-plant mismatch detection by utilizing model residuals along with disturbance innovations as performance benchmark (Sun *et al.*, 2013). The above model-plant mismatch detection and diagnosis methods are for transfer function model formulations in multivariable MPC systems. However, state-space models are widely used in the design and implementation of MIMO MPC controllers. A state-space formulation based model-plant mismatch detection approach is proposed for open-loop systems but not directly applicable to closed-loop systems with MPC controllers (Jiang *et al.*, 2006).

In our research, a novel closed-loop model-plant mismatch detection and isolation method is proposed within state-space formulations without any open-loop step tests. Three quadratic indices are developed from routine closed-loop operating data in order

to identify the statistically significant mismatches. Furthermore, various kinds of subspace projections are designed to eliminate effects of system feedback. Meanwhile, the quadratic form of the indices and the corresponding statistical hypothesis testing are developed for conducting model-plant mismatch detection and isolation. The rest of the paper is organized as follows. The model-plant mismatch detection and isolation problem based on the state-space framework is formulated in Section 2. Then quadratic indices along with the corresponding confidence limits for model mismatch detection and isolation are derived in Section 3. In Section 4, the proposed method is demonstrated with a simulated example of multivariate paper machine headbox control system. Finally, the concluding remarks and future research directions are provided in Section 5.

4.2 Problem formulations

Consider the discrete-time state-space representation of a linear time-invariant process in the innovation form at the k -th sampling instant as follows

$$x_{k+1} = Ax_k + Bu_k + Ko_k \quad (4.1a)$$

$$y_k = Cx_k + o_k \quad (4.1b)$$

where A , B and C are the system matrices of the actual state-space plant model, $y_k \in \mathbb{R}^{n_y}$ consists of the observed output signals, $x_k \in \mathbb{R}^n$ is the state vector, $u_k \in \mathbb{R}^{n_u}$ contains the observed input sequence, $o_k \in \mathbb{R}^{n_y}$ is the white noise sequence, and $K \in \mathbb{R}^{n \times n_y}$ is the steady-state Kalman gain that can be obtained from an algebraic Ricatti equation (McKelvey *et al.*, 1996). The block diagram of closed-loop MPC system under state-space representations is shown in Fig. 4.1, where Q denotes a multivariate

MPC controller and r is the vector of set-point signals. Assume that $\{\Delta A, \Delta B, \Delta C\}$ denote the model-plant mismatches and thus the model-plant mismatch detection problem is mathematically equivalent to determining whether or not $\{\Delta A, \Delta B, \Delta C\}$ are zero given the closed-loop operating data. Further, the state-space representation of the model used in the MPC controllers can be expressed as

$$\hat{x}_{k+1} = \hat{A}\hat{x}_k + \hat{B}u_k + Ko_k \quad (4.2a)$$

$$\hat{y}_k = \hat{C}\hat{x}_k + o_k \quad (4.2b)$$

where $\hat{A} = A - \Delta A$, $\hat{B} = B - \Delta B$ and $\hat{C} = C - \Delta C$ are the system matrices of the controller model with potential mismatches $\{\Delta A, \Delta B, \Delta C\}$, and $\hat{y}_k$ and $\hat{x}_k$ denote the system output and state vectors, respectively. Using the model-plant mismatch terms, the real plant model in Eq. (4.1) can be rewritten as follows

$$x_{k+1} = \hat{A}x_k + \hat{B}u_k + Ko_k + \Delta Ax_k + \Delta Bu_k \quad (4.3a)$$

$$y_k = \hat{C}x_k + o_k + \Delta Cx_k \quad (4.3b)$$

The following general assumptions are defined

A1: The system given in Eq. (4.1) is asymptotically stable;

A2: The pair (A, C) is observable

A3: The pair $(A, [B, K])$ is reachable;

A4: The innovation sequence o_k is stationary white noise with zero mean and assumed to be one-way uncorrelated with input signals u_k , i.e.,

$$\bar{E}[o_k u_t^T] = 0, k > t, \quad (4.4)$$

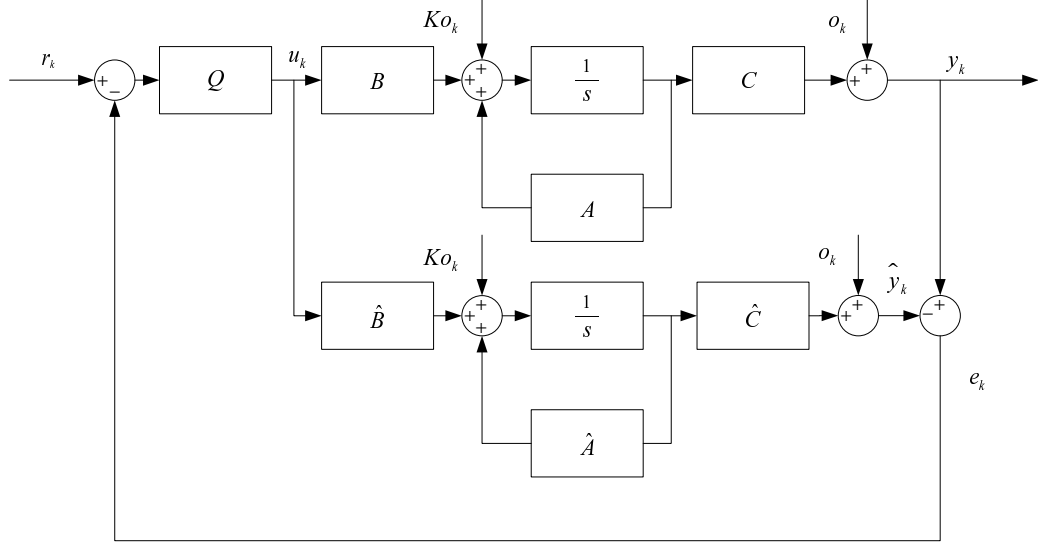


Figure 4.1: Model residual form of closed-loop MPC system in state-space representation

where the asymptotic expectation $\bar{E}$ is defined as (Ljung, 1999)

$$\bar{E}\{\cdot\} = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_{k=1}^N E\{\cdot\} \quad (4.5)$$

A5: There is no significant mismatch in the disturbance model.

