Quality-Oriented Statistical Process Control Utilizing Bayesian Modeling

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Abstract—**Quality control is an important issue in semiconductor manufacturing. Statistical process control (SPC) is known as a powerful method for accomplishing process stability and reducing variability. In this paper, we adopt the quality-oriented statistical process control (QOSPC) method. In QOSPC, product quality test data, such as electrical performance and product reliability, are incorporated into the process control procedure. QOSPC has two major challenges: extracting process variables that affect product quality, and determining quality control limits (QCLs) for each variable. In this work, we fully exploit a Bayesian approach to resolve both of these challenges simultaneously. We introduced a linear bathtub model that contains parameters corresponding to QCLs as obvious change points and fit the model to the observed data by Bayesian inference (BI). In our experiments with artificial datasets, we demonstrated that the values of QCLs and their confidence, by which we can judge whether the measured process variable is related to product quality, are estimated successfully by BI. We verified the robustness of our method by testing it repeatedly. The proposed method reduced the human labor cost for extracting quality-related process variables and determining QCLs by 93%.**

Index Terms—**Bayesian inference, Bayesian modeling, machine learning, quality control, statistical process control.**

I. Introduction

QUALITY control is important to assure that products conform to a set of required specifications in semiconductor manufacturing. Statistical process control (SPC) is known as a powerful quality control method for realizing process stability and reducing variability. Control charts are the most significant tools in SPC for monitoring process performance. A control chart is a display of the measurement data of a process variable, such as a critical dimension or a film thickness, in relation to time. The chart contains upper and lower control limits determined based on a statistical value of past measurement data (e.g. standard deviation) such that points that plot outside the control limits indicate the occurrence of shifts of process performance over time [1], [2].

In this paper, we adopt the quality-oriented statistical process control (QOSPC) method, which is illustrated in Fig. 1. In QOSPC, product quality test data, such as electrical performance and product reliability, are incorporated in the process control procedure for manufacturing operations. The typical application of QOSPC is for setting quality control limits (QCLs), which are selected such that points that plot outside the QCLs directly predict the degradation of product quality. When a QCL is set inside the control limit of an SPC, as in Fig. 1, a stricter process control must be implemented to achieve further reduction in variability. Recently, process control based on the product quality or reliability has attracted more attention and is becoming increasingly important [3], [4].

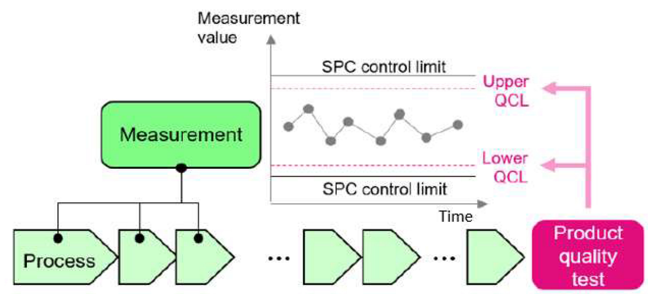

Fig. 1. Quality-oriented statistical process control (QOSPC) procedure. Quality control limits (QCLs) are determined in consideration of product quality, while SPC control limits are determined based on a statistical value of past measurement data.

Although the advantages of QOSPC are readily understood, there are some obstacles that prevent its practical use. In a real-world production line, QOSPC has two major challenges: extracting process variables that affect product quality and determining QCLs for each variable. To address the first challenge, multivariate statistical models, such as partial least squares regression, are often used (e.g., [5]), but it is difficult to construct a robust model with a small amount of data. For the second challenge, as described in Section II, an unclear boundary makes it difficult to determine QCLs. In addition, these two issues are usually addressed in sequence, resulting in unacceptable costs in terms of time and labor.

In this work, we devised a method for determining QCLs by using Bayesian modeling. The Bayesian approach enables us to infer not only the positions of QCLs but also their credibility. When the credibility is high, we can accept the inferred values as QCLs; that is, we can conclude that the process variable is related to the product quality and should be controlled by the QCLs. However, when the credibility is low, we do not select the inferred values as QCLs. Our method resolves the two abovementioned challenges simultaneously and makes QOSPC feasible even when there are a large number of process variables to be measured in a production line.

