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SCIENCE DIRECT®
Computers and Chemical Engineering 27 (2003) 327–346
Computers & Chemical Engineering
www.elsevier.com/locate/compchemeng

A review of process fault detection and diagnosis Part III: Process history based methods

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Received 12 February 2001; accepted 22 April 2002

Abstract

In this final part, we discuss fault diagnosis methods that are based on historic process knowledge. We also compare and evaluate the various methodologies reviewed in this series in terms of the set of desirable characteristics we proposed in Part I. This comparative study reveals the relative strengths and weaknesses of the different approaches. One realizes that no single method has all the desirable features one would like a diagnostic system to possess. It is our view that some of these methods can complement one another resulting in better diagnostic systems. Integrating these complementary features is one way to develop hybrid systems that could overcome the limitations of individual solution strategies. The important role of fault diagnosis in the broader context of process operations is also outlined. We also discuss the technical challenges in research and development that need to be addressed for the successful design and implementation of practical intelligent supervisory control systems for the process industries.

Keywords: Supervisory control; Diagnosis; Hybrid system

1. Introduction

In contrast to the model-based approaches where a priori knowledge (either quantitative or qualitative) about the process is needed, in process history based methods, only the availability of large amount of historical process data is needed. There are different ways in which this data can be transformed and presented as a priori knowledge to a diagnostic system. This is known as feature extraction. This extraction process can be either qualitative or quantitative in nature. Two of the major methods that extract qualitative history information are the expert systems and trend modelling methods. Methods that extract quantitative information can be broadly classified as non-statistical or statistical methods. Neural networks are an important class of non-statistical classifiers. Principal component analysis (PCA)/partial least squares (PLS) and statistical pattern classifiers form a major component of statistical feature extraction methods. The different ways in which knowledge can be extracted from process history are schematically presented in Fig. 1. We review these approaches in this part of the review paper.

We also compare and evaluate the various methodologies reviewed in this three part series in terms of the set of desirable characteristics we proposed in Part I. This comparative study identifies the relative strengths and weaknesses of the different approaches. It also reveals that no single method has all the desirable features we stipulated for a diagnostic system. It is our view that some of these methods can complement one another resulting in better diagnostic systems. Integrating these complementary features is one way to develop hybrid methods that could overcome the limitations of indivi-

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0098-1354/02/$ - see front matter © 2002 Published by Elsevier Science Ltd.
PII: S0098-1354(02)00162-X

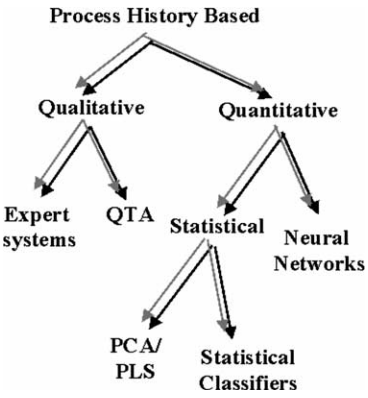

Fig. 1. Classification of process history-based methods

dual solution strategies. We review some recent trends in this direction. The important role of fault diagnosis in the broader context of process operations is also outlined. Finally, we also discuss the technical challenges in research and development that need to be addressed for the successful design and implementation of practical intelligent supervisory control systems for the process industries.

2. Qualitative feature extraction

As mentioned earlier two of the important methods that employ qualitative feature extraction are the expert systems and trend modelling approaches. In this section we review these two approaches.

2.1. Expert systems

Rule-based feature extraction has been widely used in expert systems for many applications. An expert system is generally a very specialized system that solves problems in a narrow domain of expertise. The main components in an expert system development include: knowledge acquisition, choice of knowledge representation, the coding of knowledge in a knowledge base, the development of inference procedures for diagnostic reasoning and the development of input–output interfaces. The main advantages in the development of expert systems for diagnostic problem-solving are: ease of development, transparent reasoning, the ability to reason under uncertainty and the ability to provide explanations for the solutions provided.

There are a number of papers that discuss expert system applications for fault diagnosis of specific systems. Initial attempts at the application of expert systems for fault diagnosis can be found in Henley (1984), Chester, Lamb, and Dhurjati (1984) and Niida (1985). Rich, Venkatasubramanian, Nasrallah, and Matteo (1989) discuss a diagnostic expert system for a whipped topping process. The objectives of this expert system were twofold. First, the system classifies the reasons for the observed problem as an operator error, equipment failure or system disturbance. Second, the expert system offers prescriptive remedies to restore the process to normal operation.

Structuring the knowledge-base through hierarchical classification can be found in Ramesh, Shum, and Davis (1988) and an application of an expert system for catcracker diagnosis can be found in Ramesh, Davis, and Schwenzer (1989). Several large systems have been built using such an approach and constitutes an improvement over the unstructured rule-based systems. Ideas on knowledge-based diagnostic systems based on the task framework can be found in Ramesh, Davis, and Schwenzer (1992). A rule-based expert system for fault diagnosis in a cracker unit is described in Venkatasubramanian (1989) and a specialized shell for diagnostic expert systems can be found in Venkatasubramanian (1988). A discussion on different forms of reasoning in expert systems can be found in Ungar and Venkatasubramanian (1990). More work on expert systems in fault diagnosis can be found in Quantrille and Liu (1991). A framework to represent the uncertain elements of the diagnostic problem using belief networks, and the use of distributed network (parallel) computations to determine the most probable diagnostic hypotheses can be found in RojasGuzman and Kramer (1993).

There are a number of other researchers who have worked on application of expert systems for diagnostic problems. Basila, Stefanek, and Cinar (1990) have developed a supervisory expert system that uses object-based knowledge representation to represent heuristic and model-based knowledge. A prototype has been applied to improve the behavior of a packed-bed tubular CO oxidation reactor under auto-thermal operation. Zhang and Roberts (1991) have presented a methodology for formulating diagnostic rules from the knowledge of system structures and component functions. This approach has been tested on a pilot scale mixing process and a simulated CSTR system. Chen and Modarres (1992) have developed an expert system, called FAX, to address the determination of the root cause of process malfunctions and suggestions for corrective action(s) to avert abnormal situations. Becraft and Lee (1993) have proposed an integrated framework comprising of a neural network and an expert system. A neural network is used as a first-level filter to diagnose the most commonly encountered faults in chemical process plants. Once the faults are localized within a particular process by the neural network, a deep knowledge expert system analyzes the result, and either confirms the diagnosis or else offers an alternative solution. Tarifa and Scenna (1997) have proposed a hybrid system that uses signed directed graphs (SDG) and fuzzy logic. The SDG model of the process is used to perform qualitative simulation to predict possible process behaviors for

various faults. Those predictions are used to generate *if–then* rules that are evaluated by an expert system using information about the actual process state and fuzzy logic. Zhao, Chen, and Shen (1997) have presented a wavelet-sigmoid basis neural network and expert system based integrated framework for fault diagnosis of a hydrocracking process. Wo, Gui, Shen, and Wang (2000) have presented an expert fault diagnostic system that uses rules with certainty factors. Leung and Romagnoli (2000) have presented a probabilistic model-based expert system for fault diagnosis. Possible cause and effect graph, an enhanced SDG has been used for qualitative modelling. The diagnostic system has been applied to a pilot scale distillation column. Tarifa and Scenna (1998) discuss an expert system for fault diagnosis of a multistage flash desalination process. An expert system approach for fault diagnosis in batch processes is discussed in Scenna (2000).

There are a number of other papers that discuss specific applications of expert systems for fault diagnosis. However, in all the applications, the limitations of an expert system approach is obvious. Knowledge-based systems developed from expert rules are very system-specific, their representation power is quite limited, and they are difficult to update (Rich & Venkatasubramanian, 1987). The advantage though is the ease of development and transparent reasoning.

2.2. Qualitative trend analysis (QTA)

A second approach to qualitative feature extraction is the abstraction of trend information. Trend analysis and prediction are important components of process monitoring and supervisory control. Trend modelling can be used to explain the various important events happening in the process, do malfunction diagnosis and predict future states. From a procedural perspective, in order to obtain a signal trend not too susceptible to momentary variations due to noise, some kind of filtering needs to be employed. For example, time series representations assume, a priori, certain behavior as they are identified using a known process behavior. Alternatively, one may simply use a filter (such as an auto-regressive filter) with a priori chosen filter coefficients (specifying the required degree of smoothing). Both types of filters suffer from the fact that they cannot distinguish well between a transient and true instability (Gertler, 1989). The essential qualitative characters might be distorted by these filters. Avoiding this problem requires that the trend be viewed from different time scales or different levels of abstraction. Qualitative abstraction allows for a compact representation of the trend by representing only the significant events. For tasks such as diagnosis, qualitative trend representation often provides valuable information that facilitates reasoning about the process behavior. In a majority of cases, process malfunctions leave a distinct trend in the sensors monitored. These distinct trends can be suitably utilized in identifying the underlying abnormality in the process. Thus, a suitable classification and analysis of process trends can detect the fault earlier and lead to quick control. Also, qualitative trend representation can pave way for efficient data compression.

