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ORIGINAL ARTICLE

Identifying the time of step change in binary profiles

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Abstract Control charts are intended to aid quality practitioners in monitoring whether a change has occurred in a process. When a control chart indicates an out-of-control signal, it means that the process has changed. However, control chart signals do not indicate the real time of process changes; so estimators are applied to indicate the time when a change in the process takes place, which is referred to as the change point. This paper provides a maximum likelihood estimator to identify the real time of a step change in phase II monitoring of binary profiles, in which the quality of a process is characterized by a logistic regression between the response and predictor variables. Simulation studies are provided to evaluate the effectiveness of the change point estimator.

Keywords Change point · Binary profiles · Maximum likelihood estimator (MLE) · Statistical process control (SPC)

1 Introduction

Control charts are the most popular statistical process control (SPC) tools used to monitor process changes. Once a control chart signals, quality engineers should identify and remove the special cause of variability and return the process to the state of statistical control. Helpful information to aid them is the real time that the special cause first appears in the process that is referred to as the change point. However, control chart signals do not indicate the change point and a change usually occurs much earlier than the time it is detected. Authors have suggested several methods including cumulative sum (CUSUM) control chart [1], exponentially weighted moving average (EWMA) control chart [2], and maximum likelihood estimator (MLE) [3, 4], etc., to identify the change point. In addition to the proposed methods, change point problems are classified according to change types including step, drift, and monotonic changes. Accordingly, Samuel et al. [5, 6] proposed MLE methods for the time of step changes in the mean and variance of a normal distribution, respectively. Pignatiello and Samuel [7–10] proposed a maximum likelihood estimator in different control charts to find the real time of change point under a step change. Perry and Pignatiello [11, 12] considered a linear trend change in the mean of a normal process. Samuel and Pignatiello [10] and Perry and Pignatiello [11] showed that the performance of the MLE is better than the estimators of EWMA and CUSUM in identifying the change point of a normal and Poisson process, respectively. For a comprehensive review on change point estimation methods, refer to Amiri and Allahyari [13].

Another popular topic in the SPC is profile monitoring which is paid attention by researchers recently. Profiles are useful when a quality characteristic is functionally dependent on one or more explanatory, or independent, variables. Mestek et al. [14], Kang and Albin [15], Mahmoud and Woodall [16], and Amiri et al. [17] presented different applications of profiles in SPC. Profile monitoring using control charts can be seen as a two-stage process, phases I

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and II. For phase I analysis, Mestek et al. [14], Kim et al. [18], Mahmoud and Woodall [16], Mahmoud et al. [19], and Kazemzadeh et al. [20] have studied phase I monitoring of linear profiles. Kang and Albin [15], Kim et al. [18], Gupta et al. [21], Zou et al. [22, 23], Saghaei et al. [24], Zhang et al. [25], Kazemzadeh et al. [26], and Amiri et al. [27] have investigated phase II monitoring of linear profiles. Nonlinear profile monitoring have also been considered by several authors including Walker and Wright [28], Ding et al. [29], Williams et al. [30], and Veghefi et al. [31].

Identifying the change point in profiles has been studied by some researchers. Mahmoud et al. [19] used a likelihood ratio-based method to identify the real time of a step change in phase I monitoring of a simple linear profiles. Zou et al. [22] proposed a method based on likelihood ratio statistics that is able to identify the real time of a step change in simple linear profiles in phase II. Kazemzadeh et al. [20] used an MLE method to estimate the change point in polynomial profiles under a step change in phase I.

All of the aforementioned researchers assume that the response variable is continuous (usually normal) and characterize profiles with linear or nonlinear models. However, in many industrial applications, the response variable is discrete such as binary (as in the case of a product can be classified as defective or nondefective) or countable (as the number of defect products or number of patients in a hospital). However, profile monitoring when the response is binary has received very little attention in the literature. Yeh et al. [32] studied binary profiles in phase I. They proposed different T^2 control charts for monitoring logistic regression profiles. Nevertheless, to the best of our knowledge, there is not any method to estimate the real time of a step change in binary profiles in both phases I and II .In this paper, we propose an MLE method to estimate step changes in phase II of the binary profile based on the logistic regression model. The rest of this paper is organized as follows: Section 2 illustrates logistic regression model and explains the steps of estimating the model parameters; Section 3 presents the change point model and assumptions of the problem. The performance of the proposed model is investigated in Section 4. Conclusions and some future researches are provided in the final section.

