An Online Anomaly Detection System Supporting Batch-Process Operator Decision-Making

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In recent years, the need for automatic supervision through the use of process data has increased. In this paper we propose multivariate time-series shape analysis (MTSA) modeling, which allows an entire process to be modeled without the detailed knowledge of the process that is conventionally required. This technique is particularly intended for batch processes whose operation control is complicated.

With the use of this technique, processes can be automatically monitored, and any detected deviations of process variables, as well as correlations among variables, can be presented in an intuitive, easy-to-understand format. Combining this information with their own knowledge, operators are able to analyze the root cause of anomalies and take action at an early stage.

1. Introduction

Recently, with the remarkable development of information technology, we have come to see terms like big data, artificial intelligence, and the Internet of things used in every field. Efforts to utilize AI and the IoT in industry through industry-academia-government collaboration have already begun in the manufacturing industry in Japan, and outcomes have also been reported from manufacturers.

In the field of process automation (PA), the proper management of equipment and of quality has become more important than ever, so the application of these information processing technologies is to be expected. In the field of PA in recent years, as control rooms become increasingly integrated, the scope of plant operation management is expanding. As a result, there is a growing tendency for a limited number of operators to control the entire process. In addition, many skilled plant workers with abundant operational experience have reached retirement age, but there are many sites where the transmission of their knowledge and expertise has not been well executed. As a result, more attention is being paid to facility maintenance and the ensuring of product quality. Under these circumstances, it is desirable to extract useful knowledge from various types of data collected during plant operation, such as process variables stored in databases, and to make use of that knowledge for managing equipment and quality.¹

In recent years, the utilization of anomaly detection systems that apply information processing technology is spreading.² Using the automatic monitoring of facilities in real time by AI and other information processing technologies to detect abnormalities, operators can take prompt action when an anomaly is detected in order to minimize the risk of an emergency shutdown of the process due to facility failure, and the risk of producing out-of-specification products.

However, sometimes detailed knowledge about the process, such as interconnections between various facility equipment, or details of the process flow, are required for identification of causes and planning of countermeasures when an anomaly is detected. For this reason, in order to take immediate action at the work site, it is desirable to have a function capable of providing instructions to operators to assist in decisionmaking, in addition to the conventional functions of detecting and reporting the anomaly.

Particularly when an anomaly is detected in a batch process, it is likely that more knowledge about many processes is required in order to take action. A batch process is a manufacturing process in which raw materials for the particular product are repeatedly fed and processed, or products (semi-finished) are repeatedly output, as in polymerization reaction processes or semiconductor or pharmaceutical manufacturing processes. Generally in the case of batch processes, many kinds of products are manufactured by the same facility, so control is difficult and complicated. For this reason, it is difficult to make decisions after the detection of anomalies, and it is likely that sufficient sophistication of facility maintenance and quality control may not be carried out with conventional systems that simply send a notification that something is not normal.

Therefore, in this paper, we propose a new method of detecting anomalies in batch processes, multivariate time-series shape analysis (MTSA), which can also support operators' decision-making. In addition to displaying abnormalities in process variables in a way that is intuitively understandable by the operators, this method assists operators in making decisions after an anomaly is detected by inferring the structure of correlations among the variables.

2. Problems with Conventional Methods of Detecting Anomalies in Batch Processes

Regression analysis,³ one of the general methods of detecting anomalies, specifies the process variable that is most important from the viewpoint of avoiding risk as the target variable and the monitoring target. It models the behavior of variables to be monitored using the target variable and predictor variables with a high degree of association with the target variable. Although this has the advantage of higher accuracy detection than other methods, the disadvantage is that the whole process cannot be monitored.

Another method that is used is multivariate statistical process control (MSPC), which uses principal components analysis.⁴ MSPC can model the entire process without detailed knowledge of the process to be monitored, and a method of extending it for use with batch processes has been proposed. MSPC can also calculate the degree of contribution of each variable to the detected anomaly and thereby help operators to analyze the cause. However, it has been pointed out that the degree of contribution calculated by MSPC is itself affected by the abnormal data, so there is a possibility of incorrectly judging which variable is the cause of the abnormality.⁵

On the other hand, MTSA, which is introduced in this paper, is similar to MSPC in that it can model the entire process without detailed knowledge, while it can directly find the cause of the abnormality because it detects abnormality independently for each individual variable.

