Fault Diagnosis in Multivariate Manufacturing Processes

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FAULT DIAGNOSIS IN MULTIVARIATE MANUFACTURING PROCESSES

By

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ABSTRACT

As manufacturing systems are becoming more complex, the use of multivariate fault detection and diagnosis methods are increasingly important. Effective fault detection and diagnosis methods can minimize cost of rework, plant down time and maintenance time and improve reliability and safety. This thesis proposes Principal Components Analysis (PCA) based root cause identification approach for quality improvement in complex manufacturing processes. Simulation studies are presented to demonstrate the improved diagnosability of the proposed approach compared to existing methods.

Keywords: Multivariate analysis, Principal Components Analysis (PCA), Contribution Plot, Root cause identification
1 INTRODUCTION

As modern manufacturing systems are becoming more complex, the need for effective process monitoring and fault detection methods with high detection and diagnosis capability is evident, these methods are becoming increasingly popular. It has become necessary to find appropriate models for the application where the dimension is massive. For instance, in the automobile assembly process, laser sensing for coordinate measurement of key positions is commonly employed [1]. Consider a layout of 26 measurement points, each one having three coordinates \((x, y, z)\) in 3 dimensions. Then the total dimension of measurements becomes \(26 \times 3 = 78\) in this assembly process. Multivariate statistical methods are also applied in the field of image analysis to achieve higher image resolution. Consider the data which is collected by image processing software [2]. The image can be best represented in the form of an \(N\)-dimensional vector for each pixel, where \(N\) is the number of spectral bands. From a data analysis standpoint, even in terms of the three basic bands used to generate the image, the total variable space is \(3 \times \text{(number of pixels)}\), which may be beyond thousands or hundreds thousands of dimensions. Obviously, the analysis of process monitoring systems involves many details.

In the complex multivariate manufacturing processes, it is important to improve the detectability and diagnosability by monitoring, recording, analyzing and controlling the status of the system real-time. The multivariate analysis methods become the first main area to improve detectability and diagnosability.

Multivariate analysis is the collection of statistical techniques that extends univariate data to multiple dimensions. The successful application of multivariate diagnosis depends on estimating the relationship among those multiple variables. Classical statistical methods provide many useful statistical tools such as: variance-covariance matrix, correlation matrix, Mahalanobis distance and Hotelling \(T^2\). However, to discover deeper layers of relationships
among multiple variables, such as causal relationships, network-based methods such as ANN and BN have recently been proposed.

Bayesian Network, which is a network method of probabilistic graphical modeling, can be used to model complex interdependencies and causal relationships among a large number of variables. It uses directed acyclic graph (DAG) to show probabilistic dependencies between those variables, as in Figure 1.1. Researchers have studied and developed sophisticated methods or algorithms for inferencing and learning BN with arbitrary DAG. However, network structure learning is still an active topic of research. Structure learning is a model selection and parameter estimation approach based on a set of observed data. Basically, there are two main approaches to learn BN structure [3]. The first is dependence analysis which usually uses statistical hypothesis test to discover the interdependencies from data. The second approach formulates the BN-structure learning problem as an optimization problem, and it utilizes searching and scoring methods. The algorithm used in this thesis is based on the dependence analysis.

Figure 1.1 DAG of Bayesian Network
BN is widely used in various areas. Raval, Ghahramani, and Wild [4] utilized BN modeling for protein fold recognition. Florian [5] is using BN to reconstruct the gene regulation network [5]. Cano, and Sordo [6] present some applications of Bayesian Networks in meteorology. They tried standard learning algorithm, then improved it to apply to different meteorological problems including weather forecast and stochastic weather generation [6]. Today BN methods are being utilized by corporations to help their risk analysis, strategic planning and decision support [35].

BN is powerful in multivariate analysis because it can accurately capture probabilistic information from data using DAG. It can also update probabilities when data becomes available. Thus, BN offers a tractable and interpretable method which can help us to solve various multivariate problems.

The second way to improve detectability and diagnosability is using enhanced process monitoring methods, which involve the use of data collected by a variety of sensor technologies, including piezoelectric accelerometer, force sensor, pressure sensor, velocity sensor, shock sensor, speed sensor, tachometers etc. Improvement in the capacity of monitoring methods can also be achieved by better measurement layout of the sensors. The more accurate the data collected from measurement equipment, the more predictions can be made.

In process monitoring method, the term: Condition Monitoring (CM) means the use of different technologies in order to determine equipment condition. These technologies includes: (1) Vibration Measurement and Analysis; (2) Infrared Thermography; (3) Oil Analysis and Tribology; (4) Ultrasonics; (5) Motor Current Analysis [9]. Clearly, there are a large number of performance measures that we can select for analysis, but, it is important to select only a few of the most important performance measures. The selection should be considered in terms of the following characteristics of the performance measures: [9]
(1) Relevance – is there a key link between this measure and the organization’s overall mission/vision/goals

(2) Reliability – does the suggested performance measure accurately reflect performance in the selected area?

(3) Understanding – how well is the performance measure understood by those whose performance is going to be measured?

(4) Availability of Data – is the data required to calculate the measure readily available, or easily obtainable?

(5) Timeliness – how quickly does the measure respond to changes or improvements that may have been made? Is the measure a “leading” or a “lagging” measure of performance?

(6) Controllability – to what extent can the person or group, to whom the measure is being reported, influence performance, as reported by the measure?

With the improved detectability and diagnosability, the system will have the benefits of lower cost of rework, reduced down time and maintenance time, higher reliability, availability, maintainability and safety. For instance, if we consider the example of a power plant, the power electronics will be more reliable if we have better detectability and diagnosability on its increase or disturbance of resistance. The minimum measurement configuration with a pump-pipe system can be found using the better diagnosability method. The improved detectability and diagnosability can also reduce the cost of maintenance in a pump-pipe system by controlling the flow rate. Successfully detecting and diagnosing faults in an automotive suspension system will significantly increase the safety of driving the vehicle. And diagnosis in tire pressure will be directly related to the capability of the automobile.
We all know mechanical failures are a critical problem in the manufacturing system. Mechanical failures represent a cost of billions of dollars every year to the manufacturing industry [10]. It is often cheaper and more feasible to replace or fix a soon-to-fail component than to wait until a catastrophic failure occurs. Condition Based Maintenance (CBM) methods, that combine condition monitoring and predictive maintenance, have been recently studied by many researchers. CBM uses reliability models and condition (sensor) data to predict the remaining service life of machine components and schedule preventive maintenance actions before the failure occurs.

When equipment fails, people’s biggest concern is to make the equipment functional again. However, to discover why the equipment failed and how such failure can be prevented is equally important. Preventive maintenance is the class of regular equipment maintenance practices implemented in order to avoid future problems. An important first step in any predictive maintenance program is learning to identify the root causes of equipment failure. Once the cause of failure is determined, one can take the necessary steps to avoid the problem in the future. The major economic benefits derived from employing predictive maintenance is the ability to predict with reasonable certainty how much longer a machine can safely operate, often a matter of several months from when incipient faults are first detected [39].