4.3 Subspace projection based model-plant mismatch detection

The past and future plant input vectors $u_p(k) \in \mathbb{R}^{n_u p}$ and $u_f(k) \in \mathbb{R}^{n_u f}$ and Hankel matrices $U_p \in \mathbb{R}^{n_u p \times N}$ and $U_f \in \mathbb{R}^{n_u f \times N}$ are arranged in the following form

$$u_p(k) = \begin{bmatrix} u_{k-p} \\ u_{k-p+1} \\ \vdots \\ u_{k-1} \end{bmatrix} \quad (4.6)$$

$$u_f(k) = \begin{bmatrix} u_k \\ u_{k+1} \\ \vdots \\ u_{k+f-1} \end{bmatrix} \quad (4.7)$$

$$U_p = \begin{bmatrix} u_p(k) & u_p(k+1) & \cdots & u_p(k+N-1) \end{bmatrix} \quad (4.8)$$

$$U_f = \begin{bmatrix} u_f(k) & u_f(k+1) & \cdots & u_f(k+N-1) \end{bmatrix} \quad (4.9)$$

where p and f are the past and future window sizes that should be greater than the number of state variables n while the subscripts p and f denote the past and future horizons (Jansson and Wahlberg, 1998). The Hankel matrices of the past and future system output observations, estimations and innovations, $Y_p \in \mathbb{R}^{n_y p \times N}$, $Y_f \in \mathbb{R}^{n_y f \times N}$, $\hat{Y}_p \in \mathbb{R}^{n_y p \times N}$, $\hat{Y}_f \in \mathbb{R}^{n_y f \times N}$, $O_p \in \mathbb{R}^{n_y p \times N}$ and $O_f \in \mathbb{R}^{n_y f \times N}$, are

constructed in the identical way as U_p and U_f . Moreover, the past and future plant state sequences are defined as $X_p = \begin{bmatrix} x_{k-p} & x_{k-p+1} & \cdots & x_{k-p+N-1} \end{bmatrix} \in \mathbb{R}^{n \times N}$ and $X_f = \begin{bmatrix} x_k & x_{k+1} & \cdots & x_{k+N-1} \end{bmatrix} \in \mathbb{R}^{n \times N}$ and the model state sequences $\hat{X}_p \in \mathbb{R}^{n \times N}$ and $\hat{X}_f \in \mathbb{R}^{n \times N}$ are defined in the identical fashion. It is assumed that the closed-loop operating data of u_k , y_k , and $\hat{y}_k$ are available for $k = 1, 2, \dots, N + p + f - 1$.

Through the iterations of the system equations in Eq. (4.2), it is straightforward to get the subspace matrix equations characterizing the MIMO model used in the MPC controllers as follows (Chiuso and Picci, 2005; Qin, 2006)

$$\hat{Y}_p = \Gamma_p \hat{X}_p + H_p^d U_p + H_p^s O_p \quad (4.10)$$

$$\hat{Y}_f = \Gamma_f \hat{X}_f + H_f^d U_f + H_f^s O_f \quad (4.11)$$

Similarly, the following subspace matrix equations characterizing the actual plant can be derived by iterating the system equations in Eq. (4.3)

$$Y_p = \Gamma_p X_p + H_p^d U_p + H_p^s O_p + C_p + G_p^s [A_p + B_p] \quad (4.12)$$

$$Y_f = \Gamma_f X_f + H_f^d U_f + H_f^s O_f + C_f + G_f^s [A_f + B_f] \quad (4.13)$$

The extended observability matrices $\Gamma_p \in \mathbb{R}^{n_y p \times n}$ and $\Gamma_f \in \mathbb{R}^{n_y f \times n}$ with full column

rank n are defined as

$$\Gamma_p = \begin{bmatrix} \hat{C} \\ \hat{C}\hat{A} \\ \hat{C}\hat{A}^2 \\ \vdots \\ \hat{C}\hat{A}^{p-1} \end{bmatrix} \quad (4.14)$$

$$\Gamma_f = \begin{bmatrix} \hat{C} \\ \hat{C}\hat{A} \\ \hat{C}\hat{A}^2 \\ \vdots \\ \hat{C}\hat{A}^{f-1} \end{bmatrix} \quad (4.15)$$

Then the lower triangular block-Toeplitz matrices H_p^d , H_p^s , H_f^d , H_f^s , G_p^s and G_f^s can be expressed as

$$H_p^d = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \hat{C}\hat{B} & 0 & 0 & \cdots & 0 \\ \hat{C}\hat{A}\hat{B} & \hat{C}\hat{B} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \hat{C}\hat{A}^{p-2}\hat{B} & \hat{C}\hat{A}^{p-3}\hat{B} & \hat{C}\hat{A}^{p-4}\hat{B} & \cdots & 0 \end{bmatrix} \quad (4.16)$$

$$H_f^d = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \hat{C}\hat{B} & 0 & 0 & \cdots & 0 \\ \hat{C}\hat{A}\hat{B} & \hat{C}\hat{B} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \hat{C}\hat{A}^{f-2}\hat{B} & \hat{C}\hat{A}^{f-3}\hat{B} & \hat{C}\hat{A}^{f-4}\hat{B} & \cdots & 0 \end{bmatrix} \quad (4.17)$$

$$H_p^s = \begin{bmatrix} I & 0 & 0 & \cdots & 0 \\ \hat{C}K & I & 0 & \cdots & 0 \\ \hat{C}\hat{A}K & \hat{C}K & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \hat{C}\hat{A}^{p-2}K & \hat{C}\hat{A}^{p-3}K & \hat{C}\hat{A}^{p-4}K & \cdots & I \end{bmatrix} \quad (4.18)$$

$$H_f^s = \begin{bmatrix} I & 0 & 0 & \cdots & 0 \\ \hat{C}K & I & 0 & \cdots & 0 \\ \hat{C}\hat{A}K & \hat{C}K & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \hat{C}\hat{A}^{f-2}K & \hat{C}\hat{A}^{f-3}K & \hat{C}\hat{A}^{f-4}K & \cdots & I \end{bmatrix} \quad (4.19)$$

$$G_p^s = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \hat{C} & 0 & 0 & \cdots & 0 \\ \hat{C}\hat{A} & \hat{C} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \hat{C}\hat{A}^{p-2} & \hat{C}\hat{A}^{p-3} & \hat{C}\hat{A}^{p-4} & \cdots & 0 \end{bmatrix} \quad (4.20)$$

$$G_f^s = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 \\ \hat{C} & 0 & 0 & \cdots & 0 \\ \hat{C}\hat{A} & \hat{C} & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ \hat{C}\hat{A}^{f-2} & \hat{C}\hat{A}^{f-3} & \hat{C}\hat{A}^{f-4} & \cdots & 0 \end{bmatrix} \quad (4.21)$$

where $H_p^d \in \mathbb{R}^{n_y p \times n_u p}$, $H_f^d \in \mathbb{R}^{n_y f \times n_u f}$, $H_p^s \in \mathbb{R}^{n_y p \times n_y p}$, $H_f^s \in \mathbb{R}^{n_y f \times n_y f}$, $G_p^s \in \mathbb{R}^{n_y p \times n_p}$, and $G_f^s \in \mathbb{R}^{n_y f \times n_f}$.