3. MTSA, a Method of Detecting Anomalies in Batch Processes

3.1 Overview

MTSA is an online anomaly detection method for batch processes. Figure 3-1 gives an overview of this method. MTSA provides two functions: realtime evaluation of the degree of abnormality of the monitoring target (section 3.2) and extraction of the structure of correlation among the monitored process variables (section 3.3).



Fig. 3-1. Overview of MTSA

3.2 MTSA function #1: evaluation

The evaluation by MTSA is calculated by guantifying the degree of divergence when the process data to be checked is superimposed on data from a normal period (hereinafter "normal data") delimited by the start and end of the batch process (fig. 3-1). In this step, since the progress of the batch process will vary depending on conditions such as the external temperature and the purity of the raw material, the data is superimposed after adjusting it along the time axis. In actual processing, synchronization is carried out in advance only among the normal data. When running real-time abnormality detection, the batch data to be checked (hereinafter test data) is synchronized using the synchronized normal data, so the degree of divergence of each variable against the normal data can be obtained as the evaluated divergence.

3.2.1 Synchronization

The synchronization and quantification of the degree of divergence will be described here in greater detail. Synchronization is accomplished using dynamic time warping (DTW), which is able to obtain the correspondences among the sampled data of the multiple time series data (fig. 3-2).⁶

Since DTW is a method for univariate time series data, it is difficult to apply it directly to a batch process that has multivariate data. Therefore, several existing methods have been proposed, such as obtaining the correspondences in each sample with reference to an indicator variable that shows the degree of progress of the batch process,⁷ or weighting each variable based on the result of synchronization between the variable and the normal data, and then obtaining the correspondences among the sampled data with reference to a variable that is heavily weighted.⁸



Fig. 3-2. DTW (dynamic time warping)

However, when these methods are applied to online anomaly detection, if an abnormality occurs in the variable that is set as the reference for synchronization, there is a possibility that the wrong variable will be judged to be abnormal. Figure 3-3 shows an example of the failure of synchronization of normal data with test data having the four variables A, B, C, and D. Since variable C, which is abnormal, is used as the reference for synchronization, the data after the occurrence of the abnormality is unnaturally extended. As a result, although variable D is essentially normal, it is erroneously detected as abnormal.

In order to prevent this problem, the method we are proposing dynamically decides whether each variable is appropriate as a reference before executing synchronization. This is done by determining whether the data corresponding to neighborhood ε on the time axis falls within the allowable error σ for each sample. Figure 3-4 shows an example of the method. For the sample at point a, where no abnormality has yet occurred, the sample test data for neighborhood ϵ falls within the allowable error σ and is used for synchronization. On the other hand, at point b, after the occurrence of an abnormality, since all samples in neighborhood ε are outside the allowable error, the sample of variable C is not used, and synchronization is carried out with reference to other variables. In this manner, inappropriate synchronization can be

prevented by dynamically selecting the sample used for synchronization. With this method, the general shape of the trends in each variable is similar in every sampling lot, a fact that is based on the characteristic of batch process data that the process values are close if the elapsed time from the start of the batch is approximately the same.



Fig. 3-4. Evaluating variables for use in synchronization

3.2.2 Quantifying the degree of divergence

In quantification of the degree of divergence, each variable is individually evaluated as to whether it is abnormal or not. In conventional univariate monitoring, the three-sigma method is used to determine abnormality, which is said to exist if the deviation exceeds three times the standard deviation at a normal time.9 With the three-sigma method it is assumed that the variables to be monitored are symmetrically distributed around the expected value, but the data from an actual batch process does not necessarily have to be symmetrically distributed due to differences in the amount of loaded raw material, outside air temperature, operating conditions, etc. In the MTSA method, kernel density estimation (KDE), which can express any distribution, is used for monitoring.¹⁰ Based on the finite data obtained, KDE enables one to estimate the overall probability distribution that generates the data (fig. 3-5).

If the probability distribution of the normal data has been estimated, the probability p of the occurrence of the test data can be obtained. If the test data is abnormal p is small, and if it is normal p is large, so evaluated value can be calculated using p. The abnormality of the test data is evaluated by checking whether or not evaluated value exceeds the threshold value calculated beforehand using the normal data.