The remainder of this paper is organized as follows. The difficulty in determining QCLs is described in Section II. The

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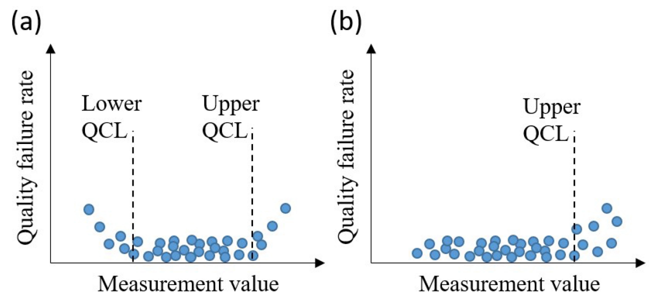

Fig. 2. Illustration of difficulty in determining QCLs. QCLs are determined from the relationship between quality failure rate and measurement values. Setting a QCL is difficult, as shown in (b), where the boundary is blurred (on the right side), or uncertain (on the left side).

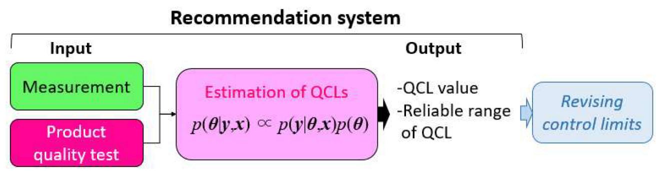

Fig. 3. Recommendation system for reducing the time-consuming process of determining QCLs. Engineers can easily decide whether to adopt a recommended QCL value by referring to its reliable range.

method for determining QCLs involving Bayesian modeling is introduced in Section III. In Section IV, we demonstrate the effectiveness of our method by using artificial data imitating a real-world dataset of a production line. We extended our method to 2-dimensional measured variables in Section V, and in Section VI we present the conclusions of this work.

II. Difficulties in Determining QCLs

Difficulties in determining QCLs are illustrated in Fig. 2. The plot shows the relationship between the quality failure rate (y-axis) and the measurement value of a process variable (x-axis). When there is an obvious increase in the quality failure rate at the edge of the measurement values, as in Fig. 2(a), it is relatively easy to visually recognize QCLs. However, it is still difficult even for skilled engineers to establish an accurate QCL value with few data. When the boundary is unclear or uncertain, as in Fig. 2(b), it becomes more difficult to specify the existence of valid QCLs, that is, whether or not the process variables related to the product quality. It is possible to select an intuitive QCL by sight, but unnecessarily strict process control has a risk of increasing cost, and moreover, it is time-consuming and unrealistic to visually identify QCLs for the tens of thousands of process variables measured in a production line.

III. Proposed Method

We devised an automated method for determining the values of QCLs that replace human labor and assists engineers by providing recommendations (Fig. 3). In this work, we fully exploit a Bayesian approach to the estimation, which is one of the most powerful techniques in the field of machine learning. Whereas point estimation methods such as maximum likelihood estimation (MLE), provide only optimal values, Bayesian methods are known to also quantify the uncertainty of estimation [6]. Because QCLs are blurred and unclear and

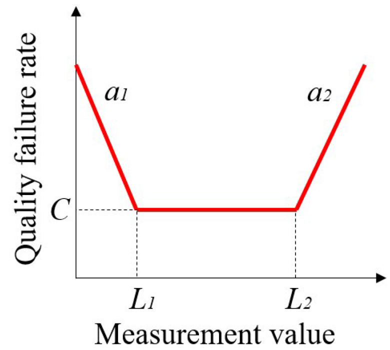

Fig. 4. Illustration of the linear bathtub model. This model is introduced based on the experience that the failure rate may increase at the edge of measurement values.