Furthermore, $A_p \in \mathbb{R}^{n_p \times N}$, $B_p \in \mathbb{R}^{n_p \times N}$, $C_p \in \mathbb{R}^{n_y p \times N}$, $A_f \in \mathbb{R}^{n_f \times N}$, $B_f \in \mathbb{R}^{n_f \times N}$ and $C_f \in \mathbb{R}^{n_y f \times N}$ account for the effects of model-plant mismatches $\{\Delta A, \Delta B, \Delta C\}$ on the system in consideration

$$A_p(k) = \begin{bmatrix} \Delta A x_{k-p} \\ \Delta A x_{k-p+1} \\ \vdots \\ \Delta A x_{k-1} \end{bmatrix}, A_f(k) = \begin{bmatrix} \Delta A x_k \\ \Delta A x_{k+1} \\ \vdots \\ \Delta A x_{k+f-1} \end{bmatrix} \quad (4.22)$$

$$B_p(k) = \begin{bmatrix} \Delta B u_{k-p} \\ \Delta B u_{k-p+1} \\ \vdots \\ \Delta B u_{k-1} \end{bmatrix}, B_f(k) = \begin{bmatrix} \Delta B u_k \\ \Delta B u_{k+1} \\ \vdots \\ \Delta B u_{k+f-1} \end{bmatrix} \quad (4.23)$$

$$C_p(k) = \begin{bmatrix} \Delta C x_{k-p} \\ \Delta C x_{k-p+1} \\ \vdots \\ \Delta C x_{k-1} \end{bmatrix}, C_f(k) = \begin{bmatrix} \Delta C x_k \\ \Delta C x_{k+1} \\ \vdots \\ \Delta C x_{k+f-1} \end{bmatrix} \quad (4.24)$$

where A_p and A_f can be constructed as

$$A_p = \begin{bmatrix} A_p(k) & A_p(k+1) & \cdots & A_p(k+N-1) \end{bmatrix} \quad (4.25)$$

$$A_f = \begin{bmatrix} A_f(k) & A_f(k+1) & \cdots & A_f(k+N-1) \end{bmatrix} \quad (4.26)$$

Similarly, B_p , C_p , B_f and C_f can be formulated in the same way. Given the above formulations, the model-plant mismatch detection is equivalent to determining whether A_p , B_p and C_p or A_f , B_f and C_f are zero or not.

The model residual $e_k = y_k - \hat{y}_k$ represents the difference between the plant output and model output and such residual signal can be feedbacked to MPC controller in closed-loop system. The following subspace equation of the model residual for future horizon E_f can be derived by subtracting (4.11) from (4.13)

$$E_f = Y_f - \hat{Y}_f = \Gamma_f(X_f - \hat{X}_f) + C_f + G_f^s[A_f + B_f] \quad (4.27)$$

Given the assumption A5, all the disturbances are properly accounted for in the disturbance model and the plant model residual will not be zero if there is any model-plant mismatch.

4.3.1 Detection of model-plant mismatch in system matrix A , B or C

In order to detect any model-plant mismatch in system matrix A , B or C , a residual based model quality index e_{ABC} is derived in this subsection. Pre-multiplying Eq. (4.27) by the orthogonal column space of Γ_f , denoted by $(\Gamma_f^\perp)^T \in \mathbb{R}^{(n_{yf}-n) \times n_{yf}}$ can yield

$$(\Gamma_f^\perp)^T E_f = (\Gamma_f^\perp)^T \Gamma_f (X_f - \hat{X}_f) + (\Gamma_f^\perp)^T C_f + (\Gamma_f^\perp)^T G_f^s [A_f + B_f] \quad (4.28)$$

Since $(\Gamma_f^\perp)^T \Gamma_f = 0$, the above expression can be simplified as

$$(\Gamma_f^\perp)^T E_f = (\Gamma_f^\perp)^T \begin{bmatrix} G_f^s & I_{n_{yf}} \end{bmatrix} \begin{bmatrix} A_f + B_f \\ C_f \end{bmatrix} \quad (4.29)$$

where $I_{n_{yf}}$ denotes the $n_{yf} \times n_{yf}$ identity matrix. The above expression can be further defined as an index

$$e_{ABC}(k) \triangleq (\Gamma_f^\perp)^T E_f(k) = (\Gamma_f^\perp)^T \begin{bmatrix} G_f^s & I_{n_{yf}} \end{bmatrix} \begin{bmatrix} A_f + B_f \\ C_f \end{bmatrix} \quad (4.30)$$

where the left hand side $(\Gamma_f^\perp)^T E_f$ is the numerical computation form of e_{ABC} and the right hand side $(\Gamma_f^\perp)^T \begin{bmatrix} G_f^s & I_{n_{yf}} \end{bmatrix} \begin{bmatrix} A_f + B_f \\ C_f(k) \end{bmatrix}$ determines the model-plant mismatch in system matrix A , B or C . If there is no mismatch in A , B or C , then $A_f(k)$, $B_f(k)$ and $C_f(k)$ should be zero. Hence, e_{ABC} is zero accordingly. On the other hand, if there is any mismatch in A , B or C , then $A_f(k)$, $B_f(k)$ or $C_f(k)$ becomes non-zero and thus e_{ABC} does not equal zero. Therefore, any mismatch in system matrix A , B

or C can be detected through the above model residual based index e_{ABC} .

4.3.2 Detection of model-plant mismatch in A or C

A residual based model quality index e_{AC} is proposed in order to detect any model-plant mismatch in A or C in this subsection. As defined in Eq. (4.23), B_f includes the effect of model-plant mismatch in system matrix B acting on the system and can be further formulated as

$$B_f = \begin{bmatrix} \Delta B & 0 & 0 & \cdots & 0 \\ 0 & \Delta B & 0 & \cdots & 0 \\ 0 & 0 & \Delta B & \cdots & 0 \\ \vdots & \vdots & \ddots & \cdots & \vdots \\ 0 & 0 & 0 & \cdots & \Delta B \end{bmatrix} U_f \quad (4.31)$$

Post-multiplying Eq. (4.29) by $\Pi_{U_f}^\perp$ yields

$$(\Gamma_f^\perp)^T E_f \Pi_{U_f}^\perp = (\Gamma_f^\perp)^T \begin{bmatrix} G_f^s & I_{n_{yf}} \end{bmatrix} \begin{bmatrix} A_f \\ C_f \end{bmatrix} \Pi_{U_f}^\perp + (\Gamma_f^\perp)^T B_f \Pi_{U_f}^\perp \quad (4.32)$$

where $\Pi_{U_f}^\perp = I - U_f^\dagger U_f$ is the orthogonal projector onto the kernel of U_f and $U_f^\dagger$ is the pseudo-inverse of U_f . Since $U_f \Pi_{U_f}^\perp = 0$ and $B_f \Pi_{U_f}^\perp = 0$, the last term of Eq. (4.32) is zero and then Eq. (4.32) can be rewritten as follows

$$(\Gamma_f^\perp)^T E_f \Pi_{U_f}^\perp = (\Gamma_f^\perp)^T \begin{bmatrix} G_f^s & I_{n_{yf}} \end{bmatrix} \begin{bmatrix} A_f \\ C_f \end{bmatrix} \Pi_{U_f}^\perp \quad (4.33)$$

Through the subspace projection, any effect of model-plant mismatch related to system matrix B is eliminated in the above equation. Define the following index e_{AC}

$$e_{AC}(k) \triangleq (\Gamma_f^\perp)^T E_f(k) \Pi_{U_f}^\perp \quad (4.34)$$

With the right hand side $(\Gamma_f^\perp)^T \begin{bmatrix} G_f^s & I_{n_{yf}} \end{bmatrix} \begin{bmatrix} A_f \\ C_f \end{bmatrix} \Pi_{U_f}^\perp$ being the internal form of e_{AC} defined in Eq. (4.34), any mismatch in A or C will result in a non-zero e_{AC} value. Otherwise, e_{AC} will be zero if there is no mismatch in A or C . Therefore, any model-plant mismatch in system matrix A or C can be detected through the above model residual based index e_{AC} .