Cheung and Stephanopoulos (1990) have built a formal framework for the representation of process trends. They introduce triangulation to represent trends. Triangulation is a method where each segment of a trend is represented by its initial slope, its final slope (at each point, or critical point of the trend) and a line segment connecting the two critical points. A series of triangles constitute a process trend. Through this method, the actual trend always lies within the bounding triangle, which illustrates the maximum error in the representation of the trend. Janusz and Venkatasubramanian (1991) identify a comprehensive set of primitives using which any trend can be represented. They use a finite difference method to calculate the first and second derivative of the process trend changes and based on these values, the primitives are identified. This qualitative formalism readily lends itself to hierarchic representations as well. Rengaswamy and Venkatasubramanian (1995) have shown how primitives can be extracted from raw noisy sensor data by treating the problem of primitive identification as a classification problem using neural networks. Each data set in a given time window would be classified to one of the primitives. This work is oriented towards a syntactic pattern recognition approach. Syntactic approaches are suitable for hierarchical representation of the trend information and are suitable for developing error correcting code, which eliminates the effects of high noise and outliers. At a lower level, a pattern classification approach like neural networks is used to identify the fundamental features of the trends observed. At a higher level, the syntactic information is abstracted and represented in a hierarchical fashion with the error correcting code smoothing out the errors made at the lower level. Vedam and Venkatasubramanian (1997) proposed a wavelet theory based adaptive trend analysis framework and later proposed a dyadic B-Splines based trend analysis algorithm (Vedam, Venkatasubramanian, & Bhalodia, 1998). Recently, Rengaswamy, Hagglund, and Venkatasubramanian (2001) have discussed the utility of trend modelling in control loop performance assessment.

Konstantinov and Yoshida (1992) proposed a qualitative analysis procedure with the help of an expandable shape library that stores shapes like decreasing concavely, decreasing convexly and so on. The first step in their method is the approximation of state variables by a proper analytic function. The analytic noise-free model is then converted into a qualitative form and the

qualitative shapes are concatenated to describe the overall trend. Whiteley and Davis (1992) discuss qualitative interpretations from sensor data as an adaptive pattern recognition problem.

Multilevel abstraction of important events in a process trend is possible through scale-space filtering through the use of a bank of filters each sensitive to certain localized region in the time–frequency domain (Marr & Hildreth, 1980). There are two underlying ideas in the use of multilevel abstraction of process trends: (a) changes in trends occur at different scales and their optimal detection requires the use of filters or operators of different sizes, and (b) a sudden change will give rise to a peak or trough in the first derivative, or equivalently, to a zero-crossing in the second derivative (a zero-crossing is a place where the value of a function changes sign, say from positive to negative). The interest in zero-crossings stems from the fact that they are very rich in information on the changes in a trend. This leads one to search for filters with two salient characteristics. First, it should be a differential operator, taking first, second or higher-order spatial derivatives of the function. Second, it should be capable of being tuned to any desirable scale, so that filters with small scale capture gradual changes in the trend. An example of such a filter that has been extensively used in image processing is a Gaussian filter (Marr & Hildreth, 1980). The main problem with a Gaussian filter is that, the representation is highly redundant and the computational time for the filters might become prohibitive. Bakshi and Stephanopoulos (1992) propose multi-scale filtering using wavelet transforms to handle this problem. In their procedure, the process trends are decomposed at different scales using wavelet transforms. At different scales, the temporal characteristics are captured using triangular episodes to facilitate pattern matching for fault diagnosis and supervisory control.

3. Quantitative feature extraction

In this section we will discuss the methods that are based on quantitative feature extraction. The quantitative approaches essentially formulate the diagnostic problem-solving as a pattern recognition problem. The goal of pattern recognition is the classification of data points to, in general, pre-determined classes. Statistical methods use knowledge of a priori class distributions to perform classification. An example is a Bayes classifier which uses the density functions of the respective classes. Approaches like PCA, on the other hand, extract information about major trends in the data using a small number of relevant factors. Neural networks assume a functional form for the decision rule thus parameterizing the classifier. We review these methods in this section.

3.1. Statistical feature extraction from process data

In real process operations, one is faced with the problem of dealing with systems subject to random disturbances. In contrast to deterministic systems, the future state of stochastic systems is not completely determined by the past and present states and future control actions. The measurements are considered to be statistical time series—a single realization of an underlying stochastic process. Since the systems are under random influences, it is reasonable or sometimes necessary to formulate the systems in a probabilistic setting. When the process is under control, the observations have probability distributions corresponding to the normal mode of operation. The underlying distributions change when the process is out of control. In general, probability distributions are characterized by their parameters when a parametric approach is used. For instance, if the underlying distribution of a monitored variable is normal, then the parameters of interest are the values of its mean and the standard deviation. Under faulty conditions, either the mean or the standard deviation may deviate from their nominal values. A composite change can occur as well. Accordingly, fault diagnosis can be stated as the problem of detecting changes in the parameters of a static or dynamic stochastic system. Basseville and Nikiforov (1993) presented the design of on-line change detection algorithms and an analysis of their performance under a unified framework. Both the Bayesian and the non-Bayesian approaches are discussed therein.

In on-line statistical approach, samples are taken sequentially and decisions are made based on the observations up to the current time. If the decision is made from the values of observations directly, then when the observations $\mathbf{x}(t) = [x_1(t),\ x_2(t),\ldots,\ x_n(t)]' \in R_n$ where R_n is the so-called stopping region in statistics, it is concluded that there is a change in the process. More often a statistic $\mathbf{g}(t)$, a function of observation $\mathbf{x}(t)$, is designed and the decision is made according to the comparison of $\mathbf{g}(t)$ with some threshold value $\mathbf{c}$. This idea can be translated into a 'stopping rule' problem with a standard form

$$\tau = \inf\{t \geq 1;\ \mathbf{g}(t) \geq \mathbf{c}\}.$$

τ is the greatest lower bound, i.e., the first time when $\mathbf{g}(t)$ is greater than $\mathbf{c}$. In on-line detection, it is desirable to detect the change as soon as it occurs, i.e., to detect it at the first time when $\mathbf{x}(t) \in R_n$ or $\mathbf{g}(t) > \mathbf{c}$. Thus, the fault (change) detection amounts to the design of the stopping rules or proper choices of statistic $\mathbf{g}(t)$ and threshold $\mathbf{c}$. Obviously a good detector must be sensitive to change. However, the sensitivity to the process noise usually increases along with the sensitivity to real change. In other words, as the failure and delay of the detection decrease, the number of false alarm tends to

increase, which is certainly undesirable. A good design is usually defined as one which will minimize the failure and delay at a fixed false alarm rate.

Quality control represented one of the earliest attempts of using statistics in on-line monitoring and change detection. Shewhart control charts were introduced in 1931 (Shewhart, 1931) followed by others such as the cumulative sums chart in 1954 (Page, 1954). Control charts approach is based on the assumption that a process subject to its natural variability (common cause variation) will remain in a state of statistical control under which certain process and/or product variables remain close to their desired values. Therefore, by monitoring the performance of a process over time, abnormal events can be detected as soon as they occur. If the causes for such events can be diagnosed and the problem can be corrected, the process is driven back to its normal operation. The growing demand for product quality and process reliability has led to an extensive use of statistical process control (SPC) charts. Although the basic concepts behind such SPC methods are still valid, the charting methods used to implement them cannot accommodate the progress in data acquisition technology. In addition, in the event that the parameters monitored are not independent, the use of univariate control chart may be misleading and may cause confusion due to the fact that the univariate method cannot handle correlation.

Multivariate statistical techniques are powerful tools capable of compressing data and reducing its dimensionality so that essential information is retained and easier to analyze than the original huge data set; and they are also able to handle noise and correlation to extract true information effectively. PCA method, initially proposed by Pearson (1901) and later developed by Hotelling (1947), is a standard multivariate technique and has been included in many textbooks (Anderson, 1984; Jackson, 1991) as well as research papers (Wold, 1978; Wold, Esbensen, & Geladi, 1987). The main function of multivariate statistical techniques is to transform a number of related process variables to a smaller set of uncorrelated variables.

Originating from the pioneering work of Wold (1982) between the mid 1960s and early 1980s PLS method was further developed by Wold and coworkers (Wold, Albano, Dunn III, Edland, Esbensen, Geladi, Hellberg, Johansson, Lindberg, & Sjostrom (1984a), Wold, Esbensen, & Geladi (1987) and Wold, Ruhe, Wold, & Dunn (1984b)) in the mid and late 1980s. Similar to PCA, conceptually, PLS is useful in reducing the dimensions of both process variables and product quality variables to be analyzed.

3.1.1. Principal component analysis/partial least squares

Theoretically, PCA is based on an orthogonal decomposition of the covariance matrix of the process variables along directions that explain the maximum variation of the data. The main purpose of using PCA is to find factors that have a much lower dimension than the original data set which can properly describe the major trends in the original data set.