it is often unknown whether they exist at all, as in Fig. 2, we take full advantage of Bayesian uncertainty quantification for automated estimation of a reliable range for the QCLs. Given that the quality failure rate may increase at the edge of measurement values as in Fig. 2(a), we introduced a complex model to summarize the relationship between product quality and measurement data as follows:

$$f_{LBM}(x) = \begin{cases} a_1(L_1 - x) + C & (x < L_1) \\ C & (L_1 \le x < L_2) \\ a_2(x - L_2) + C & (x \ge L_2) \end{cases} \quad (1)$$

Fig. 4 shows an illustration of (1). The reason for using this model is that we can directly regard estimated L_1 and L_2 values as QCLs. We call this model the linear bathtub model (LBM). The parameters of LBM $\boldsymbol{\theta}(\boldsymbol{\theta} = [L_1, L_2, a_1, a_2, C])$ are estimated by Bayesian inference (BI), which is a method of statistical inference based on Bayes' theorem $p(\boldsymbol{\theta}|\boldsymbol{y}, \boldsymbol{x}) \propto p(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{x})p(\boldsymbol{\theta})$, where $p(\boldsymbol{\theta}|\boldsymbol{y}, \boldsymbol{x})$ is the posterior distribution, $p(\boldsymbol{y}|\boldsymbol{\theta}, \boldsymbol{x})$ is the likelihood function and $p(\boldsymbol{\theta})$ is the prior distribution. The likelihood function of our method is a probability distribution whose expected value is calculated by (1). The probability distribution is selected depending on the data type of $\boldsymbol{y}$; for example, a Bernoulli distribution is selected when $\boldsymbol{y}$ are binary data and discrete distributions such as Poisson distribution and binomial distribution are selected when $\boldsymbol{y}$ are countable data.

IV. Verification Experiment

To verify the effectiveness of our method, we performed an experiment to estimate QCLs with artificial data such that failure rates increase when the measured value exceeds a certain value. In this experiment, we verified that QCLs estimated by our method correspond with the preset theoretical values. For comparison with our method, we also performed a QCL estimation experiment using a point estimation method involving LBM and MLE.

A. Dataset

For this experiment, we prepared artificial data corresponding to the case shown in Fig. 2(b) for this experiment. The artificial data consist of simulated measurement values $\boldsymbol{x}$ and quality test data $\boldsymbol{y}$, where $\boldsymbol{x}$ are random numbers generated from a standard normal distribution and $\boldsymbol{y}$ are binary data ($y = 1$ indicates failure) generated based on failure rate $\boldsymbol{p}$.

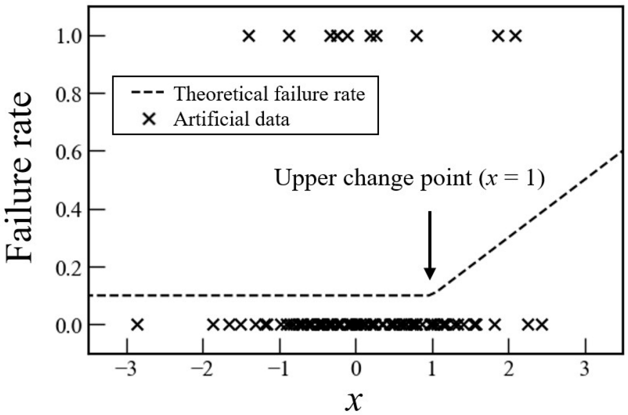

Fig. 5. The theoretical failure rate line and 100 artificial data. Upper change point is x = 1 and lower change point does not exist.

TABLE I
PRIOR PROBABILITIES OF LBM PARAMETERS

Parameter	Prior probability
L_1, L_2	Normal(0, 10)
a_1, a_2	Half-Cauchy(1)
C	Uniform(0,1)

Rate $\boldsymbol{p}$ is calculated as the following model that combines straight lines:

$$p_i = \begin{cases} 0.1 & (x_i < 1) \\ 0.2(x_i - 1) + 0.1 & (1 \leq x_i < 5.5) \\ 1 & (x_i \geq 5.5) \end{cases} \tag{2}$$

Fig. 5 shows the theoretical failure rate line based on (2) and an example of artificial data randomly generated from the theoretical failure model. As shown in Fig. 5, the change point of the failure rate is only on the upper side and does not exist on the lower side.