4.3.3 Detection of model-plant mismatch in C

In order to detect any model-plant mismatch in system matrix C , a residual based model quality index e_C is derived in this subsection. Eq. (4.27) can be rewritten in the following form

$$E_f = \begin{bmatrix} \Gamma_f & G_f^s \end{bmatrix} \begin{bmatrix} X_f - \hat{X}_f \\ A_f + B_f \end{bmatrix} + C_f \quad (4.35)$$

Define $\alpha_f = \begin{bmatrix} \Gamma_f & G_f^s \end{bmatrix}$ with rank m and select the matrix $(\alpha_f^\perp)^T \in \mathbb{R}^{(n_{yf}-m) \times n_{yf}}$ that is located in the orthogonal column space of α_f , i.e. $(\alpha_f^\perp)^T \alpha_f = 0$. Now pre-multiplying Eq. (4.35) by $(\alpha_f^\perp)^T$ can lead to

$$(\alpha_f^\perp)^T E_f = (\alpha_f^\perp)^T C_f \quad (4.36)$$

Given the fact that only a C_f related term is present in the right hand side of Eq. (4.36), any model-plant mismatch in system matrix C can be detected through the model residual based index e_C .

It is known that

$$\text{rank}(\alpha_f^T) + \text{nullity}(\alpha_f^T) = n_y f \quad (4.37)$$

and

$$\text{rank}(\alpha_f^T) = \text{rank}(\alpha_f) = m \quad (4.38)$$

Thus we have

$$\text{nullity}(\alpha_f^T) = n_y f - \text{rank}(\alpha_f^T) = n_y f - m \quad (4.39)$$

If $m \geq n_y f$, $\text{nullity}(\alpha_f^T)$ becomes zero and then the null space of α_f^T is empty. On the contrary, if $m < n_y f$ then the null space of α_f^T is not empty and exists. Since the left null space of α_f is equivalent to the null space of α_f^T , the orthogonal column space of α_f exists only if $m < n_y f$. Therefore, the residual based model quality index $e_C(k)$ exists only if $m < n_y f$.

4.3.4 Model-plant mismatch isolation based on different model quality indices

With the derived model quality indices e_{ABC} , e_{AC} and e_C , the model-plant mismatch detection problem is equivalent to the hypothesis testing of whether each of the model indices has zero mean or not. All these indices can be assumed to follow a multivariate Gaussian distribution under the Central Limit Theorem. Then, the following quadratic index $\mu(k)$ can be further defined for the purpose of statistically significant

model-plant mismatch detection

$$\mu(k) = e(k)^T R_e^{-1} e(k) \quad (4.40)$$

where $e(k)$ is one of the derived model quality indices e_{ABC} , e_{AC} and e_C , and R_e denotes the corresponding covariance matrix of $e(k)$.

For $e(k)$ following multivariate Gaussian distribution, $\mu(k)$ will follow a Chi-square distribution with l degrees of freedom

$$\mu(k) \sim \chi_l^2 \quad (4.41)$$

where $l = n_y f - n$ for e_{ABC} and e_{AC} while $l = n_y f - m$ for e_C (Anderson, 2003). Given the statistical confidence level $(1 - \alpha) \times 100\%$, the hypothesis testing for model-plant mismatch detection can be achieved by comparing $\mu(k)$ with the corresponding statistical confidence limit $\chi_l^2(\alpha)$. If we have

$$\mu(k) \leq \chi_{n_y f - n}^2(\alpha) \quad (4.42)$$

then it indicates that there is no significant model-plant mismatch in the system matrices related to the above quadratic index. On the contrary, if

$$\mu_{ABC}(k) > \chi_{n_y f - n}^2(\alpha) \quad (4.43)$$

it means that there is significant model-plant mismatch in the corresponding system matrices.

The obtained quadratic indices μ_{ABC} , μ_{AC} and μ_C under closed-loop operating

conditions can be integrated into a unified framework for model-plant mismatch isolation of different state-space system matrices. Since indices μ_{ABC} can detect the model-plant mismatch in system matrix A , B or C , the first level of detection is based upon μ_{ABC} . If $\mu_{ABC}(k) < \chi_{n_y f-n}^2(\alpha)$, it indicates that there is no significant mismatch in any of the system matrixes A , B and C and thus no further detection is needed. Otherwise, it means that there is significant mismatch in A , B or C and thereby μ_{AC} is further used in the second level of detection. If $\mu_{AC} > \chi_{n_y f-n}^2(\alpha)$, it implies that there is significant model-plant mismatch in system matrix A or C . Otherwise, it means that there is no significant mismatch in A or C and thus the model mismatch occurs in B . Finally, μ_C is utilized in the third level of detection only if $\mu_{AC}(k) \geq \chi_{n_y f-n}^2(\alpha)$. If $\mu_C < \chi_{n_y f-m}^2(\alpha)$, then there is no significant mismatch in C . Otherwise, there is significant model-plant mismatch in C . The established model-plant mismatch isolation logic is shown in Fig. 4.2.