Let us consider gearbox reliability monitoring as an example. The gearbox is one of the most critical components of power generating machinery. Figure 1.2 illustrates the gearbox of a wind turbine system.
The gearbox is an important component in a wind turbine because it transfers the power from blades to generator. Usually the speed of wind is slow, simply not fast enough to meet the speed requirement of the generator. So, the gearbox is needed to achieve the function of increasing speed. Gearbox is important not only because it has the function of transferring power and changing speed, but also of changing direction of transmission, changing torque, serving as a clutch and allocating power. So, its performance and structural integrity are crucial for the whole system.

Identifying causes of gearbox failure is a crucial step in preventing future equipment problems. To determine the root cause of failure, oil analysis and vibration analysis are the commonly applied methods, in addition to visual inspections [9]. These diagnostic
techniques are usually required to monitor the condition of plant machinery and to control the causes of machine failure.

Vibration measurement and analysis is considered the most general basis for gear fault detection [11]. This thesis focuses on vibration analysis, which is an effective technique for monitoring the condition of the gears and bearings, and determining the root cause of machine failure. The following types of root-causes are typical in gear-box failures: (1) Gear pitting (Figure 1.3 and 1.4); (2) Bearing defects (cage fractures, inner/outer ring damage); (3) Alignment errors; (4) Looseness; (5) Imbalance; (6) Resonance areas.

![Figure 1.3 Hard contact areas with gear pitting](image)

Figure 1.3 Hard contact areas with gear pitting

![Figure 1.4 Initial/Incipient Pitting (Left) and Destructive Pitting (Right)](image)

Figure 1.4 Initial/Incipient Pitting (Left) and Destructive Pitting (Right)
Because the faulty gearbox produces specific patterns in vibration data, these patterns can be used to classify the type of damage in the gear box. The most widely used method in rotating machinery condition monitoring, due to its ability to provide early prediction of developing defects, is Fast Fourier Transformation (FFT) [7].

The preventive maintenance analysis for gearbox systems consists of the following steps: (1) Establish a baseline of the system; (2) Early detection of failure, data preparation; (3) Root-cause identification by tracing back from conditioning monitoring outputs to physical problems; (4) Predict future failure.

The gearbox is one type of rotating machinery. In condition monitoring of rotating machinery, frequency domain methods based on Fourier Transformation (FT) are traditionally employed to identify defect frequencies and their change in amplitude. The Fast Fourier Transform (FFT) is an efficient and improved algorithm for FT. Figure 1.5 shows the FFT of a set of hypothetical vibration data. Any periodic function can be expressed as the sum of a series of sines and cosines (of varying amplitudes) functions. FFT is a systematic way to decompose this “generic” function into a superposition of “symmetric” functions based on Laplace transform [8]. These symmetric functions often are trigonometric functions: \( \sin(x) \) or \( \cos(x) \). The Fourier Transform decomposes a function into components, that correspond to different frequencies. In real application, FFT is often used because this algorithm focused on discrete Fourier Transform and decomposed function into fewer components, and each component has a range of frequencies rather than purely single frequency. In our gearbox case, the domain frequency corresponds to the fault frequency range of interest.
Figure 1.5 Matlab-based FFT
2 LITERATURE REVIEW

The development of expanding process automation has caused increasing demand on better performance of multivariate process detection and diagnosis methods.

2.1 Multivariate process monitoring and fault detection methods

Fault monitoring and detection means to recognise when the process is out-of-control. Detectability means the ability to correctly detect the out-of-control signal.

2.1.1 Hotelling $T^2$ control chart

In fault detection of manufacturing processes with single quality characteristic, the Shewhart X-bar control chart is the traditional approach. But in many cases, there will be more than one measurement process to monitor. The widely used multivariate monitoring control chart is the Hotelling $T^2$ control chart, which is effective in detecting faults in multivariate processes. It is based on the Hotelling $T^2$ statistic:

$$T^2 = (X - \mu)^T \Sigma_X^{-1} (X - \mu) \sim \chi^2_p$$  \hspace{1cm} (2.1)

Where $\chi^2_p$ represents a $\chi^2$ distribution with $p$ degrees of freedom. $\Sigma_X$ is the variance-covariance matrix estimated from the observed data matrix $X_{nxp}$. $n$ is the number of observations and $p$ is the number of variables.

In $T^2$ control chart, the control limit is computed based on the chi-square distribution. Given $p$ and the desired significance level $\alpha$, if the observed $T^2$ statistic exceeds this limits, the control chart shows that there is evidence in the data that the process has gone out of control (for example, some faults have occurred). See Figure 2.1, the control limit is $\chi^2_{p,\alpha}$. 
However, after the above analysis, the analyst knows when the system has faults. For example, from Figure 2.1, we know after observation 26, there should be some faults in the system. But this chart can not help to locate the root-causes of the faults (for example, which variables experience a shift).

2.1.2 Multivariate CUSUM control chart

Multivariate Cumulative Sum (CUSUM) charts extend the univariate case in CUSUM charts, this has been shown to be more efficient in detecting small shifts in the mean of a process. Analysis shows that they are better than Shewhart control charts when it is desired to detect shifts in the mean that are 2 sigma or less [52].

In univariate case, CUSUM charts are constructed by calculating and plotting a cumulative sum based on the data. Let $X_1, X_2, \ldots, X_n$ represent n data points. Based on this, the cumulative sums $S_0, S_1, \ldots, S_n$ are calculated. Notice that n data points leads to n+1 (0 through n) sums. The cumulative sums are calculated as follows: First calculate the average:
Then calculate the cumulative sum at zero by setting $S_0 = 0$. Next calculate the other cumulative sums by adding the difference between current value and the average to the previous sum, for example:

$$S_i = S_{i-1} + (X_i - \bar{X})$$

Where $i=1,2,...,n$.

The multivariate CUSUM charts are considered for detecting a shift in either mean vector or covariance matrix. It is better than Shewhart control charts when it is desired to detect small shifts.

2.1.3 Principal Components Analysis (PCA)

In multivariate case, it is normal to observe large number of dimensions in response. For instance, with electronic and other automated methods of data collection, it is not uncommon for data to be collected on 20 or more process variables. Major chemical and drug companies report measuring over 100 process variables, including temperature, pressure, concentration, and weight, at various positions along the production process [37]. So, the data reduction and interpretation is very important. One of the Principal Components’ goals is data reduction. Data reduction means express analysis in terms of as few covariances of $X$ as possible, or in terms of as few linear combinations in these covariances. In principal component analysis, although $p$ components are required to reproduce the total system variability, often much of this variability can be accounted for by a small number $k$ of their principal components (Richard and Wichern [37]).
In the fault detection stage, instead of using $T^2$ control chart (see equation 2.1), PCA uses the dominant principal components variables, which can explain the total variance of the original data much better, to detect the out of control signal [43]:

$$T^2 = X^T G V^{-1} G X \sim \chi_k^2$$  \hspace{1cm} 2.1

Where the $G$ is the first $k$ eigen vectors of the covariance matrix of original data, $V$ is a diagonal matrix and its diagonal entries are the first eigen values of the covariance matrix of original data. The $k$, which is the number of chosen principal components, is decided by how much of the total variance the components can explain. By using this equation instead of original data to determine when the process is out of control, PCA performs better than traditional Hotelling $T^2$ because it ignores the noise effect.