Let p denote the number of measured process variables; $\mathbf{X}$ be an $n \times p$ matrix representing the mean centered and scaled measurement whose covariance matrix is Σ. The rows in $\mathbf{X}$, $\mathbf{x}_1$, $\mathbf{x}_2$,..., $\mathbf{x}_n$, are p dimensional vectors corresponding to samples; whereas the columns are n dimensional vectors corresponding to variables. From matrix algebra, Σ may be reduced to a diagonal matrix $\mathbf{L}$ by a particular orthonormal $p \times p$ matrix $\mathbf{U}$, i.e., $\Sigma = \mathbf{ULU}'$. The columns of $\mathbf{U}$, $\mathbf{u}_1$, $\mathbf{u}_2$,..., $\mathbf{u}_p$ are known as the *principal component loading vectors*. The diagonal elements of $\mathbf{L}$, λ_1, λ_2,..., λ_p are ordered eigenvalues of Σ. They define the amount of variance explained by each corresponding eigenvector. The principal component transformation is given by

$$\mathbf{T} = \mathbf{XU} \quad \text{or} \quad \theta_i = \mathbf{Xu}_i \tag{1}$$

Equivalently, $\mathbf{X}$ is decomposed by PCA as

$$\mathbf{X} = \mathbf{TU}' = \sum_{i=1}^{p} \theta_i \mathbf{u}'_i \tag{2}$$

The $n \times p$ matrix $\mathbf{T} = (\theta_1, \theta_2, \ldots, \theta_p)$ contains the so-called *principal component scores* that are defined as the observed values of the principal components for all n observations. Given the fact that covariance of $\mathbf{T}$ is a diagonal matrix, θ_i vectors are uncorrelated. In addition, the θ_i, $\mathbf{u}_i$ pairs are arranged in descending order according to their associated λ_i. Furthermore, one rarely needs to compute all the p eigenvectors in practice, since most of the variation in the data can be captured by the first few PC's. If a lower number $a < p$ is used, the decomposition becomes

$$\mathbf{X} = \theta_1 \mathbf{u}'_1 + \theta_2 \mathbf{u}'_2 + \cdots + \theta_a \mathbf{u}'_a + \mathbf{E} = \sum_{i=1}^{a} \theta_i \mathbf{u}'_i + \mathbf{E}, \tag{3}$$

where $\mathbf{E}$ is the residual term. It has been found that the first two or three PC's are often sufficient to explain the variability. Hence the dimensionality is greatly reduced. By providing linear combinations with large variances, PCA is useful in finding factors that describe major trends and is capable of reducing the number of variables.

When using PCA in process monitoring and quality control, several steps are needed. An 'in-control' model has to be established. From basic statistics, for a $p \times 1$ normally distributed random vector $\mathbf{z}$ having mean τ and covariance matrix Σ, the statistic

$$\chi^2 = (\mathbf{z} - \tau)' \, \Sigma^{-1} (\mathbf{z} - \tau)$$

has a central χ^2 distribution with p degrees of freedom. χ^2 control chart can then be established with a lower

control limit 0 and an upper control limit χ^2_α where α is a properly chosen significance level.

For the situation where Σ is unknown and must be established, the Hotelling's T^2-statistic (Hotelling, 1947) can be used to replace χ^2 distribution. With an 'in-control' model established based on historical data during normal operation, process monitoring is achieved by comparing the factors against this nominal model. By projecting new observations onto the plane defined by the PCA loading vectors, the score and the residuals can be obtained, the multivariate control charts based on T^2 can in turn be plotted, and the decision is made based on the first a principal components.

PCA is a procedure used for a single data matrix, e.g., the matrix of the process variable **X**. Oftentimes we also have an additional group of data, e.g., product quality variables **Y**. It is desirable to include all the data available in the monitoring procedure and to use the process variables **X** to predict and to detect changes in the product quality variables **Y**. One way of doing this is to use PLS method. It models the relationship between two blocks of data while compressing them simultaneously. It is used to extract latent variables that not only explain the variation in the process data **X** but also that variation in **X** most predictive of the quality data **Y**. The first PLS latent variable is the linear combination of the process variables that maximizes the covariance between them and the quality variable.

3.1.2. Applications of PCA and PLS

SPC has evolved from charting methods for univariate systems or sets of independent variables to multivariate statistical projection methods. Other approaches such as incorporating multivariate SPC with neural networks have also been proposed and studied (Hoskins, Kaliyur, & Himmelblau, 1991; Nomikos & MacGregor, 1994). The successful applications of multivariate statistical methods such as PCA and PLS have been extensively reported in the literature. Overviews of using PCA and PLS in process analysis and control, fault detection and diagnosis were given by MacGregor, Marlin, Kresta, and Skagerberg (1991) and MacGregor, Jacckle, Kiparissides, and Koutondi (1994) and MacGregor and Kourti (1995).

In an earlier work, Kresta, MacGregor, and Marlin (1991) laid out the basic methodology of using multivariate SPC procedure to handle large numbers of process and quality variables for continuous process. Later on, Nomikos and MacGregor (1994) extended the use of multivariate projection methods to batch processes by using multiway PCA. To deal with nonlinearity, Qin and McAvoy (1992) proposed a neural net PLS approach that incorporated feedforward networks into the PLS modelling. In order to handle nonlinearity in batch processes, Dong and McAvoy (1996) utilized a nonlinear PCA method. To facilitate the diagnosis procedure in very large processes, new hierarchical multivariate monitoring methods based on multiblock PLS algorithm were presented by MacGregor, Jacckle, Kipparissides, & Koutondi (1994). Raich and Cinar (1996) proposed an integral statistical methodology combining PCA and discrimination analysis techniques. Based on angle discriminants, a novel disturbance diagnosis approach (Raich & Cinar, 1997) was later introduced that provides better results for cases in which distance based discrimination is not accurate enough.

Chemometrics is a data analysis technique which has been successfully applied in spectroscopy to reduce large quantity of data into meaningful information. Chemometric techniques have been applied to chemical engineering processes (Kaspar & Ray, 1992; Piovoso, Kosanovich, & Pearson, 1992; Piovoso, Kosanovich, & Yuk, 1992) in recent years. These approaches rely on the formation of a statistical model obtained from historical data. Special events can be detected when the process data deviate significantly from the nominal operation model. Piovoso, Kasanovich, & Yuk (1992) considered the use of chemometrics as a multivariate analyzer to provide a composite measurement of the state of a chemical process operation. Their technique uses PLS to establish a correlation between the dominant effect in the process and its relationship to other process sensors; then apply PCA to build a model of the process behavior unaccounted for by that dominant effect. Dunia, Qin, Edgar, and McAvoy (1996) used PCA for sensor fault detection and identification via reconstruction. In their approach, for validation, it is assumed that one sensor has failed and the remaining sensors are used for reconstruction using the PCA model. This procedure is followed sequentially until all the sensors are validated.

A major limitation of PCA-based monitoring is that the PCA model is time invariant, while most of the real processes are time-varying. Hence the PCA model should also be recursively updated. A comprehensive scheme for recursive PCA update should include: mean, covariance, principal components including number of components to be retained, and the confidence limits for T^2 and Q (squared prediction error). Algorithms utilizing rank-one modification and Lauczos tridiagonalization have been presented for recursive PCA by Li, Yue, Valle-Cervantes, and Qin (2000). The recursive PCA approach is demonstrated on adaptive monitoring of a rapid thermal annealing process. A similar algorithm for recursive PLS for adaptive modelling has been presented by Qin (1998). It has been shown that the algorithm is quite efficient as compared to the traditional PLS both in terms of memory requirements and computational speed. Two approaches, viz. moving window-based adaptation and forgetting factor-based adaptation

have been presented and applied to adaptive modelling of a catalytic reformer.

The detection, identification and reconstruction of faulty sensors is discussed in Qin and Li (1999). Structured residuals approach with maximum sensitivity (SRAMS) is used for sensor validation. The approach is based on PCA and works well for quasi-steady-state processes (i.e. no dramatic transients). The residuals are designed such that each residual is insensitive to a particular fault (or a particular group of faults) and it is most sensitive to other faults. The SRAMS are subjected to exponentially weighted moving average to smoothen the effect of noise and transients, and they are obtained using statistical methods. Indices such as generalized likelihood ratio (GLR), Q_{sum} (cumulative sum) and V_{sum} (cumulative variance) of the SRAMS are used for identification of various types of sensor faults.

Dunia and Qin (1998) present a methodology that analyzes the fault subspace for process and sensor fault detection. Necessary and sufficiency conditions for detectability (occurrence of a fault), partial and complete reconstructability (reconstruction of the measured variables if the fault is known), identifiablity (deciding a particular fault among a set of faults) and partial and complete isolability of a fault from other faults have been presented. This methodology has been explained by its application on a separation process comprising of two separation columns. Another work on improved PCA for failure identification is presented by Wachs and Lewin (1999). The idea of recursive summation of the last few PCA scores to generate descriptive statistics for process monitoring and improved resolution by enhancing the correlations through optimal time shifting are discussed in their work.