2 Logistic regression model

Many categorical response variables have only two categories: for example, whether you take public transportation today (yes, no), or whether you have had a physical exam in the past year (yes, no). Denote a binary response variable by y and $E(y)=\pi$. The value of π can vary as the value of independent variables (experimental) (x) changes, hence, we replace π by $\pi(x)$. Suppose that there are n independent variables in each setting. The relationships between $\pi(x)$ and x are usually nonlinear and the S-shaped curves are often realistic shapes for this relationship which are called the logistic regression models.

In a general logistic regression model, there are p predictor variables for any of n independent experimental sets, which is shown by $X_i = (x_{i1}, x_{i2}, \ldots, x_{ip})^T$ as well as corresponding Bernoulli response variables namely z_i for $i=1,2,\ldots,n$. The probability of success in each set is denoted by π_i and each π_i is a function of X_i. In the logistic regression model, this function is characterized by the link function $g(\pi_i)$, defined as

$$g(\pi_i) = \frac{\log(\pi_i)}{1-\log(\pi_i)} = \beta_1 x_{i1} + \beta_2 x_{i2} + \ldots + \beta_p x_{ip} \tag{1}$$

where $\beta = (\beta_1, \beta_2, \ldots, \beta_p)^T$ is the regression parameters vector. It is usual to set $x_{i1} \equiv 1$ in order to β_1 be the intercept of the model. The alternative Eq. 1, directly specifying π_i, is

$$\pi_i = \frac{\exp(X_i^T\beta)}{1+\exp(X_i^T\beta)} = \frac{\exp(\eta_i)}{1+\exp(\eta_i)}, \tag{2}$$

In this equation, $\eta_i = X_i^T\beta = \sum_{k=1}^{p} \beta_k x_{ik}$. We also assume that data are grouped so that for the i th setting of the predictor variables, there are m_i observations, $i = 1, 2, \ldots, n$. $M = \sum_{i=1}^{n} m_i$ is the total number of observations. The response variable is $y_i = \sum_{k=1}^{m_i} z_{ik}$, where z_{ik} is the k th observation (0 or 1) in i th predictor variable settings, y_i follows a binomial distribution with parameters m_i, and π_i. Albert and Anderson [33] proposed MLE method to estimate the model parameters. They used the following likelihood function:

$$L(\pi, y) = \prod_{i=1}^{n} \binom{m_i}{y_i} [\pi_i]^{y_i} [1-\pi_i]^{m_i - y_i}, \tag{3}$$

where $\pi = (\pi_1, \pi_2, ..., \pi_n)^T$ and $y = (y_1, y_2, \ldots, y_n)^T$. Taking the logarithm of Eq. 3 and using $\eta_i = X_i^T\beta = \sum_{k=1}^{p} \beta_k x_{ik} = \log\frac{\pi_i}{1-\pi_i}$, one can reexpress the log-likelihood as

$$l(\beta, y) = \sum_{i=1}^{n} \log\binom{m_i}{y_i} + \sum_{i=1}^{n}\sum_{k=1}^{p} y_i \beta_k x_{ik} - \sum_{i=1}^{n} m_i \log \left[1 + \exp\left(\sum_{k=1}^{p} \beta_k x_{ik}\right)\right], \tag{4}$$