### 2.2 Multivariate process fault diagnosis methods

Once we find where the fault is during the process, the next step is to find which variable(s) cause this fault. Fault diagnosis means to locate which variables cause the mean shift or mean change. Diagnosability means the ability to correctly identify the root-cause variables.

#### 2.2.1 $T^2$ decomposition approach

Mason, Tracy, and Young [12] proposed a method to decompose $T^2$ statistic into independent parts. These independent components can then be used to determine which characteristics are most significantly contributing to the out of control signals.

In order to decompose the $T^2$ statistic given in the equation 2.1 into independent components, we first group first $p-1$ variables together and to isolate the $p^{th}$ variable. This can be done as:
$T^2 = T^2_{p-1} + T^2_{p-1,...,p-1}$

Where the $T^2_{p-1}$ is Hotelling $T^2$ statistic using the first $p-1$ variables, and it has the form:

$$T^2_{p-1} = (X^{(p-1)} - \mu^{(p-1)})^T \Sigma^{-1}_{(p-1) \times (p-1)} (X^{(p-1)} - \mu^{(p-1)})$$

And $T^2_{p-1,...,p-1}$ is the $p$th component of $X$ adjusted by the estimates of the mean and standard deviation of the conditional distribution of $X_p$ given $X_1, X_2, ..., X_{p-1}$.

Since the term $T^2_{p-1}$ is a $T^2$ statistic on $p-1$ variables, we can partition it into two parts:

$$T^2_{p-1} = T^2_{p-2} + T^2_{p-1,1,...,p-2}$$

Repeating this procedure for all variables yields the following general decomposition of Hotelling’s $T^2$ for $p$ variables:

$$T^2 = T^2_1 + T^2_{2,1} + T^2_{3,1,2} + T^2_{4,1,2,3} + \cdots + T^2_{p,1,...,p-1} = T^2_1 + \sum_{j=1}^{p-1} T^2_{j+1,1,...,j} \quad (2.1)$$

It can be shown that each independent $T^2$ term is distributed as a constant times an $F$ distribution having 1 and $n-1$ degrees of freedom:

$$T^2_{j+1,1,...,j} \sim \frac{n + 1}{n} F(1,n-1)$$

Use the following equations to calculate the term $T^2_{p-1,...,p-1}$:

$$T_{X_j,PA}(x_j) = \frac{X_j - \mu_{X_j,PA}(x_j)}{\sigma_{X_j,PA}(x_j)}$$

Where

$$\mu_{X_j,PA}(x_j) = \sum_{i=1}^{j-1} \beta_i x_i$$

$\beta_i$ (i=1,...,j-1) are the regression coefficients of $X_j$ regressed on its parents $X_i$.  

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\[ \sigma_{X \mid \mathcal{PA}(X)} = 1 - \sum_{i=1}^{j-1} \beta_i \rho(X_i, X_j) \]

Where the \( \rho(X_i, X_j) \) is the correlation coefficient between \( X_i \) and \( X_j \).

By using this distribution one can identify which variables are contributing to out of control signals in a \( T^2 \) control chart.

Because there are \( p! \) different orders when decomposing \( T^2 \) to \( p \) partitions, it is difficult to find the most efficient order to locate the significant variable when \( p \) is large.

### 2.2.2 Causation-based \( T^2 \) (CBT) decomposition approach

Li and Shi [26] proposed a causation-based \( T^2 \) decomposition to improve the diagnosability performance of the \( T^2 \) decomposition approach. They model the causal relationship between variables by a Bayesian Network and utilize the \( T^2 \) decomposition procedure to locate root-causes of out-of-control signals.

In \( T^2 \) decomposition approach [12], all the possibilities of decomposition are considered. In multivariate case, the number of variables may be large. The \( p! \) different orders may become a huge number, it is difficult to find the most efficient order to locate the significant variable when \( p \) is large.

Li and Shi [26] use BN as tool to improve the efficiency of \( T^2 \) decomposition approach. By discovering the causal relationships among the \( p \) variables, they can find out the most efficient order to decompose the \( T^2 \) statistic. Once a failure analysis has been completed and the root cause of failure determined, it is imperative that the results be fed back into the design or maintenance process [10].

There are two steps in learning a BN. The first step is learning the structure and learning the parameters given the BN structure [26]. The structure can be learned from
manufacturing domain knowledge or from data. One commonly used data-driven algorithm for structure learning is called PC by Spirtes et al [35], which uses a series of statistical significance tests of conditional independence. Learning the parameters is based on the sample correlation matrix of all variables in the BN:

$$\begin{bmatrix} \hat{p}(PA_1(Z_j),Z_j), \ldots, \hat{p}(PA_m(Z_j),Z_j) \end{bmatrix}^T = \tilde{c}\tilde{r}(PA(Z_j),PA(Z_j))^{-1} \tilde{c}\tilde{r}(PA(Z_j),Z_j)^T$$

Where $\tilde{c}\tilde{r}(\cdot,\cdot)$ stands for the sample correlation matrix between two sets of variables. $
\hat{p}(PA_i(Z_j),Z_j) \ (i=1,...,m)$ is the path coefficient of the BN between $Z_j$ and its parent $PA(Z_i)$.

The PC algorithm is the most classic method in BN area based on independence tests. It starts with a fully connected undirected graph, where all variables are linked with all other variables by undirected arcs.

The second step is to remove the undirected arcs by conditional independent test in this multivariate case. We use Fisher’s Z-transform for testing an approximate partial correlation coefficients significance:

$$Z(r_{XY,Z}) = \frac{1}{2} \ln \left( \frac{1 + r_{XY,Z}}{1 - r_{XY,Z}} \right)$$

Where $r_{XY,Z}$ denotes the partial correlation between $X$ and $Y$ given a set of controlling variable $Z$:

$$r_{XY,Z} = \frac{r_{XY} - r_{XZ}r_{YZ}}{\sqrt{1 - r_{XZ}^2}\sqrt{1 - r_{YZ}^2}}$$

Where $r_{i,j}$ is the correlation coefficient between variable $i$ and $j$.

