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Processing History Dependent Control Parameter Estimation in Multi-step Batch Processes

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Abstract: In this study, we propose a method to estimate the parameters of a control model for a batch process by using previous batch data. We focus on the case of multistep batch processing, where appropriate control input values often exhibit strong dependency on the prior processing history of the feed (called "feed characteristics" hereafter), *e.g.,* the equipment or operating conditions used in the previous processing steps. In such cases, it is a common practice to use the data from those previous batches with identical feed characteristics as the new batch. As batch operations become more complicated, however, the variety of feed characteristics is increased and consequently the chance of finding recent batch data with identical feed characteristics is reduced. To combat the shortage of usable data in this context, it is important to enable the utilization of not only data from batches of identical feed characteristics but also those from batches of "similar" feed characteristics. This paper attempts to address this need in a practical manner. By using MANOVA (multivariate analysis of variance), a popular statistical inference method, statistical similarities among the estimated parameter values for different feed characteristics can be evaluated and substitutable sets of the feed characteristics can be identified. Results from the statistical analysis can increase the amount and/or recency of the data used in the batch control input calculation. We suggest some specific rules for selecting among available previous batch data by considering both the feed characteristic similarity and time-immediacy. The proposed method has been tested on real manufacturing industrial data and the results showed practical viability and significant potentials of the method.

Keywords: multi-step batch process, run-to-run control, parameter estimation, multivariate analysis of variance (MANOVA), statistical analysis

1. INTRODUCTION

Batch processing plays an important role in the production of specialty products, such as pharmaceuticals, fine chemicals, and semiconductors. Batch processing has been used mostly for small-volume production of high value-added products, but it has not been adopted for large-scale product chemical production. One of the reasons for this is that batch processing presents difficult control challenges such as run-to-run variations in the feed and equipment conditions, nonlinear process dynamics due to non-stationary operating conditions, and the lack of on-line quality measurements (Berber (1966), Lee and Lee (2007)) .

The principal objective of batch processing is to meet the product quality specifications with consistency. Various batch process control approaches have been developed (Chin et al. (2000), Chen and Liu (2002)). In a typical batch operation setting, after the completion of each batch run, the product quality is analyzed and stored in the database. The product quality measurements are then used to update the parameters of a regression model that describes the relationship between the product quality and the control inputs. The updated model in turn can be used to determine the control inputs for a new batch run (Fig. 1) (Lee (2013)).

Such is the basic idea of `run-to-run' (R2R) control where R2R feedback is used to improve the control performance

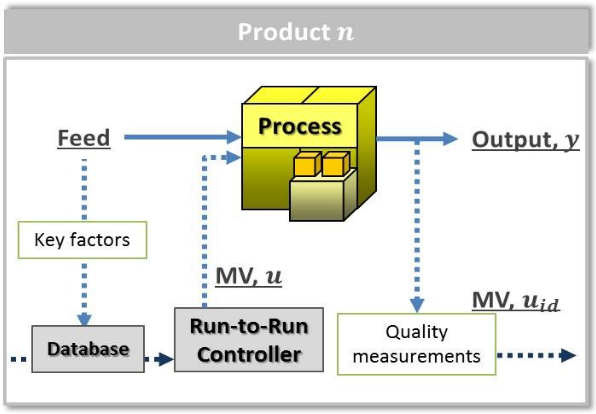

Fig. 1. Typical information flow in the run-to-run control of a batch process

(Chin et al. (2000)). R2R control is popular for discrete manufacturing processes and machine controls in which the product recipe associated with a particular machine and machine process is modified at an ex-situ run-to-run level as opposed to an in-situ level, i.e., the product recipe is modified between machine runs rather than during runs. This type of discrete control utilizes process and equipment data collected ex-situ along with historical knowledge of the process and equipment to suggest process recipe modifications so as to maintain or better achieve process output target values in subsequent process runs (Moyne et al. (1993)).