B. Statistical Model

The quality test data $\boldsymbol{y}$ are drawn according to the following generative process.

$$y_i \sim \text{Bernoulli}(p_i) \tag{3}$$

$$p_i = \begin{cases} 0 & (f_{LBM}(x_i) < 0) \\ f_{LBM}(x_i) & (0 \leq f_{LBM}(x_i) < 1) \\ 1 & (f_{LBM}(x_i) \geq 1) \end{cases} \tag{4}$$

Here, $f_{LBM}(x)$ is the LBM function. Table I shows the prior distributions of the parameters of LBM. The prior distributions of L_1 and L_2 are widespread normal distributions based on the real world, where we have no information about the position or existence of change points in advance. The prior distributions of a_1 and a_2 are half-Cauchy distributions because a_1 and a_2 values must be positive for the LBM to produce the shape of a bathtub. Given that the posterior distribution cannot be calculated analytically, we used the No-U-Turn Sampler (NUTS), which is a Markov chain Monte Carlo (MCMC) sampling method [7]. In MLE, we used a grid-search method to estimate the values of LBM parameters.

C. Results

Table II and Fig. 6 show the estimation results of the parameters of the LBM for the certain dataset (N = 10,000) generated from the theoretical failure model (2). A 95% credible interval indicates the uncertainty of estimation, and the narrower the interval, the higher the confidence of the estimated values. As shown in Table II, the theoretical values of L_2, a_2, and C are estimated correctly by both methods. However, the estimated L_1 values differ significantly between the two methods, as shown in Fig. 6. In MLE, the L_1 value is forcibly estimated as a single value although the lower change point does not exist in the theoretical model, meaning that we might set an excessive and unnecessary QCL. Meanwhile, in BI, the 95% credible interval of the estimated L_1 value is too wide to determine the value of QCL, indicating that we do not need to set a lower QCL.

TABLE II
ESTIMATED VALUES OF THE LBM PARAMETERS

Method	Parameter	Theoretical value	Estimated value	95% credible interval
BI	L_1	-	-7.8	-18.3 to -1.7
	L_2	1.0	0.9	0.8 to 1.0
	a_1	-	0.61	0.00 to 1.70
	a_2	0.2	0.20	0.16 to 0.23
	C	0.1	0.10	0.10 to 0.11
MLE	L_1	-	-2.1	NA
	L_2	1.0	0.9	
	a_1	-	0.22	
	a_2	0.2	0.20	
	C	0.1	0.09	

Fig. 7 shows the result of repeating the same experiment 100 times. The datasets are created with different random seeds for each experiment. As shown in Fig. 7, both BI and MLE can estimate L_2 values correctly at all iterations. However, MLE erroneously estimated L_1 values within the range of x46 times out of 100. In contrast, BI estimated L_1 values with wide credible intervals at all iterations.

These evaluation results show that the existence of change points and their values can always be estimated more robustly by BI than by MLE.

D. Experiments With Dataset Generated From Non-Linear Modes

The previous section presented the experimental results using datasets generated from the model having clear change points. However, in the real world, the change point of the theoretical model is often unclear. The following model is one of the example of such a model.

$$p_i = 0.1 + 0.9\left(\frac{1}{1 + e^{-(2x_i+5)}}\right) \tag{5}$$

Fig. 8 shows the theoretical failure rate line based on (5) and the example of artificial data randomly generated from the theoretical failure model (5). The failure rate increases as x increases, but the upper change point is unclear.

Table III and Fig. 9 show the results of fitting the LBM to the artificial data generated from (5) by BI. The L_2 value is estimated as the point at which the failure rate starts to increase visually. This result shows that our method can propose a practically useful QCL even in cases where the change point is not clear.