For higher order partial correlation, $r_{i,q+1,...,p}$ can be calculated as (Johnson, Wichern 1988):

$$r_{i,q+1,...,p} = \frac{r_{i,q+2,...,p} - r_{i,q+1,q+2,...,p} \cdot r_{j,q+1,q+2,...,p}}{\sqrt{1 - r_{i,q+1,q+2,...,p}^2}\sqrt{1 - r_{j,q+1,q+2,...,p}^2}}$$
The undirected arc between each pair of variables is removed if we do not reject the null hypothesis: \( H_0: r_{ij\cdot q+1\ldots p} = 0 \), which means they are conditional independent.

We reject \( H_0 \) at significance level \( \alpha \) if

\[
\sqrt{N - (p - q) - 3|Z(r_{xy.z})|} > \Phi^{-1}(1 - \alpha/2)
\]

Continue doing the remove by testing the first order partial correlation coefficients through the sequence to arrive at the available highest order partial correlation coefficients, we will get, for example:

![Figure 2.2 Removing arcs using conditional independence test](image)

The following diagram shows the procedure of PC algorithm to remove arcs:
The next step is to direct the arcs. According to PC algorithm, for each triple of variables, orient $X_r-X_j-X_k$ as $X_r \rightarrow X_j \leftarrow X_k$ if $X_i$ and $X_k$ are found to be independent (or uncorrelated) given a set of variables that do not contain $X_j$. For remaining variables, we will orient the arcs so that no cycles are produced. In addition to the PC algorithm, some orientations may be achieved through manufacturing domain knowledge or first principles. For example, if $X_i$ is known to occur before $X_j$ and there is no feedback control in the system, then direct $X_r \rightarrow X_j$. 

Figure 2.3 PC algorithm's logic to remove arcs
We need to notice that causality is not correlation. The relationship BN shows is beyond what correlation matrix can tell.

Based on $T^2$ decomposition approach and the information provided from BN structure, causation-based $T^2$ decomposition allows us to identify which variable significantly contributes to an out-of-control variable more efficiently.

Consider the hot forming example ($p=5$), which we already have the BN structure, know the parents of each variable. Different from the general decomposition of Hotelling’s $T^2$ for $p$ variables (see equation 2.1), the causation-based $T^2$ decomposition of a $T^2$ is:

$$T^2 = T^2_{1,P_A(X_1)} + T^2_{2,P_A(X_2)} + T^2_{3,P_A(X_3)} + T^2_{4,P_A(X_4)} + T^2_{5,P_A(X_5)}$$

The same as $T^2$ decomposition approach, each term of $T^2_{i,P_A(X_i)}$ should be calculated using the equations and conditional mean in 2.2.1.

The procedure of CBT approach can be concluded as follows:
(1) To detect out-of-control signal use $T^2$ control chart (see equation 2.1). Case j is out of control if $|T^2| > \chi^2_{p,\alpha}$

(2) To determine the root cause(s) of the out-of-control signal use $T^2_{i,PA(x_i)}$. Because $T_{i,PA(x_i)}$ follows a normal distribution [26], variable j is a root cause if $|T_{X_j,PA(X_j)}| > Z_{\alpha/2}$

Compare the performance of causation-based $T^2$ decomposition method with $T^2$ decomposition approach, type I and type II error rate are considered. The type I error rate is defined as the error rate of falsely identifying a mean shift; type II error rate is the error rate of misdetecting this mean shift if $X_j$ truly has a mean shift. The simulation results show that the causation-based $T^2$ decomposition method is significantly better than the $T^2$ decomposition approach in type I error rate. But in type II error rate the two approaches are comparable.

However, compare to PCA, which makes the interpretation easier because PCA representation can reveal physical relationships in the manufacturing processes [43], BN can be hard to interpret for some process models. Several authors have recommended BN models for describing processes with hierarchical structure [26]. For example, automobile sheet-metal assembly process where there are large of assembly stages conducted sequentially. But if there is no clear layered structure, then BN model may not be physically intuitive.

Also, the Bayesian Network method require conditionals independence test, which consists of testing the significance of the first, second, and so on up to $(p-2)^{th}$ order conditional correlation coefficients. For example, if we have $p=5$ variables, we need to calculate up to 3rd order conditional independence test. The total number of testing is $\binom{5}{2} \times \left( \binom{3}{1} + \binom{3}{2} + \binom{3}{3} \right) = 70$. If there are large number of variables, the BN will involve huge number of testing, which is computationally intensive.
2.2.3 Other fault analysis methods

Several recent papers address the problem of how to improve the detectability of traditional Hotelling $T^2$ control charts. James et al. [10] proposed a new $T^2$ test statistic and an estimator of the mean to improve correct detection rate of special causes of variation. Based on their proposed three approximate distributions of $T^2$ chart statistics, the upper control limit for individual observations can be calculated more accurately. Compared to the traditional $T^2$ control chart, their method can achieve better result when the sample size is small.

Zhou, Jin, and Jin [18] improved the efficiency of detection of process changes based on monitoring cycle-based signals. A cycle-based signal is a signal obtained using automatic sensing during each repetitive operation cycle of a manufacturing process. They proposed a directionally variant control chart obtained through the combination of the multivariate chi-square chart and an univariate projection chart, which considered both the available information about the process faulty conditions and the discrimination analyses that assume that process faulty conditions are completely known, because in most cases, it is not fair to assume that process faulty conditions are known.

Marion and Keunpyo [20] use multivariate exponentially weighted moving average (MEWMA) control charts to monitor processes to detect special causes that produce changes in the process. Sequential sampling method allows us to take samples of varying sizes depending on the sampling instant. The sample size taken at a sampling point depends on current and past sample data. The authors illustrate that the MEWMA chart based on sequential sampling is much more efficient in detecting changes in the process mean vector than standard control charts based on non-sequential sampling. But their approach may be inconvenient to allow a large number of groups to be taken at a sampling point.
Marion and Gyo [15] compare the performance of using combinations of multivariate exponentially weighted moving average (MEWMA) control charts, with standard multivariate T² charts. Their conclusion is that the best overall performance is obtained by using a combination of MEWMA charts and the sum of squared regression adjusted deviations from target.

Apley and Shi [53] introduce a generalized likelihood test (GLRT) procedure by assuming different shift occurrence times. This GLRT procedure conducts a multivariate hypothesis test based on residuals. Based on GLRT, Zamba and Douglas [16] use multivariate change-point model through generalized likelihood-ratio statistics to monitor and detect change in the mean vector and/or covariance matrix, as well as the epoch of a change. Their model can monitor short runs and unknown parameter change-point processes. It is assumed that the vector of measurements \( X_i \) is distributed as:

\[
X_i \sim \begin{cases} 
N_p(\mu, \Sigma) & \text{if } i \leq \tau \\
N_p(\mu_1, \Sigma_1) & \text{if } i > \tau
\end{cases}
\]

Where \( \tau \) is the unknown change point and is unknown. The remaining parameters \( \mu, \mu_1, \Sigma, \Sigma_1 \) are known in- and out-of-control mean vector and covariance matrices.