Another promising variant of the PCA approach is the multiscale PCA (MSPCA) approach which integrates PCA and wavelet analysis (Bakshi, 1998). PCA is able to decorrelate the variables by identifying a linear relationship between variables, while wavelet analysis can extract deterministic features and approximately detect autocorrelated measurements. Thus, MSPCA is able to eliminate stationary as well as non-stationary noise better than PCA or wavelets alone. The four steps of MSPCA are: (i) wavelet decomposition of the measured data; (ii) PCA on the wavelet coefficients at each scale and selection of the number of principal components to be retained; (iii) reconstruction of the wavelet coefficients using the retained principal components and thresholding of the reconstructed wavelet coefficients; and (iv) reconstruction of the data by using inverse wavelet transform. Monitoring is performed by computing T^2 (scaled squared scores) and Q (residuals) at each scale. The limits for T^2 and Q are calculated at each scale. Slow events are detected at courser scales first, and sudden changes are detected at finer scales. Also, changes affecting measurements (though satisfying the PCA model) are identified by T^2 chart and the changes violating the PCA model are detected in the Q space.

As discussed above, improvements to the PCA approach have been approached mainly in terms of making the statistical based approaches adaptive to time varying process conditions and enhancing the resolution properties of these approaches. The dynamic enhancements seem to work satisfactory on quasi-steady-state situations and their performance in the presence of significant dynamics need to be evaluated. Further, the adaptability of these approaches to minor structural changes in the process being monitoring needs to be further investigated. While there has been some work on improving the resolution property of PCA-based approaches, they are in general restricted to linear additive faults and their applicability to other types of failure situations has to be studied further.

In summary, contrary to the model-based approach, multivariate statistical methods do not need an explicit system model. They are capable of handling high dimensional and correlated process variables and they are powerful tools of revealing the presence of the abnormalities. However, they do not possess 'fingerprint' or 'signature' properties for diagnosis, which makes the fault isolation difficult. A few techniques such as contribution charts and multi-block approaches have been proposed; however, there is no complete solution to this problem yet. There has been some effort to combine the ideas in model-based approach to that in multivariate statistical method. Gertler and McAvoy (1997) have showed that there exists a close duality between PCA and parity relations. To transfer the idea of structured residuals into PCA, they suggested an enhanced PCA method and showed that the standard PCA model is related to a subspace representation of the primary set of parity relations and that it is possible to define partial PCA models that are related to subspace representations of transformed parity relations. Since such parity relations are selectively sensitive to subsets of faults, it is possible to design an incidence matrix for a set of such partial PCA models to yield a structure similar to that in the model-based approach and having fault isolation capabilities. Their work represents a promising effort to bridge the gap between two subcultures in fault diagnosis.

3.1.3. Statistical classifiers

Fault diagnosis is essentially a classification problem and hence can be cast in a classical statistical pattern recognition framework. The Bayes classifier for a two class problem (Fukunaga, 1972), assuming Gaussian density function for the classes, is

$$d_1 = (y - m_1)^T \Sigma_1^{-1} (y - m_1)$$

$d_{2=}(y-m_2)^T\Sigma_2^{-1}\ (y-m_2)$

A discriminant function h maps the decision space to class space (with a priori probabilities for the classes being the same).

$h = d_1 - d_2$

$h < \delta$, x belongs to class I

$h > \delta$, x belongs to class II

$\delta = \log\left(\frac{|\Sigma_2|}{|\Sigma_1|}\right)$ where δ is the threshold of the classifier.

The same idea can be extended to the n class problem. The Bayes classifier is an optimal classifier (minimum classification error even when the classes overlap) when the classes are Gaussian distributions and the distribution information is available. Notice that the distance measure in the scaled form is used here. Note also that a distance based classifier which scales its distance in this fashion will be the same as the Bayes decision rule for Gaussian distributions. When $\Sigma_1 = \Sigma_2 = I$, the Gaussian classifier becomes the Euclidean distance based classifier. Distance classifiers use distance metrics to calculate the distance of a given pattern from the means of various classes and classify the pattern to the class from which it is closest. Among the distance based classifiers, the most basic classifier is the Euclidean distance based classifier. It simply uses the Euclidean distance from the means of the classes and classifies the point to the class from whose mean it is closest. This classification is exact only when the classes are spherically symmetrical with the same covariance. It would fail, for example, when the classes are elongated ellipsoids and are adjacent.

When the covariance matrices of the distributions are not identity matrices (or its scalar multiples), the distributions are no longer spherically symmetrical. In such cases, the preferred distance metric is no longer Euclidean. In fact, even when the distributions are spherically symmetrical, Euclidean distance is sufficient only when the classes have the same covariance. For a Gaussian distribution, the appropriate distance measure is a scaled form of the Euclidean distance: $(x-m)^T\ \Sigma^{-1}(x-m)$. A Gaussian distribution appears as an ellipsoid when plotted in the input variable space. The inverse of the covariance serves to transform the ellipsoid into a sphere of unit radius. Thus, the distance metric serves to transform the problem (ellipsoidal distribution) to a spherically symmetric form before classification can be done. There is another class of distribution-free classifiers that reduce the need for huge number of samples by making more precise assumptions about the functional forms of the discriminant functions. In particular, one may specify the functional form for the classifier, leaving a finite set of parameters to be estimated. The most common choices here are quadratic or piecewise classifiers.

Fault diagnosis can be considered as a problem of combining, over time, the instantaneous estimates of the classifier using the knowledge about the statistical properties of the failure modes of the system (Leonard & Kramer, 1993; Rengaswamy & Venkatasubramanian, 2000; Smyth, 1994). The failure modes could be approximated as density functions. The development of density functions is a challenging problem and has received considerable attention from various researches. One of the most popular non-parametric technique for density estimation is Parzen windows (Parzen, 1962). In this estimator, an identical basis function is centered around every data point and the density is estimated by summing up all the density functions. Johnston and Kramer (1994) introduce the idea of using hyper-elliptic basis functions for the estimation of density functions. A technique based on statistical cross validation is introduced for evaluating different density estimators. A mixture sum of multivariate Gaussians (Fukunaga, 1972) can be used to estimate probability density functions.

3.2. Neural networks

Considerable interest has been shown in the literature in the application of neural networks for the problem of fault diagnosis. Neural networks have been proposed for classification and function approximation problems. In general, neural networks that have been used for fault diagnosis can be classified along two dimensions: (i) the architecture of the network such as sigmoidal, radial basis and so on; and (ii) the learning strategy such as supervised and unsupervised learning. Different network architectures have been used for the problem of fault diagnosis and these architectures will be discussed subsequently.

In supervised learning strategies, by choosing a specific topology for the neural network, the network is parameterized in the sense that the problem at hand is reduced to the estimation of the connection weights. The connection weights are learned by explicitly utilizing the mismatch between the desired and actual values to guide the search. This makes supervised neural networks a good choice for fault classification as the networks are capable of generating, hence classifying, arbitrary regions in space (Cybenko, 1988). On the other end of the spectrum are neural network architectures which utilize unsupervised estimation techniques. These networks are popularly known as self-organizing neural networks as the structure is adaptively determined based on the input to the network. One such architecture is the ART2 network (Carpenter & Grossberg, 1988).

The most popular supervised learning strategy in neural networks has been the back-propagation algorithm. There are a number of papers that address the problem of fault detection and diagnosis using back-

propagation neural networks. In chemical engineering, Venkatasubramanian (1985) and Watanabe, Matsura, Abe, Kubota, and Himmelblau (1989) and Venkatasubramanian and Chan (1989), Ungar, Powell, and Kamens (1990) and Hoskins, Kaliyus, & Himmelblau (1991) were among the first researchers to demonstrate the usefulness of neural networks for the problem of fault diagnosis. Later, a more detailed and thorough analysis of the learning, recall and generalization characteristics of neural networks for detecting and diagnosing process failures in steady-state processes was presented by Venkatasubramanian, Vaidyanathan, and Yamamoto (1990). This work was later extended to utilize dynamic process data by Vaidyanathan and Venkatasubramanian (1992). A hierarchical neural network architecture for the detection of multiple faults was proposed by Watanabe, Hirota, Iloa, and Himmelblau (1994).

Traditionally feature extraction, which is the process of developing features, is considered as a way to retain the class discriminatory information and the reduction of class common information in the set of measurements from various classes (Himmelblau, 1978). Features developed in this way would show that a measurement is relatively similar to a particular class than others. Hence it might be a good idea to perform some feature extraction and then develop neural-net classifiers based on the feature set. There are two important issues here: (a) interclass discriminatory information; and (b) intraclass similarity information.