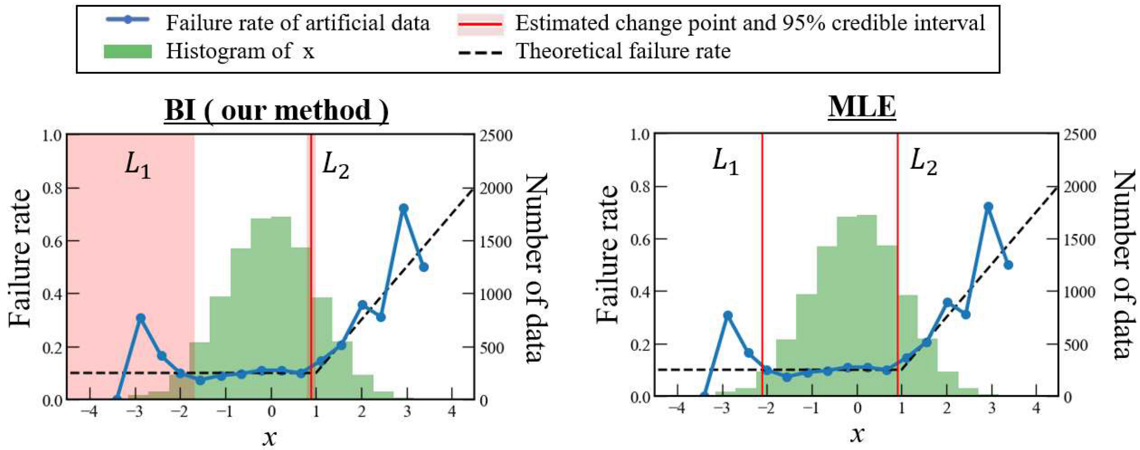

Fig. 6. Estimated change points for artificial data. Blue lines and green bars show summary values of artificial data; red lines show the estimated change points by each method.

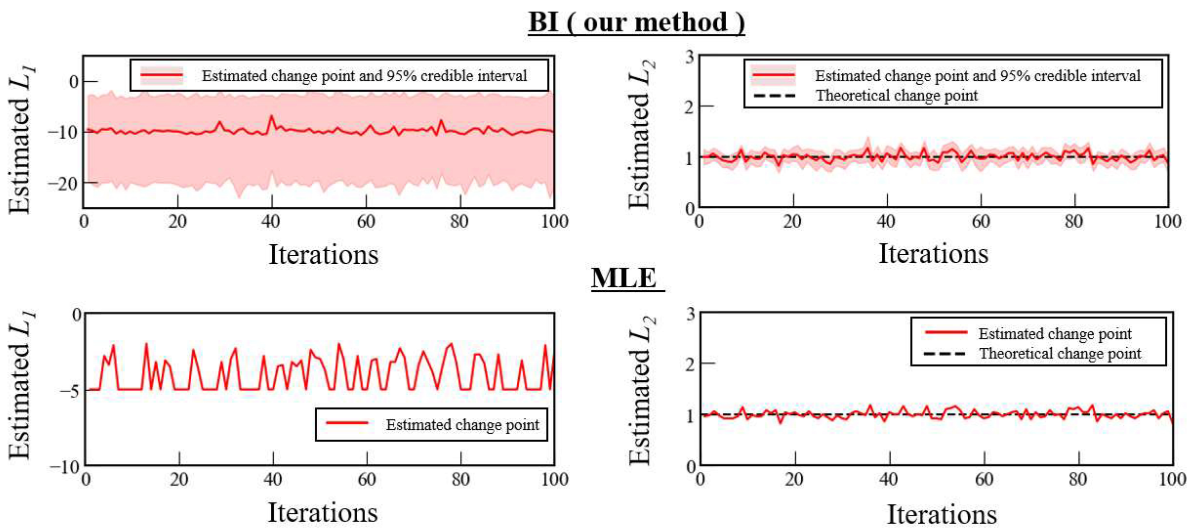

Fig. 7. Estimated change points for 100 artificial datasets. In MLE, the lower limit of the grid search range for L_1 estimation is -5; therefore, -5 indicates that L_1 does not exist within the distribution of x according to MLE.