Jiang [21] focused on monitoring multivariate autocorrelated processes. He improved the efficiency of the T² chart by employing a generalizing likelihood ratio test (GLRT). The proposed observational and innovational GLRT control chart is shown to outperform the T² chart, because it utilizes the information of \( p \) potential shift directions, where \( p \) is the number of mutually independent components of prediction errors. In his research, when the sample size is large, the proposed GLRT chart performs better than T² chart. But because the innovational GLRT chart doesn’t utilize the right shift directions, a small sample size should be avoided.

Hao, Zhou and Ding [19] use a multivariate projection chart approach to monitor a shift in the mean. Comparing to U² control chart, which is a projection chart of T² chart by Runger
[44], this approach is more suitable for monitoring the variance components: is broadly applicable, robust to noise, and having uniform responses to different fault inputs. But when the sample size is small, a systematic method for adjusting control limits require specified type I error rate.

Nedumaran, Pignatiello and Calvin [51] proposed a maximum likelihood estimator method to identify the time of step change in a multivariate process. They first detect the out-of-control signal by using standard $T^2$ chart. Then they estimate the time of change $t$ by maximizing the statistic $M_t$. Successfully locate the time of change will improve the efficiency of other fault diagnosis methods.

In manufacturing quality control area, researchers try to implement different technique to improve the diagnosability of fault detection. Li and Chen [22] aimed to detect sensor mean shift faults and distinguish them from potential process faults in discrete-part manufacturing processes. In manufacturing systems, abnormal observations may be due to process faults, such as the malfunction of tooling elements, or due to the malfunction of sensors used to take the measurements. The authors propose a $W$ control chart based on a linear fault quality model, which can effectively separate sensor faults from process faults. But when the $W$ chart indicates the presence of sensor faults, it can not directly indicate which particular sensor(s) causes the mean shift.

Lai, Tian and Lin [31] proposed a simplified method for optimal sensor distribution for process fault diagnosis in multistation assembly processes. It improves the efficiency of diagnosis in multistation assembly processes (MAPs) by reducing the number and location of the sensors. This method has been studied for the purpose of a full diagnosis of the process faults with the minimum number of sensing stations number as well as the minimum number of sensors. The existing studies in this field are time consuming with complex analysis and calculation procedures, and no intuitive principles are given directly. The optimal sensor distribution is based only on the process configuration without using
model-based matrix computation. However, the complexity of this method reduces its efficiency in the design of sensor distribution.

Wade and Woodall [41] studied cause-selecting charts using prediction limits. The cause-selecting charts, which based on regression control chart, are used to distinguish between in-coming quality problems and out-going quality problems. The authors propose to apply prediction limits to estimate the relationship between the two quality measurements and to improve the false alarm rate of cause-selecting charts.

Condition monitoring and predictive maintenance are very important because they can help achieve variability reduction and preventing catastrophic failures by increasing the ability of detecting and locating key problems in complex manufacturing processes before failures occur. Li, You and Ni [30] present a reliability-based dynamic maintenance threshold (DMT) based on the updated equipment status, to trigger maintenance work-orders. They try to improve the maintenance effectiveness and reduce equipment failures by maximizing system availability. Comparing to conventional method of fixed maintenance threshold using the lifetime distribution of each machine, DMT considers the updated state of the system, which allows to more effectively detect the onset of failures.

Farrar, Doeblng, and Nix [38] briefly reviewed structural health monitoring and the process of vibration-based damage detection using statistical pattern recognition. They partition the process into four parts: (1) operational evaluation; (2) data acquisition and cleaning; (3) feature selection and data compression; (4) statistical model development. The algorithms used in statistical model usually fall into three categories and will depend on the availability of data: group classification, analysis of outliers, and regression analysis.

Randall [39] deeply discussed fault detection, fault diagnosis, and signal processing techniques for monitoring rotating machinery. He reviewed the fundamental measurement ways of fault detection: the use of accelerometers and analyzes the physical reasons of fault
in rotating machinery, which are: (1) shaft speed faults; (2) electrical machine faults; (3) gear faults; (4) bearing faults; (5) reciprocating machine faults. He also reviewed a number of classical and newer techniques in signal processing including: (1) FFT analysis; (2) zoom FFT; (3) practical FFT analysis; (4) digital Filters; (5) MA models; (6) AR models; (7) separation of periodic and random signals; (8) order tracking; (9) adaptive noise cancellation; (10) demodulation; (11) envelope analysis; (12) phase and frequency demodulation.

Pusey [10] reviews developments and progress in the mechanical failure prevention literature, primarily over the last four decades. Three technical areas must be addressed for effective fault diagnosis using vibration: (1) condition and fault mechanisms; (2) modification of signal transmission paths; (3) signal analysis. Life extension and durability can also be examined from a different perspective to improve product performance.

Liu, Shi and Hu [32] discuss a method to identify variation sources by using interactions between potential variation sources and product quality variables in multistage manufacturing processes. The procedure does not depend on complex engineering models of the interactions between process variation sources and it is illustrated that the method by using a factor analysis approach improves the diagnostic interpretability.

Kong, Ceglarek, Dariusz and Huang [33] proposed a multiple fault diagnosis method in multistation assembly processes that involves orthogonal diagonalization and Principal Components Analysis (PCA). Orthogonal diagonalization allows estimating the statistical significance of the root cause of the identified fault. The proposed method can balance both focusing on modeling of variation propagation in complex manufacturing processes and root cause identification.

Apley and Zhang [23] focus on identifying the major sources of variation that contributes to the final product or process variability in modern manufacturing processes. Based on high dimensional manufacturing measurement data, they proposed a model for representing
nonlinear variation patterns and identifying the patterns by principal curve estimation. Their proposed methodology can overcome computational and accuracy problems caused by high dimensionality. The PCA-filtering can improve the accuracy of the variation pattern estimation.

Ding, Gupta and Apley [34] improve the standard least-squares estimation (LSE), resulting in nondiagnosable fixture errors in fixture fault diagnosis for multi-station assembly processes. They suggest a reformulation of the original error propagation model into a covariance relation. The LS criterion is then applied directly to the sample covariance matrix to estimate the variance components. The proposed methods achieve higher diagnosability in singular manufacturing systems.

Irad and Gonen [29] present a novel SPC method to monitor nonlinear and finite-state processes that often result from feedback-controlled processes. The methodology requires fewer parameters to be estimated and it can capture both linear as well as nonlinear trends in the data.

By assuming a linear model between the quality measurement and process faults, Jin and Zhou [28] proposed the identification method based on testing of the common eigenspace between the fault signatures and the covariance matrix of the newly collected samples. Their method can be used for quick root cause identification of a manufacturing process. They assume the system noise's variance follows $\sigma^2 I$, however, it may not be reasonable for some systems.