Most of the work on improvement of performance of standard back-propagation neural network for fault diagnosis is based on the idea of explicit feature presentation to the NN. There have been a number of researchers who have worked on this issue. Fan, Nikolaou, and White (1993) discuss the performance gains through the incorporation of functional inputs in addition to the normal inputs to the neural networks. Incorporation of knowledge into the NN framework for better diagnosis is discussed by Farell and Roat (1994). Data processing and filtering is shown to lead to significant performance improvement and reduced training time. Tsai and Chang (1995) propose the integration of feedforward NNs with recurrent NNs for better performance. Integration of NNs with the expert systems for fault diagnosis has been considered by Becraft and Lee (1993).

Modifications have been suggested to the standard back-propagation network for the problem of fault diagnosis also. It has been argued that basis functions generating bounded decision regions could be better suited to the problem of fault diagnosis. For example, Leonard and Kramer (1990) suggested the use of radial basis function networks for fault diagnosis applications. In classification, the decision boundary is often not unique and this requires a means of saying whether a particular boundary is desirable and how to construct a decision. For fault diagnosis, it is essential to restrict the nature of the network so that it can generate the bounded decision regions. Holcomb and Morari (1991), Kavuri and Venkatasubramanian (1993a,b, 1994) generalized radial units to Gaussian units and proposed methods to solve the hidden node problem.

Bakshi and Stephanopoulos (1993) proposed Wavenet: a multi-resolution hierarchical neural network. Wavenet is a NN with one hidden layer whose basis functions are drawn from a family of orthonormal wavelets. One important advantage of the Wavenet is that the nodes may be added or removed without retraining the network because of the orthogonality property of the wavelet basis functions. A continuum of models exist with nearest-neighbor models at one extreme, through radial basis functions, which cut the input space into larger patches, to models with global basis functions such as the hyperplanes and sigmoids. Fig. 2 shows the types of nodes traditionally used in neural networks and their classification.

There are also other architectures such as self-organizing maps (Kohonen, 1984). The objective of these methods is to give credit for patterns that are similar to group together. The similarity measure is usually a distance measure. Whenever a pattern is seen that is not similar (in a distance metric sense) to any of the previously formed classes, a new class is formed and the pattern is retained as the defining pattern for the new class and similarity is measured with respect to this pattern. The crucial elements in these kinds of architectures are the distance metric one chooses and the threshold for similarity. Clustering is a technique to group samples so as to maximize separability between these groups. Clustering algorithms specify the number of groups and maximize an objective function that is a measure of separability of these groups. In this manner, clustering becomes a well-defined optimization problem. In the clustering process credit is given to patterns exhibiting similar characteristics. Clustering procedures need two important components. First, they need a measure for estimating similarity between different data points. Without this no credit can be assigned for patterns that are similar. Second, one needs representative patterns against which the similarity of other patterns can be checked.

	Orthogonal	Nonorthogonal
Local	Wavelets	RBFs
Global	Trignometric, polynomial	Sigmoids

Fig. 2. Characteristics of nodes used in neural networks.

The most popular clustering algorithm proposed in the literature is the K-means clustering algorithm (Duda and Hart, 1973). K-means clustering pre-supposes the number of clusters needed and would cluster the data accordingly. It utilizes all the cluster centers so that each of the clusters is guaranteed at least one pattern. Kohonen's self-organizing maps (Kohonen, 1984) identifies the cluster center closest to the training pattern and updates this cluster center and all its topological neighbors. K-means clustering can be shown to be a special case of Kohonen's clustering algorithm. In Kohonen's algorithm, after the neighborhood is decided, the algorithm makes all the clusters in the neighborhood be the winners of the pattern. This leads to the problem of gravity where all the cluster centers migrate towards dense regions leaving less dense regions unrepresented. To avoid this, a fuzzy clustering approach is proposed by Kavuri and Venkatasubramanian (1993a)—here a membership function makes cluster centers relatively far off from the pattern have very little movement towards the pattern—leading to significant reduction of the gravity problem. Self-organizing neural network structures such as the ART2 network (Carpenter & Grossberg, 1988) have also been extensively used in fault diagnosis. Whiteley and Davis (1994) demonstrate the use of ART2 network for the interpretation of sensor data. Chen, Wang, Yang, and Mcgreavy (1999) and Wang, Chen, Yang, and Mcgreavy (1999) discuss the integration of wavelets with ART networks for the development of diagnostic systems. For a collection of papers on the application of neural networks in chemical engineering problems, an interested reader is referred to Venkatasubramanian and McAvoy (1992) and Bulsari (1995). There are a number of papers on neural network applications in process fault diagnosis and it is not possible to provide an exhaustive review of all the approaches here. However, the papers that we have reviewed in this part should provide the reader a good entry point to the literature in this area.

4. A comparison of various approaches

So far in this three part series, we have reviewed the three conceptually different frameworks for process fault diagnosis. In this section, we provide a comparative evaluation of these different frameworks against a common set of desirable characteristics for a diagnostic system that we proposed in part I. The evaluations are summarized in Table 2.

Quantitative model-based methods, such as parity space and observer-based approaches, have several desirable characteristics (Gertler, 1991). If one has complete knowledge of all inputs and outputs of the system, including all forms of interactions with the environment, fault diagnosis would be a well-defined problem regardless of the number of faults present. On the other hand, if there is only a single sensor indicating whether the system is normal or faulty, then nothing can be diagnosed including the proper functioning of the sensor itself. Effectiveness of any diagnostic procedure is limited by the availability of sensor information. In practice, the sensor information is between these two extremes. Given a particular choice of measurements, these methods can specify (a) whether a fault is detectable; (b) can we distinguish the fault from other unknown faults that we do not consider? (c) can we detect the fault in the presence of process and measurement noise? and (d) can we always distinguish a fault from other faults we intend to identify? In answering these questions these methods provide design schemes in which the effects of unknown disturbances can be minimized.

The cost for obtaining these advantages are mainly modelling effort and the restrictions one places on the class of acceptable models. The general state space model of the system is given by:

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}\mathbf{u}(t) + \mathbf{E}\mathbf{d}(t) + \mathbf{F}\mathbf{p}(t)$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t), \tag{4}$$

$\mathbf{E}$ is the distribution matrix for the disturbances $\mathbf{d}(t)$ which in the general case includes both structured and unstructured uncertainties. The term $\mathbf{E}\mathbf{d}(t)$ characterizes the unknown input or disturbance and represents all uncertainties acting upon the system. The major problem in this approach is in this simplistic approximation of the disturbances that include modelling errors. In the design of the nonlinear unknown input observer, more general models have been considered:

$$\mathbf{x}(t+1) = \mathbf{A}\mathbf{x}(t) + \mathbf{B}(y(t),\ \mathbf{u}(t)) + \mathbf{E}\mathbf{d}(t) + \mathbf{F}(\mathbf{x}(t))\mathbf{p}(t)$$

$$\mathbf{y}(t) = \mathbf{C}\mathbf{x}(t) + \mathbf{K}(\mathbf{x}(t))\mathbf{p}(t), \tag{5}$$

In practice, however, severe modelling uncertainties occurring due to parameter drifts come in the form of multiplicative uncertainties. This is a general limitation of all the model-based approaches that have been developed so far. In addition to difficulties related to modelling they do not support an explanation facility owing to their procedural nature. The type of models the analytical approaches can handle are limited to linear and some very specific nonlinear models. For a general nonlinear model, linear approximations can prove to be poor and hence the effectiveness of these methods might be greatly reduced. When a large-scale process is considered, the size of the bank of filters can be very large increasing the computational complexity.

Rule-based expert systems can be used where fundamental principles are lacking, where there is an abundance of experience but not enough detail is available to develop accurate quantitative models. However, its

limitations are well-known (Rich & Venkatasubramanian, 1987). Causal models are also a very good alternative when the quantitative models are not available but the functional dependencies are understood. Abstraction hierarchies help to focus the attention of the diagnostic system quickly to problem areas. One of the advantages of qualitative methods based on deep-knowledge is that they can provide an explanation of the path of propagation of a fault. This is indispensable when it comes to decision-support for operators. They can also guarantee completeness in that the actual fault(s) will not be missed in the final set of faults identified. However, they suffer from the resolution problems resulting from the ambiguity in qualitative reasoning. When quantitative information is available partially, one could use the order-of-magnitude analysis or interval-calculus to improve the resolution of purely qualitative methods.

Pattern recognition approaches or classifiers are constructed generally from historic process data. Neural network architectures, such as radial basis function networks and ellipsoidal unit networks, have been demonstrated to perform well in terms of robustness to noise and isolability requirements. There are some limitations, however, to methods which are based solely on historic process data. It is the limitation of their generalization capability outside of the training data. This problem can be alleviated by radial and ellipsoidal units by avoiding a decision in case there are no similar training patterns in that region. This allows the network to detect unfamiliar situations arising from novel faults. Besides its lack of ability to generalize to unfamiliar regions of measurements space, networks also have a difficulty with multiple faults. This brings out a crucial point of distinction between model-based approaches and classifiers based on historic process data. In the case of qualitative model-based approaches, the combinatorial complexity is unavoidable and can only be partly alleviated with efficient search (de Kleer & Brown, 1984; Reiter, 1987). Because of the combinatorially many multiple fault combinations, the search for multiple faults by specifying them explicitly as different classes and obtaining training patterns for them is not feasible. Given this limitation, the ability of neural networks to generalize to multiple faults has been tested with some success (Venkatasubramanian & Chan, 1989; Venkatasubramanian et al., 1990). Particular architectures showed a greater ability to generalize than certain others. For example, use of a mixture of Gaussians or ellipsoids can provide a good approximation of the class data (Kavuri & Venkatasubramanian, 1993a).