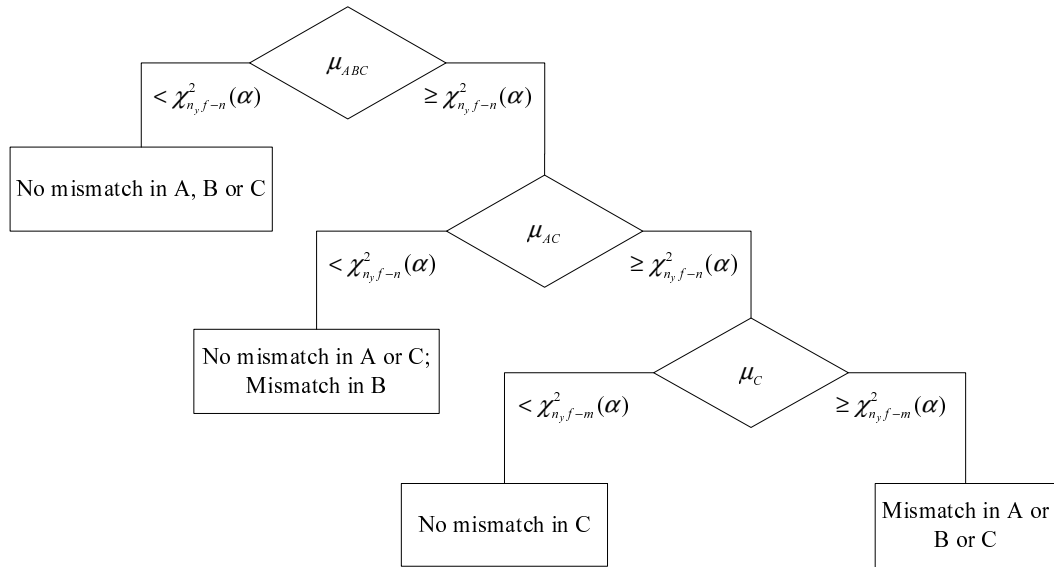


Figure 4.2: Schematic diagram of the designed model-plant mismatch isolation logic

It should be noted that the subspace projection based quadratic indices require

sufficient set-point excitation in order for the model-plant mismatches to be detected and isolated. Similar to closed-loop systems identification (Söderström and Mossberg, 2011; Söderström *et al.*, 2013), the following remarks can be made on the requirements of set-point excitation for model mismatch detection and isolation.

Remark 4.1: Set-point moves must be persistently excited in order to get informative closed-loop data for model-plant mismatch detection. With non-informative closed-loop data, the mismatched model used in the MPC controllers cannot be distinguished from the real plant model and thus the model-plant mismatch is not detectable in this situation. The quasi-stationary set-point signal $r(t)$ is persistently excited with the order s if the following matrix is positive definite

$$\begin{bmatrix} R_r(0) & R_r(1) & \cdots & R_r(s-1) \\ R_r(1) & R_r(0) & \cdots & R_r(s-2) \\ \vdots & \vdots & \ddots & \vdots \\ R_r(s-1) & R_r(s-2) & \cdots & R_r(0) \end{bmatrix} \quad (4.44)$$

where $R_r(\tau) = \bar{E}[r(t)r(t-\tau)]$ is the covariance function of the set-point r (Ljung, 1999).

Remark 4.2: Since the model residual e_k contains white noise with the same covariance as the noise covariance of the plant output y_k , the sequence of model residual will become less informative and identifiable due to the increased noise covariance. Therefore, the larger noise covariance will lead to the higher requirement of set-point excitation so that the signal-to-noise ratio is guaranteed for model-plant mismatch to be detectable by the residual based model quality indices.

4.4 Case studies

The proposed model-plant mismatch detection and isolation method is applied to a simulated multivariable model predictive control system of paper machine headbox and the schematic diagram of the headbox control problem is shown in Fig. 4.3. The state variables of the process are $x = \begin{bmatrix} H_1 & H_2 & N_1 & N_2 \end{bmatrix}^T$, where H_1 and H_2 are the liquid levels in the feed tank and headbox while N_1 and N_2 are the consistencies in the feed tank and headbox. Meanwhile, the controlled variables of MPC system are $y = \begin{bmatrix} H_2 & N_1 & N_2 \end{bmatrix}^T$ and the manipulated variables are $u = \begin{bmatrix} G_p & G_w \end{bmatrix}^T$, where G_p and G_w are the flow rates of the stock entering the feed tank and the recycled white water, respectively. The sampling time used in the simulation is 1 minute and a MIMO MPC system is implemented to control the paper machine headbox. The prediction and control horizons of MPC are set to 10 and 3 sampling periods, respectively. Moreover, the constraints of both manipulated variables are set to $(-10, 10)$. The state-space system matrices $\{A, B, C\}$ of the real plant are as follows

$$A = \begin{bmatrix} 0.145 & 0 & 0 & 0 \\ 0.133 & 0 & 0.533 & 0 \\ 0.133 & 0 & 0.533 & 0 \\ 0.212 & -0.512 & 0.244 & 0.653 \end{bmatrix} \quad (4.45)$$

$$B = \begin{bmatrix} 0.564 & 0.564 \\ 0.124 & 0.124 \\ 0.994 & -0.482 \\ 0.420 & 0.128 \end{bmatrix} \quad (4.46)$$

$$C = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \quad (4.47)$$

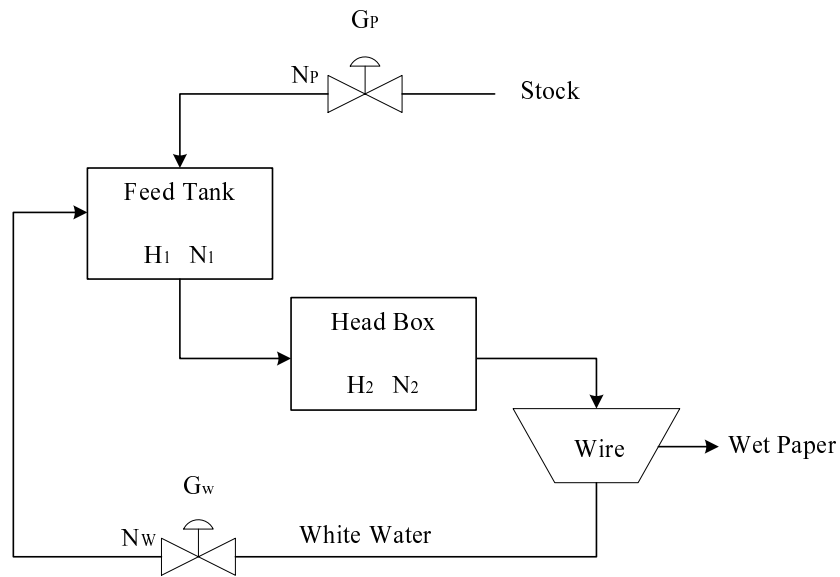


Figure 4.3: Schematic diagram of the paper machine headbox control problem

In order to examine the effectiveness of the proposed method, four test cases with different types of model-plant mismatches are designed, as listed in Table 4.1. In each test case, the initial 300 samples are simulated with no model-plant mismatch and

then a particular mismatch is applied to the model used in the MPC controller from the 301-st through the 1000-th sample. All the measurement samples are collected under the closed-loop operating conditions and the setpoint values are generated from the persistently excited pseudo random binary signals (PRBS) with amplitudes from 0 to 1. Both the future horizon f and past horizon p are set to 10 in this work. Thus the confidence limits with $\alpha = 0.05$ are $\chi_{26}^2(0.05) = 38.885$ for μ_{ABC} and μ_{AC} and $\chi_8^2(0.05) = 15.507$ for μ_C . The detection results for the four test cases are shown in Figs. 4.4, 4.5, 4.6, and 4.7, respectively.