Wang and Huang [25] apply error cancellation modeling to machining process control. They proposed the concept of Equivalent Fixture Error (EFE) embedded into a modeling methodology and developed a sequential root-cause identification procedure and EFE compensation methodology based on the process fault model. Their EFE methodology helped to reveal the structure of the matrix of the fault model.
Li and Shi [13] explain their method to improve the efficiency of learning causal relationships in BN. From observational datasets and using integrated causal modeling approach can improve an existing causal discovery algorithm by integrating manufacturing domain knowledge with the algorithm. With this causal network, the causal relationships among the variables can be identified. The manufacturing domain knowledge plays important role in causal discovery as it can effectively constrain the model search, reduce the computational complexity, increase model accuracy, and help validate, interpret the results. Based on the causal network, the causal relationship among variables can be identified both qualitatively and quantitatively.
3 METHODOLOGY

This thesis presents a new fault diagnosis approach. When a process-shift to an out-of-control state is detected the proposed principal components analysis based root-cause identification algorithm is applied to determine the variables that are the significant causes of this process shift. In order to detect the process shift (fault-detection) we employ the Hotelling $T^2$ statistic. For a $p$ dimensional quality characteristic vector $x$ that follows a multivariate normal distribution with mean $\mu$ and covariance matrix $\Sigma$, the statistic

$$T^2 = \frac{n(n-p)}{p(n+1)(n-1)} (x - \bar{x})' S^{-1} (x - \bar{x})$$

follows an $F$ distribution with $p$ and $n-p$ degrees of freedom when the process is in control. Here, $\bar{x}$ and $S$ are the sample mean vector and the sample covariance matrix estimated from $n$ reference observations of the process. The instant process shifts to an out of control state can be detected when $T^2 > F_{\alpha,p,n-p}$ at $\alpha$ level of significance. Once the faulty state is detected, the method proceeds with diagnosing the root-causes using the PCA methods, as explained in the next section. Figure 3.1 gives an overview of the proposed fault diagnosis method.

The proposed root-cause identification method integrates PCA and contribution plot into the diagnosis procedure. First represent the system $(X_1, \ldots, X_k)$ as a function of dominant principal component variables $(Z_1, \ldots, Z_m)$. Then diagnose faults based on contribution of original variables on PC variables.

![Figure 3.1 PCA approach procedure](image-url)
3.1 PCA based fault detection and diagnosis

Most production or industrial systems are characterized by large number of process variables. For example the stability of a chemical reaction process can be described by jointly monitoring the viscosity, concentration, pH and the molecular weight of the product. For such processes, efficient multivariate process monitoring and diagnosis methods therefore are of crucial practical significance.

As the number of process variables grows, the conventional control chart based methods become less effective in quickly detecting process shifts and methods that employ some form of a dimension reduction are recommended. Principal Components Analysis (PCA) is a popular dimension reduction approach. It consists of projecting the process information from the original variables, which are usually highly correlated and noisy, to a lower-dimensional subspace which consists of the important dimensions that contain relevant information about the process. The objective of PCA is to represent a data set on a large number of interrelated variables with a smaller number of variables while explaining as much of the variation in the data as possible.

Suppose \( x = (x_1, x_2, ..., x_p) \) is a random vector of observations from \( p \) variables. Assume that when the process runs within its normal operating range (when it is in control) \( x \) follows a multivariate normal distribution with mean vector \( \mu \), covariance matrix \( \Sigma \). The mean vector and covariance are estimated from a reference sample of \( n \) observations collected from in control operation of the process using sample mean vector and covariance matrix. The dimension reduction in PCA is accomplished as follows. The variability represented by \( \Sigma \) is reduced to a diagonal matrix \( \Lambda \) by applying a transformation \( A \Sigma A = \Lambda \) where \( A \) is an orthonormal matrix. The diagonal elements \( \lambda_1, \lambda_2, ..., \lambda_p \) of \( \Lambda \) are
the eigenvalues of $\Sigma$ and the column vectors $a_1, a_2, ..., a_p$ of the matrix $A$ are the eigenvectors of $\Sigma$.

PCA transforms the original variables $x = (x_1, x_2, ..., x_p)$ into the new set of variables $y = (y_1, y_2, ..., y_p)$ by applying the coordinate axes rotation 

$$y = Ax.$$ 

Therefore, the $i$th principal component of the original variables is 

$$y_i = a_i'x = a_{1i}x_1 + \cdots + a_{pi}x_p$$

for $i = 1, 2, ..., p$. The variance of the $i$th principal component is $\lambda_i$. The first principal component is the linear combination (with a coefficient vector that has unit length) of the original variables with largest variance. The second principal component is the linear combination with largest variance chosen among the unit-length coefficient vectors that are orthogonal to the coefficient vector, and so on (Richard and Wichern [37]).

If the variations in the original variables occur in a lower dimensional space then by using a few (usually 2 or 3) principal components one can explain most of the variability in the process. In this paper we select the appropriate number of principal components in order to explain 90% of the variability in the data. Thus, the first $k$ principal components are used if the following is satisfied 

$$\lambda_1 + \lambda_2 + \cdots + \lambda_k \geq 0.9(\sigma_1^2 + \cdots + \sigma_p^2)$$

where $\sigma_1^2, \sigma_2^2, ..., \sigma_p^2$ are the diagonal elements of $\Sigma$. The benefit of reduction to fewer principal component variables is that one can increase the sensitivity of the diagnosis or monitoring method to small process upsets or faults by dealing with fewer variables that explains the majority of the variations in the data.
3.2 Contribution plot

The contribution plot is a useful graphical tool for fault diagnosis [49], which can show the contribution of individual variables to the PCA representations. To calculate the contribution corresponding to each original variable, first to estimate the loadings of PCA from calibration data: \( a_1, \ldots, a_p \)

The \( i^{th} \) variable's contribution on \( j^{th} \) principal component is:

\[
C_{ij} = a_{ij} X_j
\]

Where \( a_{ij} \) is the loading value which can be known from the eigen vector of variance-covariance matrix.

The total contribution of \( i^{th} \) variable is:

\[
C_i = \sum_{j=1}^{k} C_{ij}
\]

Take an example calculation with a process with 5 variables, and introduce errors in variables 1, 2, and 3. Figure 3.2 shows the total contribution of each va

Figure 3.2 Contribution Plot
After calculation of each variable’s contribution based on PCA, next step is to diagnose the root causes. Using estimated confidence limits, variable $i$ is a potential root-cause if $C_i$ is outside the confidence limits. We test the significance of the observed contribution score $C_i$.

$$H_0: C_i = 0, \quad H_1: C_i \neq 0$$

The null hypothesis is rejected if the observed contribution falls outside the empirical 100(1-$\alpha$)% confidence interval: $[C_{i, a/2}, C_{i, 1-a/2}]$. Figure 3.3 shows the histogram of simulated contribution data and 2.5%, 97.5% points of $C_1$.