For certain types of batch processes, e.g., those within multi-step manufacturing, appropriate control input values strongly depend on the prior processing history of the feed. Hereafter, the condition of the feed as a result of several factors regarding previous processing steps will be referred to as 'feed characteristics'. The components of feed characteristics can be equipment used to perform the previous operation steps, product recipes used or status of raw material. In case that such prior history (i.e., feed characteristics) dependency exists, it is a common practice to use only the data from those batches of exactly same feed characteristics with the new batch to estimate the control inputs for controlling product quality. However, in some cases insufficient and outdated data from exactly identical feed characteristics is a problem and requires advanced methodologies. In this paper, we present a new statistical approach geared toward enlarging the amount of data to include those from batches of ``similar" feed characteristics that can be used to estimate batch control inputs.

The rest of this paper is organized as follows. Section 2 describes the problem of interest. In section 3, we introduce the statistical significance test of multivariate analysis of variance (MANOVA) to identify similarity among different feed characteristics. In section 4, we construct a new methodological framework for parameter estimation. Finally, the proposed method has been tested using data from a real industrial process and the results are presented in section 5.

2. PROBLEM DEFINITION

As mentioned previously, appropriate control parameter values can depend strongly on the feed characteristics in the context of multistep batch process manufacturing. For the determination of control inputs, let us assume that a general high regression model like Eq. (1) is used.

$$y = \beta_{00} + \beta_{10}x_1 + \beta_{01}x_2 + \beta_{20}x_1^2 + \cdots + \beta_{0n}x_2^n + \varepsilon \qquad (1)$$

Here, y is the product quality measurement that can be obtained only after the completion of each batch run, β s are the regression coefficients, and x_1 and x_2 are the two control inputs. After each run, measurement y is taken, and βs are estimated *ex post facto*, typically through the simple least squares. These values are then stored in the database so that they can be used to set the control parameters for a future batch. An important point relevant to the case at hand is that βs vary with the feed characteristics. Therefore, the parameters used to set the control inputs for a new batch run should be in accordance with its feed characteristics. Typically, data from a previous batch run of exactly equal feed characteristics are searched for in the database and used irrespective of its timing.

In today's complex batch manufacturing environment (e.g., in VLSI, bio-technology, semiconductor manufacturing), the variety of feed characteristics encountered is considerable, as they involve a large number of levels and factors. This in turn causes a shortage of data with exactly same feed characteristics and therefore increased time gaps between successive such batch data. Even though control parameters are highly correlated with the feed characteristics, they also vary with time and the use of outdated data, even of same feed characteristics, can lead to poor control results. This is because operation conditions or equipment characteristics may have shifted with time. Hence, the time immediacy of the data is as important as their match in terms of the feed characteristics.

Our objective in this work is to enable the use of previous batch data beyond those that match the feed characteristics exactly. Industries often encounter situations where a previous batch run with exactly same feed characteristics cannot be found within a sufficiently recent time window. These situations arise not only due to the increased variety of the feed characteristics but also during times of temporary data shortage when new products are introduced or an equipment maintenance run resets the process characteristics (and therefore the control parameters). Extensions to allow the use of "similar" batch run data would be highly welcome by the industries. MANOVA provides a basis to quantify the degree of similarity among different feed characteristics in terms of the regression model parameters. And feed characteristics of high similarity pairs (or groups) can then be substituted for each other in the parameter estimation. This enables us to use more recent (and higher amounts of) data, which in turn leads to more accurate predictions.

3. FUNDAMENTALS

In this research, data is analyzed by a statistical inference method of MANOVA. MANOVA enables assessment of the statistical significance of certain factors and their interactions within an experiment design (Stevens (2002)). MANOVA is essentially analysis of variance (ANOVA) but with multiple dependent variables. For further comprehension of MANOVA, understanding of ANOVA is needed.

3.1 ANOVA

ANOVA is a collection of statistical models used to analyze the differences between group means and their associated procedures. As a result, ANOVA provides a statistical test of whether or not the means of several groups are equal.