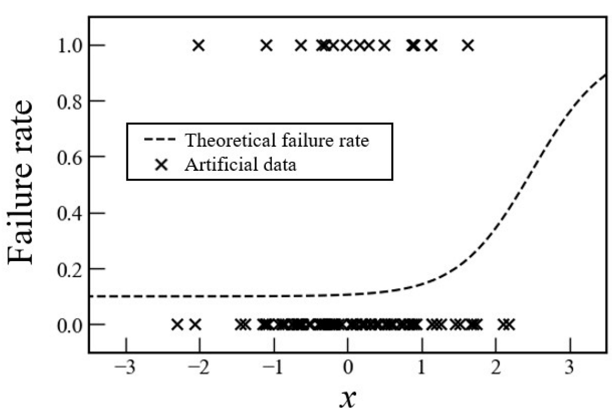

Fig. 8. The theoretical failure rate line and 100 artificial data. The upper change point is not clearly defined.

TABLE III
ESTIMATED VALUES OF THE LBM PARAMETERS FOR THE DATASETS GENERATED FROM THE NON-LINEAR MODEL

Method	Parameter	Theoretical value	Estimated value	95% credible interval
BI	L_1	-	-10.3	-20.8 to -2.4
	L_2	Unclear	1.0	0.9 to 1.1
	a_1	-	0.81	0.00 to 1.81
	a_2	Unclear	0.31	0.26 to 0.37
	C	0.1	0.11	0.10 to 0.12

V. QCLs Determination With Multidimensional Data

Our method determines the QCLs of multiple variables in consideration of the interaction effect by using the extended LBM. Fig. 10 shows the failure rate heat map of artificial data consisting of two types of measurement data ($\boldsymbol{x_1}$ and $\boldsymbol{x_2}$) as well as the test result data ($\boldsymbol{y}$ are binary data and $y = 1$ indicates failure). The failure rate increases when x_1 and x_2 exceed the two change lines on the plane of (x_1, x_2). To estimate the change lines, we introduce the 2-dimensional LBM as follows:

$$f(x_1, x_2) = \varphi_1(x_1, x_2) + \varphi_2(x_1, x_2) + C$$
$$\varphi_1(x_1, x_2)$$

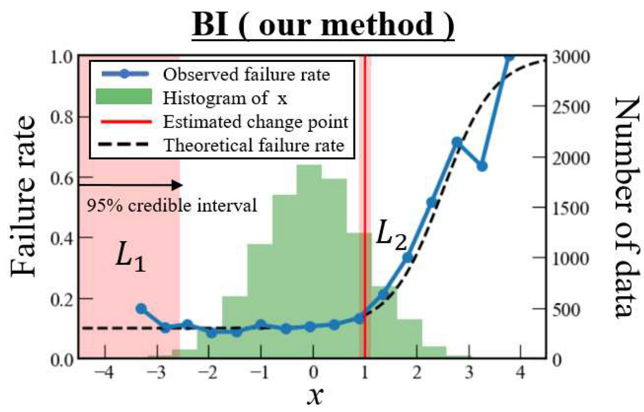

Fig. 9. Estimated change points for artificial data generated from non-linear model. Estimated L_2 value is reasonable as the upper QCL.

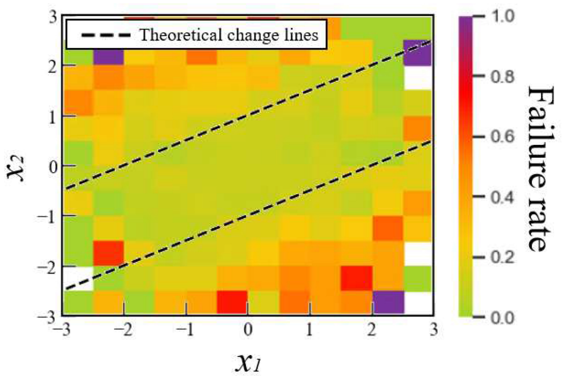

Fig. 10. Failure rate heat map of artificial data for two variables. The failure rate is set to increase as x_1 and x_2 exceed the change lines.