![Figure 3.3. Histogram of Contribution with control limits](image)

Figure 3.4 shows the contribution plot with confidence limits to determine root causes:
The confidence limits for contribution plot can be either positive or negative. And the limit is different for each variable. If $C_i > UCL_i$ or $C_i < LCL_i$ => $X_i$ is a root-cause. So, in this example, variable 1, 2, and 3 are root causes even the contribution of variable 3 is small.
4 RESULTS AND DISCUSSION

4.1 Performance measures to evaluate proposed method: type I, type II and overall error rates

We will monitor all 5 quality and process variables. The process can go out of control because of a deviation in one or more of these variables. The objective of diagnosis is to identify the variables (root-causes) that experience the shifts. To evaluate the performance of different methods, we consider type I, type II, and overall error rates.

Type I error rate is the false alarm rate. It means the possibility that process is in control but our monitoring system gives us an out-of-control alert, or variable $i$ is not root cause but our diagnosis system shows us variable $i$ is root cause. Type II error rate is the misdetection rate. It means the possibility that our monitoring system can not detect out-of-control signal, or our diagnosis system can not determine the true root causes.

Take an example of the 5-variable process that only variable 1 has mean shift. This means $X_1$ is faulty variable. Figure 4.1 shows the diagnosis results of 4 simulations:

![Figure 4.1 Calculation of Type I and Type II error rates](image)

The rows are corresponding to each simulation, and the columns are corresponding to each variable. We define the ones or zeros $d_i$. For each simulation, if $X_i$ is root cause, let
\( d_i = 1 \), otherwise, \( d_i = 0 \). Because the true root cause in this example is variable 1, the type II error rate can be estimated directly from how many zeros in the first column. Type I error rate can be estimated from how many ones in the remaining columns. In this example, type II error = \( 2/4 = 0.5 \), and type I error = \( 4/16 = 0.25 \).

The overall error means the possibility of failing to correctly diagnose all faulty variables simultaneously. It is different from type I or type II because it focused on only faulty variables.

The same as type I and type II, to take an example of the 5-variable process that only variable 1 has mean shift. Figure 4.2 shows how to diagnosis overall error rate:

<table>
<thead>
<tr>
<th></th>
<th>( X_1 )</th>
<th>( X_2 )</th>
<th>( X_3 )</th>
<th>( X_4 )</th>
<th>( X_5 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Correct diagnosis</td>
<td>1</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Correct diagnosis</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Correct diagnosis</td>
<td>1</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td>Wrong diagnosis</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>1</td>
</tr>
<tr>
<td>Wrong diagnosis</td>
<td>0</td>
<td>1</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
</tbody>
</table>

Figure 4.2 Calculation of overall error rate

To calculate overall error rate, we consider the diagnosis results of faulty variables only, which means we ignore the diagnosis results of other variables. For example, we consider row 1 to row 3 as correct diagnosis since all of the \( d_{i1} \) are 1. For row 4 and 5, even \( d_{i2} \) to \( d_{i5} \) maybe equal to 0, we still consider them as wrong diagnosis. So, in this case, the overall error = \( 2/5 = 0.4 \).
4.2 Simulation examples

The operations of the two systems described in the previous section were simulated by Monte Carlo simulation. In each simulation run we introduced random faults at various locations in the system. Simulation length in each realization was 100 and the fault was introduced at time step 50. In order to evaluate the long-run performance of the proposed fault diagnosis approach the simulation was replicated 1000 times for each scenario in the following examples.

4.2.1 Small System (Hot Forming process)

Take a hot forming process as example [26]: There is one quality variable \((X_5)\): final dimension of workpiece; and four process variables: temperature \((X_1)\), material flow stress \((X_2)\), tension in workpiece \((X_3)\), blank holding force \((X_4)\).

![Diagram of Hot Forming process](image)

Figure 4.3 Small System (Hot Forming process)

In order to compare the performance of the proposed PCA approach and causation based approach (CBT), we conduct a simulation study based on 31 different fault scenarios: Single-variable fault (1-5); Two-variable faults (6-15); Three-variable faults (16-25); Four-variable faults (26-30); Five-variable faults (31).
4.2.2 Large System (Continuous Stirred Tank Reactor system)

To illustrate the diagnosability of PCA approach and CBT approach, a large scale system is constructed as follow:

The same root cause identification procedure is applied in this large scale system, but the total number of scenarios is:

\[ n = \sum_{k=1}^{14} \binom{14}{k} = 16383 \]
It is difficult to model all the scenarios, so we consider only $X_1 \sim X_5$ has mean shift (31 scenarios) to make it is comparable to small system.

### 4.3 Simulation results

Figure 4.5 below shows one realization of $X_1$ and $X_2$ under scenario 1 (only $X_1$ is introduced a mean shift) and the corresponding contributions of $C_1$ and $C_2$ for small system.

![Figure 4.5. One realization of scenario 1 of small system](image)

We can find in this figure the $X_2$ also appears mean shift because of it is the child of $X_1$. But the contribution of $X_2$ still falls inside the control limits. Based on this property, we can use PCA approach to identify the root-causes.

Figure 4.6 and 4.7 shows the type I and type II error rates respectively in small system:
Figure 4.6 Type I error rates in small system

Figure 4.7 Type II error rates in small system
We can find that PCA approach performs better in type II errors, but worse in type I errors than CBT approach. CBT has very low type I error rate but not as good type II error rate as PCA approach.

Figure 4.8 shows what happens when we use different significance level:

![Figure 4.8 Choice of significance level to control the errors](image)

In figure 4.8, the dash line shows the error rates conducted using $\alpha=0.01$ instead of $\alpha=0.05$. We find decreasing $\alpha$ can decrease type I, but increase type II error. Because the proposed approach has better type II but worse type I, it has important meaning to control both the type I and type II in an acceptable range.
Figure 4.9 and 4.10 shows the type I and type II error rates respectively in large system:

![Type I Error Rates](image1)

**Figure 4.9** Type I error rates in large system

![Type II Error Rates](image2)

**Figure 4.10** Type II error rates in large system

41
The same we can find that PCA approach performs better in type II errors, but worse in type I errors than CBT approach. But the average of type II increases much from small system to large system because the large scale system makes diagnosis more difficult.

The overall error rates are also estimated with combined number of shifts. It means we combined the scenarios which have the same number of shifts together. For example, scenario 1 to 5 all has 1 shift, so we average all of their error rates. After doing the same thing on remaining scenarios, we get the following plot with standard errors:

![Figure 4.11 Overall error rates vs number of shifts](image)

The red line is error rate of proposed PCA approach, and blue line is CBT approach. The dash lines are corresponding large systems. We can find the proposed approach obviously performs better than CBT approach. The red dash line is lower than solid blue line, which means PCA approach in large system is even better than CBT approach in small system.

Comparing the proposed PCA approach to CBT approach, the advantage and disadvantage are apparent. PCA approach performs better in type II error rates, while CBT
approach performs better in type I error rates. However, in real manufacturing process, the type II errors are more important to quality of product than type I errors. We can find in figure 3.1, if we could not find fault at the detection stage, the faulty product will be consider as with good quality and finally reach the market, customers. The same thing happens when we could not determine the true faulty variables. This kind of errors happen when we can not find or locate fault, is type II errors, not type I errors. The faulty product goes to market and customer due to type II errors, which is not any industrial company wants to see. At the mean time, the product with good quality will be examined once again due to type I errors. It is not as serious problem as selling bad product for the industrial company. So, our proposed PCA approach is very useful in the manufacturing processes.