First of all, there are some assumptions for the ANOVA test. The following assumptions should be satisfied by the data to be tested (Manly, B.F.J. (1994)). While considering m independent groups, each of size n, X_{ij} indicates the j-th sample of the i-th group.

- **Independence of observations**: The samples from the populations are independent random samples.
- **Normal Distribution**: The dependent variables should be normally distributed within groups.

$$X_{ij} \sim N(\mu_i, {\sigma_i}^2) \qquad (2)$$
$$\mu_i: group\ mean, {\sigma_i}^2: group\ variance$$

- **Homogeneity of Variances**: The dependent variables exhibit equal levels of variance across the range of predictor variables.

$$\sigma_1 = \sigma_2 = \cdots = \sigma_m = \sigma \qquad (3)$$

Then, ANOVA approach is used for following null hypothesis (H_0) and alternative hypothesis (H_1):

$$H_0: \mu_1 = \mu_2 = \cdots = \mu_m \tag{4}$$
H_1: at least one μ is not equal to the other

The statistic

$$SS_W = \sum_{i=1}^{m}\sum_{j=1}^{n}(X_{ij} - X_{i.})^2 \tag{5}$$

is called the within groups sum of squares. And $SS_W/(nm - m)$ is an estimator of σ^2

The statistic

$$SS_b = n\sum_{i=1}^{m}(X_{i.} - X_{..})^2 \tag{6}$$

is called the between groups sum of squares. When H_0 is true, $SS_b/(m-1)$ is an estimator of σ^2

Then, test statistic is given by Eq. (7).

$$TS = \frac{SS_b/(m-1)}{SS_W/(nm-m)} \tag{7}$$

In Eq. (7), when H_0 is true, TS has an F-distribution with $m-1$ numerator and $nm-m$ denominator degrees of freedom. H_0 will be rejected when TS is sufficiently large.

The significance level α test of H_0 is as follows:

$$\begin{cases} reject\ H_0\ if\ \ TS > F_{m-1,nm-m,\alpha} \\ do\ not\ reject\ H_0\ otherwise \end{cases} \tag{8}$$

p-value given by Eq. (9) gives the critical significance level in the sense that H_0 will be accepted if the significance level α is less than the p-value.

$$p - value = P\{F_{m-1,nm-m} \geq TS\} \tag{9}$$

For more information and description, please refer to Ross, S.M. (2004).

3.2 MANOVA

MANOVA is used when there are several correlated dependent variables, and the researcher desires a single, overall statistical test on this set of variables instead of performing multiple individual tests (Carey (1998)). In other words, unlike the analysis of variance (ANOVA), MANOVA assesses the statistical significance of the effect of multiple groups on a set of two or more dependent variables (DVs) and has the ability to examine the simultaneous effect on the multiple DVs at once. Assuming that the intercorrelations between all DVs are zero, the MANOVA approach simply sums the F ratios that would result from individual ANOVAs applied to the separate DV (Li (1964)). In this paper, since a high order regression model with multiple parameters is considered, MANOVA is deemed more appropriate for deciding the similarity or discrepancy among groups. Consider p variables, the null hypothesis (H_0) and alternative hypothesis (H_1) for MANOVA can be stated as in Eq. (10). Here, μ_{ki} is the mean of the k-th variable in the i-th group (Cole et al. (1993)).

$$H_0:\ \mu_1 = \begin{bmatrix}\mu_{11}\\ \mu_{21}\\ \vdots\\ \mu_{p1}\end{bmatrix} = \begin{bmatrix}\mu_{12}\\ \mu_{22}\\ \vdots\\ \mu_{p2}\end{bmatrix} = \cdots = \begin{bmatrix}\mu_{1m}\\ \mu_{2m}\\ \vdots\\ \mu_{pm}\end{bmatrix} = \mu_m \tag{10}$$

H_1: *at least one μ is not equal to the other*

In MANVOA, all assumptions are the same as in ANOVA, but one more additional assumption is related to covariance (French et al. (2002)).