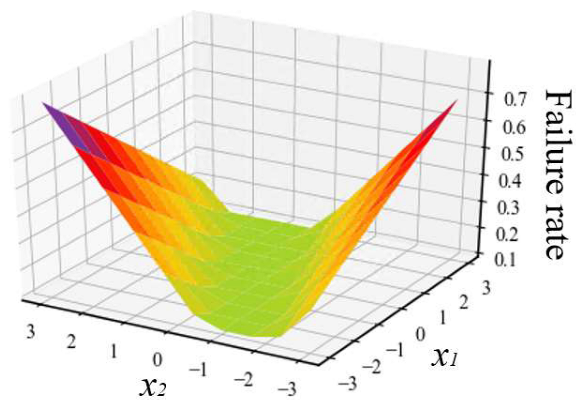

Fig. 11. Three-dimensional illustration of the result of fitting 2-dimensional LBM to the artificial data shown in Fig. 10.

$$= \begin{cases} a_1((p_1x_2 + q_1) - x_1) & (x_1 < p_1x_2 + q_1) \\ 0 & (p_1x_2 + q_1 \le x_1 < p_2x_2 + q_2) \\ a_2(x_1 - (p_2x_2 + q_2)) & (x_1 \ge p_2x_2 + q_2) \end{cases}$$

$$\varphi_2(x_1, x_2) = \begin{cases} b_1((r_1x_1 + s_1) - x_2) & (x_2 < r_1x_1 + s_1) \\ 0 & (r_1x_1 + s_1 \le x_2 < r_2x_1 + s_2) \\ b_2(x_2 - (r_2x_1 + s_2)) & (x_2 \ge r_2x_1 + s_2) \end{cases} \quad (6)$$

By fitting (6) to the observed data, change lines are estimated as straight lines on the plane of (x_1, x_2). Fig. 11 illustrates the result of fitting (6) to the artificial data shown in Fig. 10. Two-dimensional LBM has a flat bottom and its sides can be regarded as the change lines. Fig. 12 shows the estimated change lines and the credible intervals. Both theoretical change lines are within the estimated 95% credible intervals.

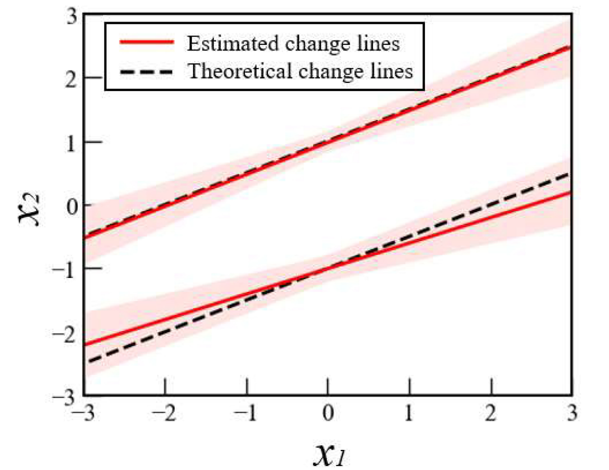

Fig. 12. Estimated change lines of artificial data shown in Fig. 10. Both theoretical change lines fall within each of the estimated 95% credible intervals.

VI. Conclusion

In this paper, we focused on determining QCLs for process variables related to product quality based on the concept of QOSPC, which aims to improve product quality by directly implementing process control procedures. To overcome the difficulties in determining QCLs, a method of fitting the LBM to the observed data by BI was presented. From the experimental results using artificial data, we verified that the proposed method successfully identified the QCL values, including their uncertainty, which gives us the criteria for whether or not to set a QCL. We demonstrated the robustness of the proposed method in the repeated experiments. Our method reduced the time-consuming human labor cost for determining QCLs by 93%, making QOSPC feasible for application to real-world production lines.

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