Fig. 3-5. Using KDE for evaluation

3.3 MTSA function #2: extracting the structure of correlations

MTSA has a function for estimating the correlation between variables in order to assist in decision-making when an abnormality is detected, and in order to better understand the process. A commonly used measure of correlation is the Pearson product-moment correlation coefficient.¹¹ By calculating it for each pair of variables, the structure of correlations for all the process variables can be obtained. However, since this correlation coefficient includes cases of spurious correlation, it is difficult to interpret the extracted structure. To solve this problem, MTSA uses the graphical lasso algorithm,¹² which can extract only the intrinsic structure of correlations by assuming that the correlations between individual variables are sparse (fig. 3-6).



After a sparse correlation structure is obtained, it can be used to narrow down the propagation paths when predicting the propagation of anomalies that have occurred, as described below in section 4.

4. Application Examples of MTSA for Detection of Anomalies

In this section, we give application examples to show how MTSA can support real-time decision-making after detecting anomalies. Azbil Corporation has already conducted feasibility studies on abnormal cases experienced by multiple end users, and has confirmed that MTSA can provide useful information for operator decision-making. Although the data used in this section is simulated, it was created on the basis of anomalies that occurred at real work sites.

4.1 Hypothetical abnormal cases

Graphs of the artificial data are shown in figure 4-1a. Ten process variables were monitored, and 20 production batches were made under the same manufacturing conditions, with the amount of time for one batch varying between approximately 300 and 350 minutes. The graphs show the normal data for five consecutive batches and the subsequent data for one batch that included an abnormality. The naming convention for each variable name is Tag[index No.]_ [device name]@[type], the index number being a unique number for each variable, the device name indicating the piece of equipment, and the type identifier showing either a measured process value (PV) or a setpoint (SP).

The assumed abnormality propagation scenario is shown in figure 4-1b. The numbers (1) to (4) in the figure correspond to the order of occurrence of the abnormalities. First, the Tag6_D@PV variable of device D does not reach the normal value at point (1) on the timeline, and the value of Tag0_A@SP and Tag1_ A@PV of device A decrease at point (2) due to the abnormality of Tag6_D@PV. Then, Tag4_C@SP and Tag5_C@PV of device C cause hunting at point (3), and finally at point (4) the values of Tag2_B@SP and Tag3_ B@PV of device B increase earlier than in the normal case. This scenario is described in figure 4-1b. The time when the operator recognizes the anomaly is indicated by \blacktriangle in figure 4-1(b). The developing problem is not recognized at points (1) to (4).

The operator does not recognize the propagation of the abnormality from device A to device C at points (2) to (3). A detailed description of the propagation of the abnormality is given in section 4.3.



Fig. 4-1. Graphs of the artificial data and timeline of abnormality propagation scenario



Fig. 4-2. Anomaly detection by MTSA

4.2 Results of applying MTSA

Figure 4-2 shows the detection of abnormalities as a result of applying MTSA to this artificial data. Additionally, figure 4-3a shows the structure of the correlation of variables according to MTSA.

In figure 4-2a, a variable evaluated to exceed the threshold value is judged to be abnormal 140 minutes before the operator recognizes the problem. MTSA detects abnormalities at points (1) and (2) in the abnormality scenario, which is to say that it detects abnormalities of device D (Tag6_D@PV) and device A (Tag0_A@SP and Tag1_A@PV) more than two hours before the operator does.

Figure 4-2b shows further variables judged to be abnormal, in addition to those detected in 4-2a, 50 minutes before the operator recognizes them. MTSA detects abnormalities at points (3) and (4) of the abnormality scenario, namely abnormalities in device C (Tag4_C@SP) and device B (Tag2_B@SP and Tag3_ B@PV).



Fig. 4-3. Propagation of abnormalities

4.3 Prediction of anomaly propagation destinations

In this section, we give a concrete example of assisting operator decision-making by predicting the destinations of abnormalities utilizing MTSA at a point 140 minutes before the operator recognizes an abnormality (fig. 4-3).

As described in section 4.2, MTSA detects abnormalities in devices D and A 140 minutes before the operator recognizes them (fig. 4-2a). Although only three variables were detected as abnormal, by using the inferred structure of correlations (fig. 4-3a) and the operator's knowledge (fig. 4-3b), it is possible to predict where the anomalies will propagate, as described below.