- **Homogeneity of Covariances**: Since there are multiple DVs, it is also required that their intercorrelations (covariances) are homogeneous across the cells of the design.

The use of two or more dependent variables in an MANOVA requires that the cross-products between different DVs as well as the sum of squares for each DV be taken into account. (Barker, H.R. (1984)) In other words, we use the statistic SSCP (sum of squares and cross-product) matrix $(p \times p)$ instead of SS (scalar). In a fashion analogous to ANOVA, the between groups SSCP ($SSCP_b$) is divided by the within group SSCP ($SSCP_W$). Then Wilks' lambda, Λ, can be calculated by Eq. (11) for MANOVA tests of statistical significance.

$$\Lambda = \prod_{i=1}^{p}(1+\lambda_i)^{-1} \tag{11}$$

Where λ_i are eigenvalues of $({SSCP_W}^{-1} \cdot SSCP_b)$ .More detailed explanation of approximation with a Chi-squared distribution from the Wilks' lamda is appeared in Mardia, K.V. (1971) and Bartlett, M.S. (1954)

The key outputs from the MANOVA test are the dimension d and p-value. d is an estimate of the dimension of the space containing the group means $(\mu_1, \mu_2, \cdots \mu_N)$. For N groups, d can take any value between *0* and $N-1$. If $d = 0$, there is no evidence to reject the null hypothesis (*i.e.,* all the group distributions are the same). If $d > 0$, then we can reject the null hypothesis at the specified significance level (usually 5%). When $d = n$, it means n groups all have different group distributions. The vector of p-value is for testing whether specific means lie in a space of dimension 0, 1, and so on.

4. METHODOLOGY

This paper proposes a new methodological framework for batch process control parameter estimation by exploring the database to identify similar feed characteristics and make use of such information in selecting data for the parameter estimation. The method entails four major steps: data preparation, identification of substitutable candidates, selection of historical data for an incoming batch run, and parameter estimation (Fig. 2).

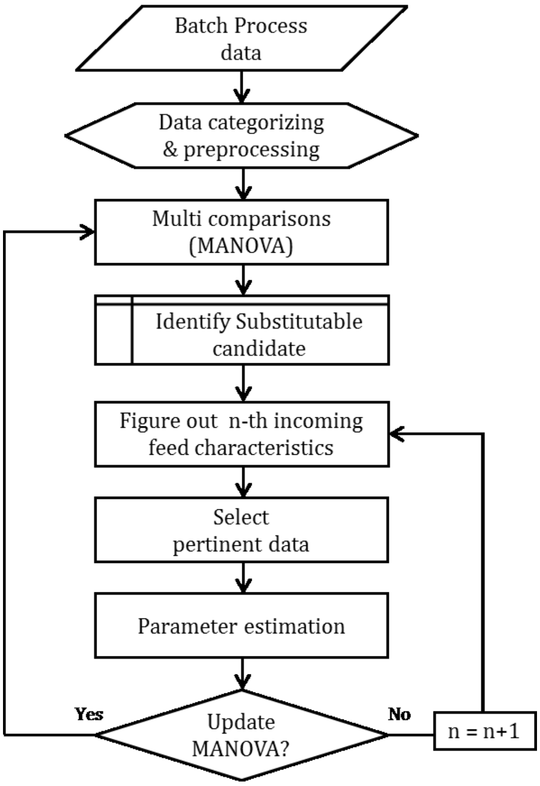

Fig. 2. Proposed Methodology

4.1 Data Preparation

During batch operations, a large amount of on- and off-line will be recorded and accumulated in the database. The collected database often includes noisy, missing and inconsistent data points. Through data preprocessing, the quality of the data and the result of data analysis can be improved. (Chien et al. (2007))