The general limitation of process history based methods is not in the classifiers that are available to them, but in the availability of only a finite sampling of the distribution of the class data in the measurement space. To explain this, consider the 3-dimensional measurement space shown in Fig. 3. Three fault classes are shown as shaded circles at three corners of the cube. Three measurement patterns—x_1, x_2 and x_3—are considered in the measurement space for generalization. Without assuming any classifier, one would expect that

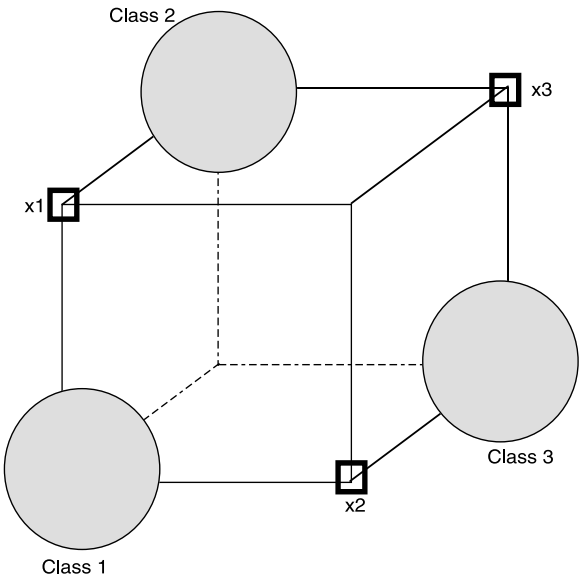

Fig. 3. Location of multiple faults in the output space.

1) x_1 is in classes 1 and 2
2) x_2 is in classes 1 and 3
3) x_3 is in classes 2 and 3

This is, in general, beyond the scope of a classifier and cannot be guaranteed. If we consider classifiers which are linear transformations, then we should expect a similar structure of the data in both the input and output space. This brings out one important point—that the structure in the input space has strong implications on what output one can expect. Thus, if the input space is such that x_1 belongs to classes 1 and 2, then distance-based classifiers can be expected to do multiple fault diagnosis of x_1 properly. However, this cannot be ensured for the measurement space. One needs to determine a proper feature space that has this property. If one uses as input the residuals from the parity equations of a parity-space approach, then the input would be as expected in Fig. 3 and a required structure is thus imposed on the input space. This suggests that, when model information is available, one should use a bank of filters to generate the inputs.

Filter banks are computationally expensive. This suggests that it would be efficient to use qualitative abstraction hierarchies to quickly reduce the focus of diagnosis and then use filter banks in the region of focus.

Table 1 summarizes the transformations that the process data goes through in a diagnostic classifier for some of the methods discussed in this three part series.

Table 1
Typical transformations in various diagnostic methods

	Observers	Digraphs	QTA	Neural networks
Measurement space	Measurements	Measurements	Measurements	Measurements
Feature space	Residuals	Qualitative state/partial pattern	Trends	Hidden nodes/any explicit feature
Decision space	Crisp residuals/fault classes	Fault classes	Likelihood measures	Output nodes
Class space	Fault classes	Fault classes	Fault classes	Fault classes

Table 2 gives a comparison of various methods in terms of the desirable characteristics of diagnostic systems. In the table only some representative methods in each of the three approaches (quantitative model-based, qualitative model-based, process history based) are chosen for comparison. A check mark would indicate that the particular method (column) satisfies the corresponding desirable property (row). A cross would indicate that the property is not satisfied and a question mark would indicate that the satisfiability of the property is case-dependent.

Consider neural networks as an example in Table 2. Quick detection, isolability, and robustness to noise properties of neural networks have been demonstrated through the use of many case studies by different researchers (Ungar, Powell, & Kamens, 1990; Leonard & Kramer, 1990; Venkatasubramanian, Vaidyanathan, & Yamamoto, 1990; Kavuri & Venkatasubramanian, 1994). Neural networks that generate bounded decision regions have been shown to exhibit the property of novelty identifiability (Leonard & Kramer, 1993; Kavuri & Venkatasubramanian, 1994). Due to the procedural nature of neural network development, they lack the explanation and adaptability properties. Further, generation of classification error estimates is difficult using the neural network approach. Since neural networks predominantly work with process history data, the modelling requirements are minimal. Further, once a neural network is trained, the on-line computations are simple function evaluations and hence the on-line computational complexity is minimal. Finally, regarding the multiple-fault identifiability property, as discussed previously in this paper, if the input data structure is favorable, then multiple fault diagnosis is possible. However, the neural network development procedure by itself does not explicitly take into account the idea of multiple fault identifiability. This can be contrasted with an observer-based approach where one could explicitly include multiple fault identifiability in the design procedure. We used similar basis for generating the entries for other methods given in Table 2.

From industrial application viewpoint, the maximum number of fault diagnostic applications in process industries are based on process history based approaches. This is due to the fact that process history based approaches are easy to implement, requiring very little modelling effort and a priori knowledge. Further, even for processes for which models are available, the models are usually steady-state models. It would require considerable effort to develop dynamic models specialized towards fault diagnosis applications. The scope of the process history based systems as applied in the industry is mainly restricted to sensor failures. There are very few industrial applications in published literature that deal with parametric failures. Among the process history based approaches, statistical approach seems to have been well studied and applied. The reason for this might be that with the current state-of-art in applications, detection seems to be a bigger concern than detailed diagnosis. Hence, statistical approaches that are easy to build and which do very well on fast detection of abnormal situations have been successfull in industrial applications. The other data based approaches that have been applied in the industry are

Table 2
Comparison of various diagnostic methods

	Observer	Digraphs	Abstraction hierarchy	Expert systems	QTA	PCA	Neural networks
Quick detection and diagnosis	✓	?	?	✓	✓	✓	✓
Isolability	✓	×	×	✓	✓	✓	✓
Robustness	✓	✓	✓	✓	✓	✓	✓
Novelty identifiability	?	✓	✓	×	?	✓	✓
Classification error	×	×	×	×	×	×	×
Adaptability	×	✓	✓	×	?	×	×
Explanation facility	×	✓	✓	✓	✓	×	×
Modelling requirement	?	✓	✓	✓	✓	✓	✓
Storage and computation	✓	?	?	✓	✓	✓	✓
Multiple fault identifiability	✓	✓	✓	×	×	×	×

ART2 networks and qualitative trend analysis (QTA). QTA approach specializes more on diagnosis than detection and hence might be a useful tool where diagnosis is of importance. QTA approach seems to be robust to routine variations in process operations; however, the time taken to customize and implement might be more than approaches such as PCA.

Though quantitative model-based approaches such as observers have made an impact in mechanical and aeronautical engineering applications, they have had very little impact in process industries. This might be due to the following reasons:

i) Chemical processes are inherently nonlinear in nature. While the theory of linear quantitative model-based approaches is quite mature, the design and implementation for nonlinear models is still an open issue.
ii) Most of the quantitative approaches are based on input–output models and if the models are restricted to linear domain, the advantages of a model-based approach over a simple statistical approach such as PCA might be minimal. Hence, it is easier to implement a PCA-based detection approach than a model-based approach.
iii) Model-based approaches have been predominantly restricted to sensor and actuator failures.

The impact of qualitative model-based approaches such as QSIM and QPT in terms of applications has been minimal. Many of the academic demonstrations of these models have been on very simplistic systems and implementing them for industrial systems is beset with problems related to computational complexity and generation of spurious solutions. Graph-based approaches have been researched upon quite extensively and they have been applied in safety studies, such as HAZOP analysis and tools are being developed for using these types of models in real-time decision making.

In general, literature on industrial applications of diagnostic systems are not many. This could be due to the proprietary nature of the development of in-house systems. Also, there seems to be a general lack of overall penetration of diagnostic systems in process industries. This might be due to the gap between academic research and industrial practice. Two of the most important considerations from an industrial viewpoint such as the adaptability of the systems and ease of deployment are seldom addressed in academic research. Most of the techniques would do poorly on the issue of ease of deployment save some detection techniques such as PCA. Contrast this with, for example, the ease with which PID controllers can be deployed. The other issue of adaptability is crucial too from industrial perspective. Process plants rarely remain invariant with periodic minor changes in operating policy, retrofit design and so on. Once a diagnostic system is deployed, it should be able to adapt with minimal effort as new situations are encountered and the scope of the system is expanded. These issue need to be investigated further for successful deployment of diagnostic systems in industrial setting.