First, the inferred structure of correlations indicates that there is a correlation between the device A variables (Tag0 A@SP and Tag1 A@PV) that were detected as abnormal and the device C variables (Tag4_C@SP and Tag5_C@PV). In other words, the propagation of the abnormality from device A to device C (from point (2) to point (3)) is suggested. As mentioned in section 4.1, this propagation is not included in the knowledge of the operator (fig. 4-3b), but the operator may be able to notice it from the inferred structure of the correlations.

Next, based on the knowledge of the operator, it can be understood that the device C abnormality (Tag4 C@SP) will propagate to device B (Tag2 B@SP and Tag3_B@PV), from point (3) to point (4). In this way, by combining the knowledge obtained from the data, namely the correlation structure, and the knowledge of the operator, it is possible to predict that the currently detected abnormality in device D (Tag6 D@PV) will ultimately propagate to device B.

As a result of propagation, if an emergency process shutdown or a particularly serious situation such as the production of out-of-spec goods is expected, the risk can be avoided by devising countermeasures at this point. Generally, when planning countermeasures, it is necessary to identify the cause of the abnormality, but since MTSA detects abnormalities in individual variables, the detected variables are themselves candidates for the cause. In this example, it can be said that there is a high possibility that the above-mentioned three variables (Tag6_D@PV, Tag0_A@SP, and Tag1_ A@PV) are the cause of the abnormalities.

On the other hand, even though an abnormality is detected, there are cases in which its propagation cannot be predicted with certainty, such as when the detected abnormality may propagate to multiple destinations. Even if the occurrence of a serious problem is predicted, in a case where it is possible to take immediate countermeasures by switching to backup equipment, for example, dealing with the initial problem may be suspended with the cause still unknown.

In such a situation, by obtaining the process data during the propagation of the abnormality, prediction can be made more reliable and utilized for making decisions. In this case, MTSA detects further anomalies in Tag4 C@SP, Tag5_C@PV, Tag2_B@SP, and Tag3_ B@PV 50 minutes before the operator recognizes them (fig. 4-2b). From this it can be known that the prediction of the propagation destinations 140 minutes previously was valid.

As described above, MTSA supports not only the detection of abnormalities but also the analysis of causes and prediction of possible further incidents. This allows operators to make smart decisions in real time based on the predicted situation and the expected difficulty of various courses of action.

5. Example of System Configuration Using **MTSA**

This section outlines a system under development for predicting anomalies in batch processes. The system consists of three modules: viewer, server, and configurator (fig. 5-1).

The viewer is a graphical user interface for informing the operator of the current state of the monitored process and for giving information in an easy-tounderstand manner to assist in decision-making when an anomaly is detected. In addition to an alarm function when an anomaly is detected, the viewer shows the structure of correlations (fig. 4-3a), graphs of individual variables, evaluations of the degree of abnormality (fig. 4-2), and the order in which abnormalities were detected. Figure 5-2 shows an example of the monitoring screen that displays graphs and evaluations.



Fig. 5-1. System configuration example

The server does online checking and detecting of abnormalities, and reports the results to the viewer. It obtains the current value of each process variable from the process database at constant intervals, synchronizes the test data and the normal data, evaluates the degree of abnormality, and then determines whether or not the values are abnormal.

The configurator is a tool for specifying the monitoring functions to the server. It obtains the normal data for the monitored process, synchronizes the data, infers the structure of the correlations, and uploads the processed data to the server.

6. Conclusions

In this paper we describe MTSA, a new anomaly detection method developed for batch processes. In addition to detecting abnormalities, this method assists operator decision-making by providing useful information for analyzing the causes of abnormalities and for predicting how abnormalities will propagate.

Azbil Corporation has already verified actual cases of anomalies in batch processes experienced by multiple end users and has confirmed the effectiveness of this method. As a next step, we will work on improving usability so that this method can be easily used at more manufacturing sites. In addition to the use of an abnormality prediction detection system for continuous processes that has been adopted at many manufacturing sites, we would be pleased if you consider using MTSA for batch processes.



Fig. 5-2. Example of viewer monitoring screen (the screen is still under development and may change in the future)

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