To define feed characteristics, engineers figure out two or three main factors that affect the control parameters. According to the chosen factors, the set of possible feed characteristics is defined. Then, the data is categorized according to the feed characteristics. There are some conditions for the categorized data to satisfy before the MANOVA test can be applied. First, the number of data points for each kind of feed characteristics should be bigger than the number of parameters. Second, outliers should be eliminated as much as possible. Since outliers affect the mean and variance significantly, MANOVA is known to be highly sensitive to them. Outliers may produce either a Type I or Type II error with no indication given as to which type of error will occur in the analysis. (French et al. (2002)) Lastly, data should satisfy the assumptions of MANOVA. The normality of distribution can be checked by using the chi-squared quantile-quantile plot (Q-Q plot). The Q-Q plot enables one to determine graphically whether the plotted data set comes from a normal distribution. (Wilk and Ganadesikan (1968)) The other assumptions, like independence of the observations and homogeneity of the variances, can be satisfied through scaling and data preprocessing.

4.2 Identification of Substitutable Candidate

After data preprocessing, MANOVA is performed to identify pairs (or groups) of substitutable feed characteristics. When MANOVA is applied to more than two groups, the results can be ambiguous as to which groups are different and which groups are similar. The multi-comparisons can be used for further clarification in this regard. The term “comparisons” in multi-comparisons refers to comparisons of two groups, which correspond to a pair of feed characteristics. When dimension $d = 1$, we can reject the null hypothesis. It means the two groups are sampled from different populations. When $d = 0$, we cannot reject the null hypothesis and the two feed characteristics can be concluded to be similar. The results help us identify groups of similar feed characteristics, which serve as a reference for determining substitutable candidates for each feed characteristic. In this step of MANOVA, moderate amounts of historical data should be used. If the amount of data is too small, MANOVA cannot be performed or the results are not reliable. On the other hand, too big a data size also causes wrong results due to potentially significant fluctuations in the data distributions over the time.

4.3 Selection of Pertinent Data for an Incoming Batch Run

This step should be performed before each new batch run is performed. The task is to extract the relevant information and data from the current database, which is continually being updated. Through MANOVA, the substitutable feed characteristics should have been identified. We can then simply look for the most recent runs with either the same or substitutable feed characteristics as that of the current batch. But this simple approach has a weakness in that, even when a fairly recent batch run with identical feed characteristics exist, it may be superceded by an even more recent batch run of a similar feed characteristics. A more reasonable solution is to apply a time limit, *i.e.,* during a specific time limit, batch runs of exactly same feed characteristics are preferentially selected. If a sufficient number (to be specified by the user) of such runs cannot be found, then runs of similar feed characteristics are selected based on their recency. This way, batch data of similar feed characteristics will be extracted only when the number of runs of identical feed characteristics within the fixed time limit is insufficient.

4.4 Parameter Estimation

Industrial data typically have large variances and noise even after elimination of obvious outliers. In addition, most parameters show time correlations. Given these, it is a common practice to use weighted moving averages to determine the control parameters of an incoming batch. Moving average is used with time series data to smooth out short-term fluctuations and highlight longer-term trends or cycles. If we assume that n data sample is chosen, the simple weighted moving average of Eq. (12) is used to estimate the parameters for the t-th incoming batch. Here, $\boldsymbol{\beta}_t$ is (p x 1) the vector form of p control parameters for the t-th batch. The latest data has the biggest weight n, and the weight is gradually decreased with time going back.

$$\boldsymbol{\beta}_t = \frac{\sum_{k=1}^{n}(n-k+1) * \boldsymbol{\beta}_{t-k}}{\sum_{k=1}^{n}(n-k+1)} = \frac{n * \boldsymbol{\beta}_{t-1} + (n-1) * \boldsymbol{\beta}_{t-1} + \cdots + \boldsymbol{\beta}_{t-n}}{n(n+1)/2} \quad (12)$$