In the first test case, there is model-plant mismatch in system matrix A only. It can be readily seen from Fig. 4.4 that the index μ_{ABC} exceeds the corresponding confidence limit from the 300-th sample, indicating model-plant mismatch in system matrices A , B or C . Furthermore, it is obvious that the mismatch is in system matrix A because the values of the index μ_{AC} is greater than the confidence limit from the 300-th sample onwards while the index values μ_C are always below the corresponding confidence limit for the entire operating period. The model-plant mismatch detection and isolation results are consistent with the simulation design.

For the second test case, model-plant mismatch only exists in system matrix B . As shown in Fig. 4.5, the index μ_{ABC} clearly points out that the model-plant mismatch occurs after the 300-th sample. The indices μ_{AC} and μ_C are further examined for the mismatch isolation. It can be seen that the values of μ_{AC} and μ_C always below the corresponding confidence limit line, even though the index values are inflated after the 300-st samples. According to the decision criteria, there is no significant model-plant mismatch in A or C . Since there must be model-plant mismatch of the system matrices as indicated by the index μ_{ABC} , the conclusion is that there is model-plant mismatch in system matrix B .

In the third test case, there are mismatches in system matrices A and C . It can

Table 4.1: Case Studies: Four Test Cases with Different Types of Model-Plant Mismatches in System Matrices

Case	Description
1	Sample 1-300: No mismatch Sample 301-1000: Mismatch in system matrix A $\hat{A} = \begin{bmatrix} 0.145 & 0.2 & 0.2 & 0.2 \\ 0.533 & 0.2 & 0.133 & 0.2 \\ 0.533 & 0.2 & 0.133 & 0.2 \\ 1.012 & -1.112 & 1.044 & 1.153 \end{bmatrix}$
2	Sample 1-300: No mismatch Sample 301-1000: Mismatch in system matrix B $\hat{B} = \begin{bmatrix} 0.564 & 0.734 \\ 0.124 & 0.161 \\ 1.889 & -1.688 \\ 0.420 & 0.167 \end{bmatrix}$
3	Sample 1-300: No mismatch Sample 301-1000: Mismatches in system matrices A and C $\hat{A} = \begin{bmatrix} 0.145 & 0.2 & 0.2 & 0.2 \\ 0.133 & 0 & 0.533 & 0 \\ 0.133 & 0 & 0.533 & 0 \\ 0.512 & -0.812 & 1.344 & 0.953 \end{bmatrix} \quad \hat{C} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$
4	Sample 1-300: No mismatch Sample 301-1000: Mismatches in system matrices A, B and C $\hat{A} = \begin{bmatrix} 0.145 & 0.2 & 0.2 & 0.2 \\ 0.133 & 0.2 & 0.533 & 0.2 \\ 0.133 & 0.2 & 0.533 & 0.2 \\ 0.512 & -0.712 & 1.344 & 0.853 \end{bmatrix}$ $\hat{B} = \begin{bmatrix} 0.734 & 0.734 \\ 0.161 & 0.161 \\ 1.292 & -0.627 \\ 0.546 & 0.167 \end{bmatrix} \quad \hat{C} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$

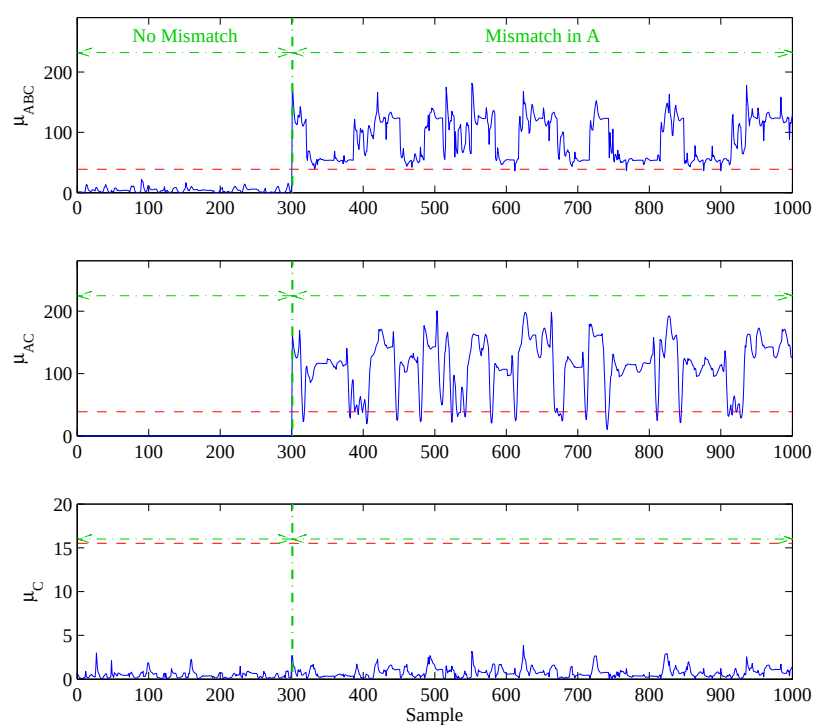


Figure 4.4: Model-plant mismatch detection results in Case 1

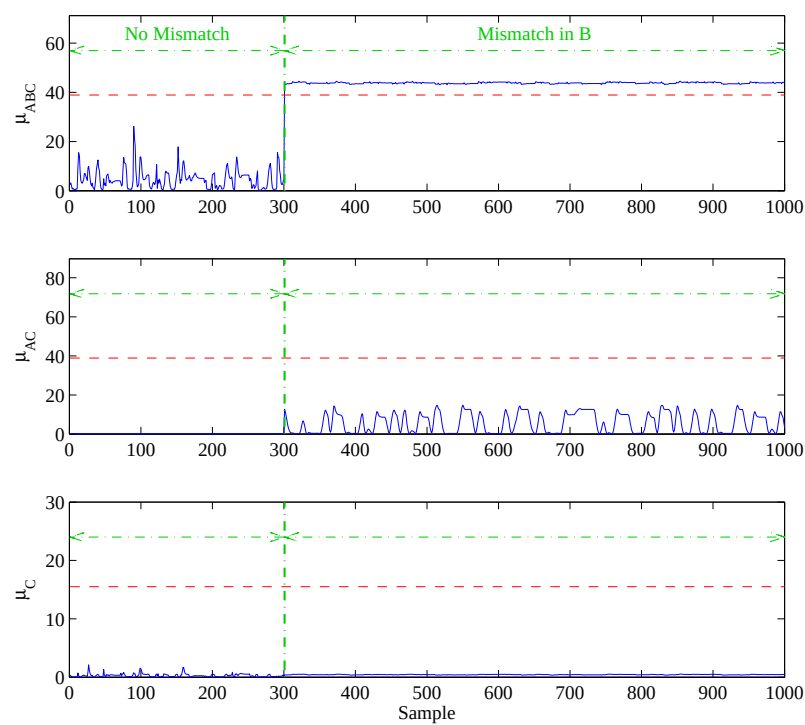


Figure 4.5: Model-plant mismatch detection results in Case 2

be readily observed from Fig. 4.6 that in the period from the first through the 300-th sample, the values of the index μ_{ABC} are always below the confidence limit. After that, the index values rise above the corresponding confidence limit, which indicates the model-plant mismatch in A , B or C . Since the mismatch in system matrix C can make both the indices μ_{AC} and μ_C above the corresponding confidence limits, the actual trends in Fig. 4.6 is consistent with the test scenario.