Another important result coming from comparison is overall error rates of PCA approach are not affected significantly from the location of the fault. Take scenario 1 to 5 (shift introduced on $X_1, \ldots, X_5$ respectively) in small system as example:

Table 4.1 Overall error rates of scenario 1 to 5

<table>
<thead>
<tr>
<th>Scenario</th>
<th>$e_{\text{CBT}}$</th>
<th>$e_{\text{PCA}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.12</td>
<td>0.01</td>
</tr>
<tr>
<td>2</td>
<td>0.02</td>
<td>0.01</td>
</tr>
<tr>
<td>3</td>
<td>0.03</td>
<td>0.01</td>
</tr>
<tr>
<td>4</td>
<td>0.09</td>
<td>0.03</td>
</tr>
<tr>
<td>5</td>
<td>0.01</td>
<td>0.01</td>
</tr>
</tbody>
</table>

We can find in CBT approach, the error rates of scenario 1 and 4 are relatively much higher than scenario 2 and 3. The error rates of scenario 2 and 3 are relatively higher than scenario 5. This is because $X_1$ and $X_4$ are at higher level in the system structure than $X_2$ and $X_3$, and $X_2$ and $X_3$ are parents of $X_5$. The CBT approach diagnosis is based on the structure,
while PCA approach does not need the hierarchy: the error rates of PCA approach are distributed normally.

Compare the diagnosability in small system to large system: In small system, type I error increased from 0.0275 (CBT) to 0.0962 (PCA), type II error decreased from 0.1511 (CBT) to 0.065 (PCA). In large system, type I error increased from 0.0223 (CBT) to 0.0834 (PCA), type II error decreased from 0.2884 (CBT) to 0.1219 (PCA). Since there is a trade-off between type I and type II error rates. When we try to decrease type II error, type I error will increase. The proposed approach can significantly decrease type II error rates without scarifying too much type I error rates. In both small system and large system, the type I error rates can be controlled under 0.1, which is acceptable level for manufacturing processes. Even in large system, the PCA approach has very low type II error rates (0.12), which illustrate that the proposed approach performs excellent in large system.

4.4 Extended PCA fault diagnosis method

In the simulation example we discussed before, we always look at the individual observation point when we detect the fault. We do not consider the lag between when the fault occurs and when we detect it, and the information between these two points. So this extended PCA diagnosis method is based on identifying the onset of a change in the mean.

Nedumaran, Pignatiello and Calvin [18] worked on identifying the time of step change using maximum likelihood estimator method. They first detect when the out-of-control signal occurs, say $\tau_2$. Then they estimate the time of change $\tau_1$ by maximizing the statistic $M_t$: 

$$\hat{\tau}_1 = \arg\max_t M_t, \quad t = 0, 1, \ldots, \tau_2$$

Where

$$M_t = \left(\bar{x}_{t,\tau_2} - \mu_0\right)^\prime\Sigma_0^{-1}\left(\bar{x}_{t,\tau_2} - \mu_0\right)$$
And where

\[ \bar{X}_{t, \tau_2} = \frac{1}{\tau_2 - t} \sum_{i=t+1}^{\tau_2} X_i \]

Figure 4.12 shows an example of identifying the time of step change: we detect the fault at time 53, but the onset of the change is at time 51.

![Figure 4.12 Example of identifying \( \tau_1 \) and \( \tau_2 \)](image)

In this method after we successfully locate the time of change, we will calculate the contribution using the average of all the observations between \( \tau_1 \) and \( \tau_2 \):

\[ C_{ij} = a_{ij} \bar{X}_j \]

And the total is:

\[ \bar{C}_i = \sum_{j=1}^{k} \bar{C}_{ij} \]

Instead of using single observation, we compare the contribution of average values from \( \tau_1 \) to \( \tau_2 \), to the control limits.

Figure 4.13 shows the results using the same procedure:
This figure shows the extended method: PCA mean method seems that it improves type I and type II slightly. To illustrate it, we take the difference between the two methods, and calculate the percentage of how many scenarios are larger than 0, which means the extended method is better.
Figure 4.14 shows the confidence intervals of reduction in type I and type II error rates by using mean method. If the intervals are greater than 0, it means we significantly improve the error rate; if the intervals contains 0, it means the improvement is not significant. Based on this figure, there is about 75% of the scenarios are improved in type I error. In type II error, it seems that only 25% of the scenarios are improved. The extended method based on averages improves type I error (incorrectly diagnosing non-causes), but does not improve type II error rates (failing to diagnose causes).
5 CONCLUSIONS

The performance of PCA based root causes identification approach is assessed in this thesis. Both small system and large system are explored to evaluate the type I, type II and overall error rate of proposed and existing methods. The proposed PCA approach is based on Principal Components Analysis and contribution plot.

The PCA is a dimension reduction method which can project data to lower dimensions to make the interpretation of high dimensional processes easier. It can improve the detection and diagnosing effectiveness by representing the data with only the dominant principal component variables and ignoring the noise effect in the original data. Contribution plots are very useful method to enhance the interpretation of the multivariate results, exploration of data and correct identification of root causes.

The proposed PCA based root causes identification approach is very useful compared to the existing method. By applying PCA, the proposed method can improve the diagnosability of existing methods with a large number of variables which means its diagnosis of faults has a low error rate compared to the causation-based (CBT) approach. The advantage of proposed PCA method is that it is easier to implement than existing approaches. It does not require learning step of BN structure. The BN structure learning algorithm is complicated procedure which contains conditional independency test, parameter learning, and directing of the arcs. All of these steps will greatly lower the efficiency of root cause identification. But the PCA approach performs better in the algorithm. It does not require complex statistical testing based on the data’s distribution or structure learning. PCA is also a dimension reduction method which can extract the most useful information by ignoring the noise effect in the original data. PCA can be applied to various processes because it does not have iid requirement, and can model dynamic processes, in which the parameter, variance covariance keeps changing during the process. The PCA approach is more efficient because it does not need complicated statistical decomposition.
The performance of PCA based root causes identification method shows quite good results in both small system and large system. The type II error rates can be significantly reduced while keeping the type I error rates in an acceptable range. Estimating the overall error rates indices also tell us the PCA approach performs much better than existing approaches both in small and large system.

Although the results are based on simulations, the PCA approach is recommended to be used for modeling online experiments because the approach works quite well for dynamic processes in high dimensions. Other identification techniques involving a regression approach will be explored to further improve the diagnosability. Also, the author will explore how to reduce the type I error in extended PCA approach by incorporating process knowledge.
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BIOGRAPHICAL SKETCH

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