A slight extension of the above estimation method can consider potentially the different confidence levels for data from batch runs of same vs. similar feed characteristics. Let us ignore the time proximity effect for the time being and only consider the priority with respect to the feed characteristics. If we assume that, among n selected data samples, m of them have the identical feed characteristics, the equations of (13), (14) may be used. Different weighting factors, w_{or} and w_{sim}, are used to weigh the data of the same and similar feed characteristics distinctively.

$$\boldsymbol{\beta}_t = \frac{\sum_{k=1}^{n} w_k * \boldsymbol{\beta}_{t-k}}{\sum_{k=1}^{n} w_k} \quad (13)$$

Here,

$$w_k = \begin{cases} w_{or} & if\ (t-k)\ th\ input\ is\ same \\ w_{sim} & if\ (t-k)\ th\ input\ is\ similar \end{cases} \quad (14)$$

5. A CASE STUDY

To test the proposed method, we conducted a test case study using real industrial data from a major microelectronics manufacturing company (the source of the data cannot be revealed due to a nondisclosure agreement). In this study, our analysis was restricted to batches making a same product in a same production line. The results obtained by using the proposed method are compared with those by using only the data of identical feed characteristics (current practice). Sum of squared error (SSE) for p control parameters was calculated between the estimated parameters and ideal parameters (those from the *ex post facto* analysis). Performance improvement was measured as the relative reduction in the SSE with respect to the SSE resulting from the current method:

$$\frac{\sum(\beta_{id} - \hat{\beta}_{or})^2 - \sum(\beta_{id} - \hat{\beta}_{new})^2}{\sum(\beta_{id} - \hat{\beta}_{or})^2} \times 100\ (\%) \quad (15)$$

The parameters calculated by the original method, $\hat{\beta}_{or}$, are estimated by Eq. (12) only with data from the runs of identical feed characteristics. On the other hand, those calculated by the proposed method, $\hat{\beta}_{new}$, are estimated by using data of both identical and similar feed characteristics. Here, β_{id} represent the values from the *ex post facto* measurements after each run.

The first step is data preparation. The feed characteristics were defined by three factors considered to be critical in determining the control inputs. Then, the data were categorized and saved by feed characteristics and obvious outliers were removed. Simple limits were used to identify outliers. If a data point was outside the range of $(\mu - 3 * \sigma, \mu + 3 * \sigma)$, then that data point was treated as an outlier. Here, μ and σ are the mean and variance of the categorized data. The normality of distribution was also ascertained by making the Q-Q plot.

Multi comparisons by MANOVA were performed to identify substitutable candidates using 1000 batch run data. Then, for additional 500 test batches, input feed characteristics were figured out and data of batch runs with identical or substitutable feed characteristics within a time limit of 60 batches were retrieved. We looked for 5 most recent runs for the parameter estimation. Among the 500 batches tested, 259 batch runs had substitutable feed characteristics candidates and data from such runs were utilized for estimating the parameters according to the procedure described previously. Among the 259 batches, 98 batches used data from runs of similar feed characteristics. In other words, our method used extra data (compared to the conventional method) in 98 of the tested batches. The rest of the 259 batches had a sufficient number of runs with identical feed characteristics within the time window even though they also had exchangeable batch runs.

Based on the analysis results and data selection, we estimated the control parameters for the 98 batch runs. The two different parameter estimation methods described were tested and compared. First is the time weighted parameter estimation method as described by Eq. (12). Because 5 data points were used, the weighting vector was set as (5, 4, 3, 2, 1). The bigger weight factor is given to the more recent data. The other method tested is as in Eq. (13). The weighting value for identical feed characteristics (w_{or}) was set as 1, and the weighting value for similar one (w_{sim}) was varied from 0.3 to 1. Through this procedure, the relative influence of the data from identical vs. similar feed characteristics could be varied. Fig. 3 shows that the overall performance of the similarity weighted method is better than that of the time weighted method except for the case of $w_{sim} = 0.3$. The similarity weighted method shows the best performance when $w_{sim} = 0.6$. Given the better performance of the similarity weighted method, we can conclude that more confidence should be given to the data from the runs of identical feed characteristics.