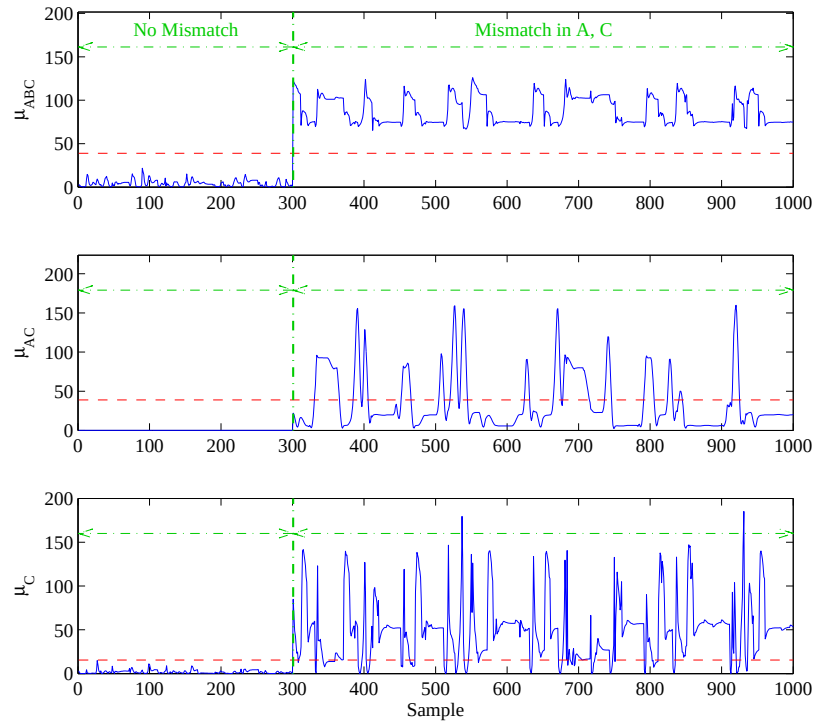


Figure 4.6: Model-plant mismatch detection results in Case 3

In the last case, model-plant mismatches are applied to system matrices A , B and C . It can be seen from Fig. 4.7 that the values of all the three indices are significantly larger than the corresponding confidence limits. It reveals that there are model-plant mismatches in all the system matrices. The results in all different test cases verify the effectiveness of the proposed model-plant mismatch detection approach for closed-loop MIMO MPC systems.

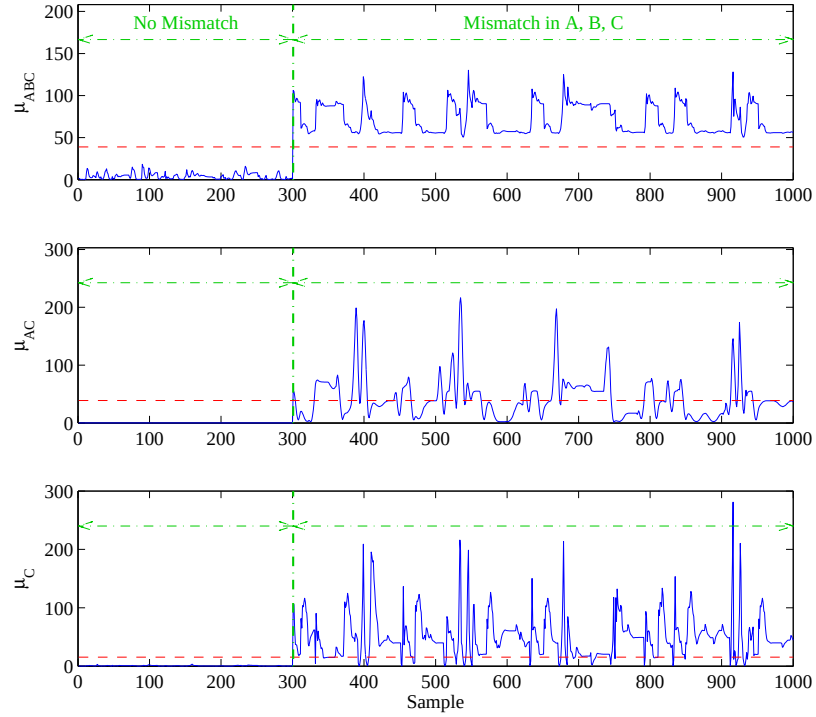


Figure 4.7: Model-plant mismatch detection results in Case 4

4.5 Conclusions

A novel subspace projection based model-plant mismatch detection and isolation method for multivariable model predictive control systems is proposed in this paper. Aimed at the closed-loop systems in state-space formulations with MPC controllers, three model residual based model quality indices are developed through different kinds of subspace projections so that the effects of system feedback and various state-space system matrices can be eliminated. Further, an integrated monitoring framework is established to isolate the significant model-plant mismatches on different system matrices by designing quadratic indices and statistical hypothesis testing. The presented method is applied to the simulated example of paper machine head-box process with MIMO MPC control system and the monitoring results indicate that

the proposed approach can reliably detect and isolate the significant model-plant mismatches in different system matrices. Therefore, this method provides an effective way for model-plant mismatch detection and isolation of closed-loop MPC systems in state-space framework. Future research may focus on the diagnosis of significantly mismatched input-output model channels of closed-loop MIMO MPC systems.

4.6 Acknowledgements

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Bibliography

- Anderson (2003). *An introduction to multivariate statistical analysis*. Wiley, New York, NY, USA, 3rd edition.
- Badwe, A., Gudi, R., Patwardhan, R., Shah, S., and Patwardhan, S. (2009). Detection of model-plant mismatch in MPC applications. *J. Process Contr.*, **19**(8), 1305–1313.
- Chiuso, A. and Picci, G. (2005). Consistency analysis of some closed-loop subspace identification methods. *Automatica*, **41**, 377–391.
- Jansson, M. and Wahlberg, B. (1998). On consistency of subspace methods for system identification. *Automatica*, **34**(12), 1507–1519.
- Jelali, M. (2006). An overview of control performance assessment technology and industrial applications. *Control Eng. Pract.*, **14**(5), 441–466.
- Jiang, H., Li, W., and Shah, S. (2006). Detection and isolation of model-plant mismatch for multivariate dynamic systems. In *IFAC Symposium on Fault Detection, Supervision and Safety of Technical Processes*, volume 6, pages 1396–1401, Beijing, China.
- Kano, M., Shigi, Y., Hasebe, S., and Ooyama, S. (2010). Detection of significant model-plant mismatch from routine operation data of model predictive control system. In *9th International Symposium on Dynamics and Control of Process Systems (DYCOPS), IFAC*, pages 685–690, Leuven, Belgium.
- Ljung, L. (1999). *System Identification: Theory for the User*. Prentice-Hall, Inc., Englewood Cliffs, NJ, USA, 2nd edition.