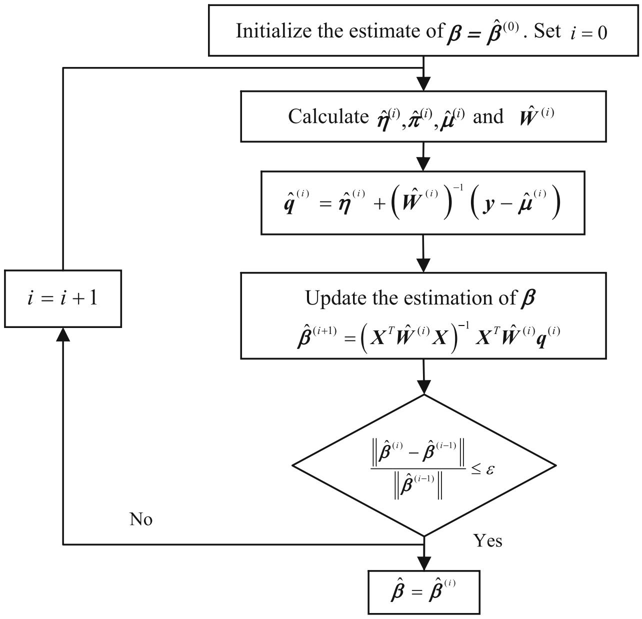

Fig. 1 The procedure of estimation of logistic regression parameters

Taking derivative of Eq. 4 with respect to β, and using iterative-weighted least-square estimation method suggested by McCullagh and Nelder [34], the logistic regression parameters can be estimated as follows:

$$\widehat{\beta} = \left(X^T\widehat{W}X\right)^{-1}X^T\widehat{W}q, \tag{5}$$

In Eq. 5, $X = (X_1, X_2, \ldots, X_n)^T$ is an $n \times p$ matrix. $\widehat{W} = \mathrm{diag}[m_1\widehat{\pi}_1(1-\widehat{\pi}), m_2\widehat{\pi}_2(1-\widehat{\pi}_2), \ldots, m_n\widehat{\pi}_n(1-\widehat{\pi}_n)]$ is an $n \times n$ diagonal matrix and $q = \widehat{\beta} + \widehat{W}^{-1}(y - \widehat{\mu})$. The procedure iterations are described in the following flowchart (Fig. 1):

McCullagh and Nelder [34] proved that as n becomes large or m_i is constant, $\widehat{\beta}$ is distributed asymptotically as a p-dimensional normal distribution $N_p\left(\beta, (X^TWX)^{-1}\right)$. This procedure will be used in MLE change point estimator described in Section 3.

3 Process behavior model and derivation of the MLE

In this model, it is assumed that the underlying process initially operates in a state of statistical control, with observations coming from a binomial distribution with the known parameters m_i and π_i; so, the mass probability function is $f(y_{ij}) = \binom{m_i}{y_{ij}}\pi_i^{y_{ij}}(1-\pi_i)^{m_i - y_{ij}}$, where y_{ij} is the value of the i th response variable in the j th profile. Following an unknown profile τ (known as the process change point), the process changes to an unknown out-of-control state such that the behavior in π_i can be described by $\pi_{i1}(\pi_{i1} > \pi_{i0})$ and it remains at the new level until the source of the assignable cause is identified and eliminated, i.e., during the formulation of profiles $j = 1, 2, \ldots, \tau$ the process parameter π_i is equal to its known in-control value. For profiles $j = \tau+1, \tau+2, \ldots, L$ the parameter π_i become equal to some unknown parameter π_{i1}, where L is the last profile sampled in which the control chart signaled an out-of-control state. Two unknown parameters in model are τ and π_{i1}, representing the last profile taken from an in-control process and the out-of-control process parameter, respectively.

This model can be used to derive the MLE of τ. We will denote the MLE of the proposed change point estimator as $\widehat{\tau}$. Assuming a process change point at τ, the likelihood function is given by

$$L(\tau, \pi_{i1}|\boldsymbol{y}) = \prod_{j=1}^{L}\prod_{i=1}^{n}\binom{m_i}{y_{ij}}\prod_{j=1}^{\tau}\prod_{i=1}^{n}\left[\frac{\pi_{i0}}{1-\pi_{i0}}\right]^{y_{ij}}[1-\pi_{i0}]^{m_i} \prod_{j=\tau+1}^{L}\prod_{i=1}^{n}\left[\frac{\pi_{i1}}{1-\pi_{i1}}\right]^{y_{ij}}[1-\pi_{i1}]^{m_i}, \tag{6}$$