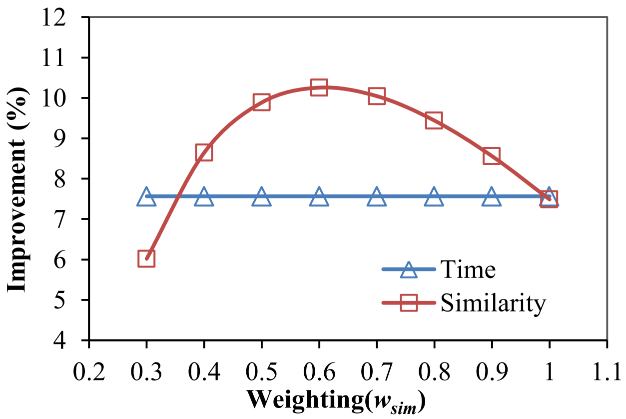

Fig. 3. Improvement of parameter estimation with time weighted (red) and similarity weighted (blue) method

In order to further demonstrate the effectiveness of the proposed control method, we have performed an extensive analysis with a large amount of industrial data. The number of batch runs used in the overall study is 3966 from product line A and 3954 from line B. For line A, among the 3966 batches, the number of cases that utilized data from runs of similar feed characteristics was 608. For line B, this number was 697. The similarity weighted parameter estimation method has been applied to such cases.

Table 1 shows the performance improvement using the new parameter estimation over the current practice. The new parameter estimation method improves the estimation results for all 4 parameters in both lines. The average improvement is 21.8% for line A and 31.0% for line B. These improvements can translate into significant economic savings due to improved yields. As a sample, detailed reduced squared error results for the second parameter for line A are shown in Fig. 4. The horizontal axis represents index of batches and the vertical axis, the normalized squared error. Fig. 4 shows most of the runs that had large squared errors with the original method had greatly improved results when the new method is applied for the parameter estimation.

Table 1. Improvement (%) of estimation for line A

Parameters	β_1	β_2	β_3	β_4
Line A (%)	24.4	32.8	21.2	8.7
Line B (%)	38.8	40.8	26.4	17.9

6. CONCLUSION

In this study, we have presented a new parameter estimation method to control batch processes the control parameters of which show strong dependency on the prior processing history of the feed. The proposed method enables the use of more data, specifically those from batch runs of "similar" feed characteristics as well as identical ones. It was suggested that by using MANOVA, the statistical significance among previous history data for different feed characteristics could be assessed. Those groups with high similarity are determined as substitutable candidates. The validity of using data from runs of similar feed characteristics has been verified with real industrial data. The case study showed that the proposed method can improve the accuracy of parameter estimation by allowing the use of a larger amount of more recent data. This approach is a more flexible and efficient solution for the case that already-mentioned data shortage.

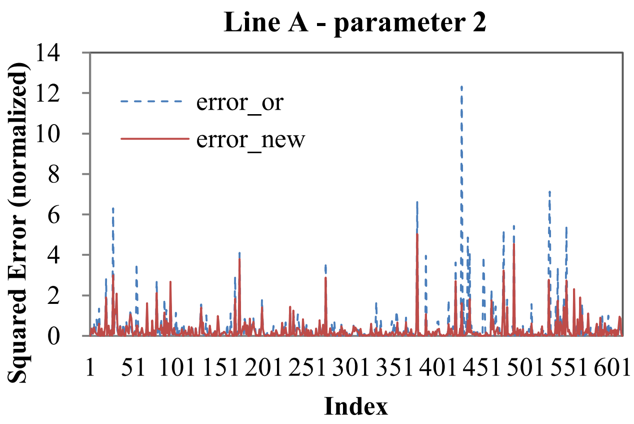

Fig. 4. Comparisons of Squared Error between original method (blue) and new method (red)

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