- Loquasto III, F. and Seborg, D. (2003). Model predictive controller monitoring based on pattern classification and PCA. In *American Control Conferenc*, volume 3, pages 1968–1973, Denver, CO, USA. IEEE.
- McKelvey, T., Akçay, H., and Ljung, L. (1996). Subspace-based multivariable system identification from frequency response data. *IEEE Trans. Autom. Control*, **41**(7), 960–979.
- Morari, M. and Lee, J. (1999). Model predictive control: past, present and future. *Comput. Chem. Eng.*, **23**(4), 667–682.
- Patwardhan, R. and Shah, S. (2002). Issues in performance diagnostics of model-based controllers. *J. Process Contr.*, **12**(3), 413–427.
- Qin, S. (2006). An overview of subspace identification. *Comput. Chem. Eng.*, **30**, 1502–1513.
- Qin, S. and Badgwell, T. (2003). A survey of industrial model predictive control technology. *Control Eng. Pract.*, **11**(7), 733–764.
- Qin, S. and Yu, J. (2007). Recent developments in multivariable controller performance monitoring. *J. Process Contr.*, **17**(3), 221–227.
- Schäfer, J. and Cinar, A. (2004). Multivariable MPC system performance assessment, monitoring, and diagnosis. *J. Process Contr.*, **14**(2), 113–129.
- Söderström, T. and Mossberg, M. (2011). Accuracy analysis of a covariance matching approach for identifying errors-in-variables systems. *Automatica*, **47**, 272–282.
- Söderström, T., Wang, L., Pintelon, R., and Schoukens, J. (2013). Can errors-in-variables systems be identified from closed-loop experiments? *Automatica*, **49**, 681–684.

- Sun, Z., Qin, S., Singhal, A., and Megan, L. (2013). Performance monitoring of model-predictive controllers via model residual assessment. *J. Process Contr.*, **23**(4), 473–482.
- Wang, H., Song, Z., and Xie, L. (2012). Parametric mismatch detection and isolation in model predictive control system. In *8th IFAC International Symposium on Advanced Control of Chemical Processes*, pages 154–159, Singapore.

Chapter 5

Conclusions and Future Work

5.1 Conclusions

This thesis has addressed three applications of statistical methods in process systems. The main theme of this thesis is based on the knowledge acquisition from industrial process data. Specifically, the performance monitoring of non-Gaussian dynamic processes with shifting operating conditions, the data-based soft sensor for online estimation of nickel pellet size distributions, and the model-plant mismatch detection for MIMO MPC performance monitoring are studied by analyzing different types of process data.

In chapter 2, an ICA mixture model dissimilarity method for multi-mode process monitoring with non-Gaussian components is developed. An ICA mixture model, which can characterize the non-Gaussian features in each mode, is first built from the multi-mode process data. Then the ICA component with the largest posterior probability is chosen as the target benchmark set and the dissimilarity index between the target benchmark and monitored sets can be evaluated for fault detection. With a window moving on the monitored set, the dependency between IC subspaces

and the non-Gaussian features in the ICA component can be extracted continuously via higher-order statistics underlying the dissimilarity factor. The proposed ICA mixture model dissimilarity method is applied to a numerical example and the Tennessee Eastman Chemical process and the monitoring results are compared to those of the eigenvalue decomposition based and the modified angle based PCA dissimilarity methods. The proposed method shows satisfied performance on not only increasing the fault detection rate but also decreasing the false alarm rate.

In chapter 3, two video analysis based nickel pellet sizing methods are developed for estimating and predicting the pellet size distribution. The first method relies on the edge detection of the free falling pellets in the filtered gray-scale video frames and can identify the diameters of pellets through the widths of the converted free falling tracks. In contrast, the second method is designed in the way of scanning the filtered gray scale images row by row in order to obtain the gray scale curves. Then Gaussian process regression model is built to decompose multi-peak curve and estimate the diameters of different pellets including the overlapped ones. Further a counting rule is established to estimate the pellet size distribution by eliminating the pellet overlapping effect along the horizontal and vertical directions. The two presented methods are applied to measure the size distribution of nickel pellets from nickel decomposer bed. The computational results demonstrate that the size distribution of nickel pellets can be more accurately predicted from the second video analysis method.

In chapter 4, a novel subspace projection based model-plant mismatch detection and isolation approach is developed. Aimed at the closed-loop systems with MPC controller in discrete time state-space representation, three quadratic indices are derived for model-plant mismatch detection and isolation assuming that the mismatch only exist in system matrixes A , B , or C . It is also assumed that there is not mismatch in disturbance model and the set-point moves are persistently excited. Under

closed-loop operating conditions, different kinds of subspace projections are designed for eliminating the feedback effects and isolating the model mismatches on various system matrices. The presented method is applied to the MPC system of the paper machine process with four different cases of model-plant mismatches. The results demonstrate that the proposed approach can accurately detect and isolate the mismatches in the simulated example. Therefore, this approach offers an effective tool for closed-loop MPC performance monitoring and especially model-plant mismatch detection.

5.2 Recommendations for Future Work

Recommendations for future work are presented below.

- (1) The processing monitoring method is proposed by using ICA mixture model dissimilarity method in chapter 2. The process fault can be detected in a real time fashion. However, the root-cause variables are unknown. Future research may focus on extending the ICA mixture model dissimilarity method for fault diagnosis to isolate the root-cause variables. On the other hand, the proposed method can be applied to real industrial process data with different operating modes.
- (2) For the nickel pellet sizing problem, more experiments are needed to determine the suitable illumination and pixel/inch ratio. When applying online, some pre-processing procedures need to be chosen to make the frames suitable for the proposed video analysis approaches. In addition, future research may focus on further improving the soft sensor prediction accuracy of pellet size distributions and extending the video analysis based soft sensors towards different industrial

applications.

- (3) In the present work of MPC performance monitoring, it is assumed that there is no mismatch in the disturbance model. Further work is recommended for isolating and detecting the model-plant mismatch in disturbance model. As mentioned in Remark 4.1, set-point moves must be persistently excited in order to get informative closed-loop data for model-plant mismatch detection. The requirement of persistent set-point moves may not be realistic during regular process operation. A possible direction of the future work will be assessing the magnitude of the set-point moves that is necessary for the proposed methodology to be successful. In particular, criteria could be developed for the minimum levels of moves to provide persistent excitation for the proposed method to work. In addition, future research may also focus on the diagnosis of significantly mismatched input-output model channels of closed-loop MIMO MPC systems.