Finally, there seems to be little articulation in the literature about the benefits that can be accrued through the deployment of diagnostic systems. There are some general guidelines based on experience on the economic impact due to abnormal situations, but there are no case studies that analyze the specific benefits that can be attained through the implementation of diagnostic systems. More research is needed on this issue in line with the work that has been carried out analyzing the benefits of implementation of advanced control systems.

4.1. Hybrid methods

One of the important points that we have tried to emphasize in this review is that no single method is adequate to handle all the requirements for a diagnostic system. Though all the methods are restricted, in the sense that they are only as good as the quality of information provided, it was shown that some methods might better suit the knowledge available than others. It is our view that some of these methods can complement one another resulting in better diagnostic systems. Integrating these complementary features is one way to develop hybrid methods that could overcome the limitations of individual solution strategies. Hence, hybrid approaches where different methods work in conjunction to solve parts of the problem are attractive.

As an example, fault explanation through a causal chain is best done through the use of digraphs, whereas, fault isolation might be very difficult using digraphs due to the qualitative ambiguity and analytical model-based methods might be superior. Hence, hybrid methods might provide a general, powerful problem-solving platform. There has already been some work on hybrid architectures. The two-tier approach by Venkatasubramanian and Rich (1988) using compiled and model-based knowledge is one of the earliest examples of a hybrid approach. Process specific knowledge, also called compiled knowledge of the process behavior can be used to give quick identification of potential suspects. This compiled knowledge can be acquired or learned during the operations. This can reduce the time of search for frequent faults. Frank (1990) advocates the use of knowledge-based methods to complement the existing analytical and algorithmic methods of fault detection. Combination of methods allows one to evaluate different kinds of knowledge in one single framework for better decision making. The resulting overall fault detection scheme would have a knowledge base consisting of both heuristic knowledge and analytical models, database, inference engine and explanation component.

A blackboard-based cooperative problem-solving framework where different diagnostic methods work in conjunction to perform collective process fault diagnosis has been proposed by Mylaraswamy (1996), Mylaraswamy and Venkatasubramanian (1997) and Vedam, Dash, and Venkatasubramanian (1999). A blackboard architecture, called Dkit, in which different diagnostic methods analyze the same problem, and a scheduler which regulates the decision-making of these methods is the central concept in this framework. The utility of such a hybrid framework for solving real-time complex fault diagnosis problems is illustrated through the use of a diagnosis study on the Amoco Model IV Fluid Catalytic Cracking Unit (FCCU) (Mylaraswamy, 1996). This framework was adopted by the Honeywell ASM Consortium for the development of a commercially-viable, next generation, intelligent control systems called AEGIS and MSEP.

5. Role of fault diagnosis in design and other process operations

Much interest has been shown in the concept of total process control (Garcia, Ramaker, & Pollard, 1991) with the realization that, due to the limitations of accurate model development, automation of decision-making requires the addition of an exception handling decision layer. These include such tasks as identifying the occurrence of events outside of normal operation, diagnosing the root cause and finally synthesizing and implementing a corrective action.

Fault diagnosis shares with other process operations the realization that with powerful knowledge representation schemes, one can capture the expertise of operators and control engineers that was gained over years of experience with process plants. Process specific knowledge can be used to improve general purpose methodologies. There is a close coupling between diagnosis and process operations and design of chemical plants. Proper design of a chemical plant can reduce the burden on the task of diagnosis. Also, the information from diagnosis can be used to continuously improve the performance of process operations. The information from fault diagnosis can be incorporated into the traditional solution paradigms of other process operations. The aim of this section is to provide a brief overview of various design and operations modules that would particularly share information with fault diagnosis module and also outline the nature of interaction that one can expect.

5.1. Optimal sensor location

Much of the information one gets about the state of the system is from its sensors. Hence, it is very important that the sensors be located optimally. This is a task that should be performed at the design stage of the plant. The basic idea is to locate sensors to enhance observability, detectability and separability (Tanaka, 1989). The detectability index characterizes the ability of the system in detecting specified faults, whereas, separability index characterizes the ease of separation of faults as a function of the minimum angle between the functional subspaces of the faults. Observability index imposes full rank conditions on the system matrix. Sensors are located based on the minimization of all three indices. Other than these indices, one can also consider other important factors like frequency of occurrence of different faults, cost of sensors, severity of faults and so on.

Recently, Rengaswamy et al. (Raghuraj, Bhushan, & Rengaswamy, 1999; Bhushan & Rengaswamy, 2000, 2002a,b) have investigated the problem of sensor location based on various fault diagnostic observability criteria. In their work, they have shown how DG and SDG can be used for deciding the location of sensors. Concepts of fault observability and resolution are introduced which then forms the basis for the sensor location algorithm. Raghuraj, Bhushan, & Rengaswamy (1999) use the DG in their sensor location algorithm. Bhushan and Rengaswamy (2000) demonstrate that better design could be achieved using the SDG of the process.

5.2. Data reconciliation

Data reconciliation is an important activity performed in the continuous process industries. Data reconciliation is essentially a quantitative fault diagnosis approach with the focus on detecting sensor faults and sensor biases. Also, another important goal is the reconciliation of measurement data. Data reconciliation usually consists of three parts: (i) identification of the biased parameter; (ii) estimation of the bias; and (iii) rectification of the sensor measurements.

Data reconciliation can be performed in both steady-state and transient conditions. Steady-state data reconciliation is the problem of removing errors from sensor variables given a collection of data points. It is usually handled using linear least squares estimation techniques and has been shown to give reliable results. In contrast, dynamic data reconciliation is the problem of removing errors under time evolutions of sensor variables. This is a significantly tougher problem due to the presence of differential constraints and the pronounced effect of nonlinearity on the solution strategy.

Instead of the purely quantitative approaches to data reconciliation one can use a combination of qualitative approaches and quantitative approaches to better solve the data reconciliation problem. The diagnostic qualitative knowledge can be used to reduce the search space

and provide good initial guesses. The usefulness of such an approach has been demonstrated by Vachhani, Rengaswamy, and Venkatasubramanian (2001).

5.3. Supervisory control

Supervisory control is an activity that falls in scope between regulatory control and planning. Planning, typically, is the task of creating schedules and making operating decisions on the time-frame of months. It becomes imperative to have a decision layer at a lower level than planning to coordinate various individual control loops and to do exception handling on a much smaller time-frame. Plant behavior in most cases is not perfectly known. Even rigorous models are not adequate to predict plant behavior with satisfying accuracy. There is a natural variability in the process due to raw material variability and due to unsteady environmental condition. This makes the closed world assumption invalid in control strategy. Once a model is obtained and the controller designed, changes in the plant operation can occur that can render the controller ineffective. For many situations this information on changes cannot be anticipated at the design stage, but the controller may be expected to perform over a different operating region or meet more stringent performance criteria than originally specified. When this happens, the controller may exhibit undesirable behavior which requires some action either by the operator or the control engineer. First some retuning may be performed on-line. If this does not correct the problem the loop would be taken off line and a complete redesign performed. As the number of loops under an engineer's supervision increases, the monitoring and correction of control loop problems can become a very time consuming task. This is where we need a supervisory control system to assist in the decision process. The supervisory control system would use the information available from the fault diagnosis system to check and monitor the loops in the regulatory control system. If there has been changes in the control loops, the supervisory control system would then look for different control configurations or set points that would improve the process operations.

For example, the controller configuration, parameters, and actions are not only determined by the mathematical models of the process and the controller, but they are also crucially dependent upon whether the assumptions that underlie the mathematical models are still valid. In many ways the assumptions may be violated. For instance, the controller's effectiveness depends on getting reliable data from the sensors. This is one of the key assumptions underlying the models. If a sensor is faulty, the controller action may become ineffective or it may even cause adverse process behavior. The model could have been linearized near the steady-state operating condition, but due to some equipment malfunction the process could have drifted towards a new steady state. There could be other equipment malfunctions which would make the controller ineffective. There could be changes in the process parameters due to external influences, which could call for a different control configuration, or different set points and gains.

Hence, fault diagnosis is an important module that can help with information for supervisory decision-making. At a lower level, ideas from diagnosis can be used to perform controller diagnostics. Kraus and Myron (1984) discuss an Expert Adaptive Controller Tuning (EXACT) Controller using ideas from pattern recognition approach. Gertler (1989) discusses an intelligent supervisory control which supplements a basic feedback loop with an outer adaptation loop, consisting of an identifier and a tuner. Identification means the estimation of the plant model on the basis of a sequence of input–output measurements. Tuning would require both monitoring the system and adaptation based on the tests performed. The monitoring part of the algorithm does excitation monitoring, stability monitoring and trend filtering. Tuning would then be performed to improve process operations or restore stability as the case may be.

6. Conclusions and future directions

The basic aim of this paper is to organize, classify, review and compare various approaches to fault diagnosis from different perspectives. Towards that goal, we classify the different methods into three categories: (i) quantitative model-based methods; (ii) qualitative model-based methods; and (iii) process history based methods. We also present a framework that shows how these different approaches relate to and differ from each other regarding the transformation of information from the measurement space to the decision space. The important components in the transformation are the transformation from measurement to feature space and the transformation from feature to decision space. A priori process knowledge is used in the first transformation and different search techniques are used in the second transformation. This led to the discussion on diagnostic systems in terms of the typology of a priori knowledge used.

We also propose a list of ten desirable characteristics that one would like a diagnostic system to possess. We compare and evaluate the various methodologies in terms of these characteristics. This comparative study identifies the relative strengths and weaknesses of the different approaches. It also reveals that no single method has all the desirable features we stipulated for a diagnostic system. It is our view that some of these methods can complement one another resulting in better

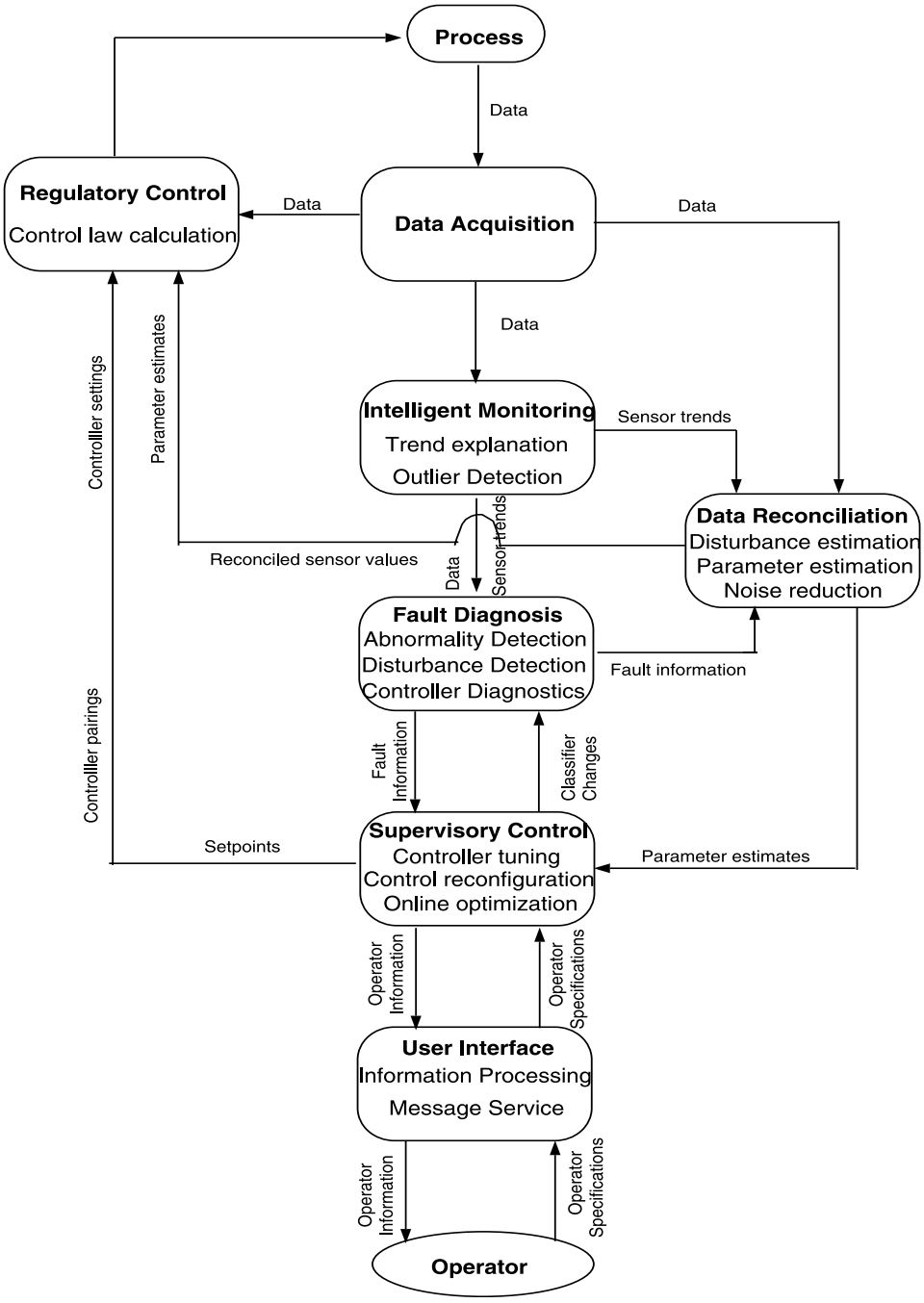

Fig. 4. Integration framework.

diagnostic systems. Integrating these complementary features is one way to develop hybrid systems that could overcome the limitations of individual solution strategies. We think that hybrid systems are an important future direction for research and development in diagnostic systems. Two other areas of equal importance for future research are: (i) integration of diagnostic methods with other process operations for a more comprehensive and effective intelligent supervisory control system; and (ii) implementational issues for large-scale industrial applications. Even though we have broadly classified the future directions into three categories, they are, however, not insulated from each other. They are indeed related to one another. We discuss below the key issues involved in these three future directions of research briefly.

As noted before, the drawbacks of single-method based diagnostic systems are serious enough to limit their applications to small case studies and render them unsuitable for large-scale industrial situations. This makes the design and development of hybrid systems important. Such considerations led to the first attempt

towards hybrid systems in the form of the Dkit diagnostic system that was demonstrated on a large-scale FCCU and BRCP case studies (Mylaraswamy, 1996; Mylaraswamy and Venkatasubramanian, 1997; Vedam, Dash, & Venkatasubramanian, 1999; Vedam, 1999). For similar reasons, the Honeywell ASM Consortium adopted the Dkit architecture as its AEGIS prototype, a next-generation intelligent control system for operator support. Our experience in designing such systems suggests that a practically successful hybrid system is likely to have at least three diagnostic components: (i) a quantitative method such as PCA for quick detection, (ii) a trend-based diagnostic method (e.g. QTA, wavelets) for explicitly assessing process trends, and (iii) a qualitative causal model approach (e.g. SDGs, abstraction hierarchies) to provide explanations and cause–effect reasoning for the operator. Despite such promising starts towards hybrid systems, much work still remains to be done.

Another important direction for research is the integration of diagnostic tasks with other process operations such as regulatory control, data reconciliation, and supervisory control tasks as depicted in Fig. 4 (Rengaswamy, 1995). The overall problem of process operations management involves several subproblem areas that are related to each other and cannot really be treated as individual problems in isolation. For example, the operating targets via refinery scheduling linear programs, constructed using average operating values, have often been found to be infeasible for implementation at the process control level and hence are routinely ignored (Lasdon & Baker, 1986). In the case of data reconciliation, traditionally one does not consider parameter drifts and structural faults as part of the problem. However, an integrated view is necessary for reconciliation of measured data in the presence of process faults. Low-level events such as sensor failure or some other equipment malfunction, can have a significant impact on the higher level plans by calling for the revision of previous schedules. Likewise, higher level decisions have a serious impact on lower level activities such as supervisory and regulatory control. Thus, while these operational tasks may be intrinsically different from each other, they are, however, closely related to each other and cannot be treated as isolated tasks. Hence, one needs an approach wherein all these different tasks can be integrated into a single unified framework so that the operational decision-making can be made more comprehensively and more effectively.

Despite the close connection of diagnosis with control, it is striking that researchers, particularly in academia, have largely tended to treat them as separate problems. This artificial separation needs to disappear in order for real progress to be made in this area. This creates great research opportunities for the traditional diagnostic and control communities.

The third direction of implementational issues for large-scale diagnostic problems raises important challenges in software architecture, real-time hardware, field testing and validation, maintenance, user interface and operator training and acceptance. The design and implementation of hybrid systems as well as integration of diagnosis with other process operations face several technical challenges. Without going into detail, we would like to list some key ones here:

i) Ability to reason about process operations without assuming accurate models.
ii) Ability to reason with incomplete and/or uncertain information about the process.
iii) Ability to understand, and hence represent, process behavior at different levels of detail depending on the nature of the task.
iv) Ability to make assumptions about a process when modelling or describing it. One has to ensure the validity and consistency of these assumptions.
v) Ability to integrate different problem-solving paradigms, knowledge representation schemes, and search techniques.
vi) Ability to maintain global database and global management of process knowledge.
vii) Ability to cope with data explosion and the need for effective compression.
viii) Ability to keep the role of an operator primary and active, not secondary and passive, in the operating environment that is managed with the assistance of on-line intelligent systems.

Developing solutions to overcome these difficult issues towards the design of intelligent supervisory control systems will set the pace of research and development for the coming decade and beyond for engineers in academia and industry. Indeed, we see the successful design and implementation of intelligent supervisory control systems for operator support in a variety of large-scale process applications as the next grand challenge problem for process control engineers.

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