The MLE of τ is the value of τ that maximizes the likelihood function in Eq. 6 or, equivalently, its logarithm. Taking the logarithm of Eq. 6

$$\begin{aligned} LnL(\tau, \pi_{i1}|\boldsymbol{y}) = &\sum_{j=1}^{L}\sum_{i=1}^{n}Ln\binom{m_i}{y_{ij}} + \sum_{j=1}^{\tau}\sum_{i=1}^{n}y_{ij}Ln\left[\tfrac{\pi_{i0}}{1-\pi_{i0}}\right] \\ &+ \sum_{j=1}^{\tau}\sum_{i=1}^{n}m_iLn(1-\pi_{i0}) + \sum_{j=\tau+1}^{L}\sum_{i=1}^{n}y_{ij}Ln\left[\tfrac{\pi_{i1}}{1-\pi_{i1}}\right] \\ &+ \sum_{j=\tau+1}^{L}\sum_{i=1}^{n}m_iLn(1-\pi_{i1}), \end{aligned} \tag{7}$$

As the values of τ and π_{i1} are unknown, they must be estimated. This involves finding estimates for τ and π_{i1} which maximize the logarithm of likelihood function in Eq. 7, denoted as $\widehat{\tau}$ and $\widehat{\pi}_{i1}$. Obtaining this expression is not a trivial task. The partial derivative of Eq. 7 with respect to π_{i1} is given by

$$\frac{\partial LnL(\tau, \pi_i|y)}{\partial \pi_{i1}} = \sum_{j=\tau+1}^{L}\sum_{i=1}^{n}\frac{y_{ij}}{(1-\pi_{i1})\pi_{i1}} - \sum_{j=\tau+1}^{L}\sum_{i=1}^{n}m_i\frac{1}{(1-\pi_{i1})}, \tag{8}$$

In Eq. 8, there is no closed-form solution for π_{i1}. Thus, a numerical method such as Newton–Raphson is needed for finding successively better approximations to the roots of a real valued function. Perry and Pignatiello [12] used this method to find the MLE of the slope parameter, in Poisson process. Accordingly, we use Newton's method to find the MLE of the out-of-control parameter, π_{i1}, and denote it as $\widehat{\pi}_{i1}$. By obtaining $\widehat{\pi}_{i1}$, replacing it in Eq. 8 and calculating the logarithm of the likelihood function in Eq. 7 for all possible change point values, the MLE of the change point τ is the value which maximize the expression and can be written as follows:

$$\widehat{\tau} = \arg\max\left\{ \sum_{j=1}^{\tau}\sum_{i=1}^{n} y_{ij} Ln\left[\frac{\pi_{i0}}{1-\pi_{i0}}\right] + \sum_{j=1}^{\tau}\sum_{i=1}^{n} m_i Ln(1-\pi_{i0}) + \sum_{j=\tau+1}^{L}\sum_{i=1}^{n} y_{ij} Ln\left[\frac{\widehat{\pi}_{i1}}{1-\widehat{\pi}_{i1}}\right] + \sum_{j=\tau+1}^{L}\sum_{i=1}^{n} m_i Ln(1-\widehat{\pi}_{i1}) \right\}, \tag{9}$$

where $\widehat{\tau}$ is the MLE of the change point. Note that the arg max stands for the argument of the maximum, that is to say, the set of points of the given argument by which the given function obtains its maximum value.

Yeh et al. [32] introduced five Hotelling control charts to monitor binary profiles in phase I. The plotting statistic for profile j is defined as

$$T_j^2 = \left(\widehat{\beta}_j - \beta\right)^T S^{-1}\left(\widehat{\beta}_j - \beta\right), \tag{10}$$

where $\widehat{\beta}_j$ is estimator of the logistic regression parameters in j th profile and S is the variance covariance matrix of $\widehat{\beta}_j$. Any of these T^2 charts presents a different way to estimate β and S. They showed T_I^2 control chart which estimates the covariance matrix by averaging the covariance estimates of each given sample, is more effective in detecting both step and drift changes. This control chart also can be used in phase II. So we used T_I^2 control chart to detect the out-of-control state in phase II. The upper control limit for the proposed control chart is equal to $\chi^2_{2,\alpha}$, the α percentile points of the chi-square distribution with 2 degrees of freedom. Covariance matrix in phase II is also computed using the following equation:

$$\sum = (\mathrm{X}^T\mathrm{WX})^{-1}, \tag{11}$$

where W is equal to $\mathrm{diag}\{m_1\pi_1(1-\pi_1), m_2\pi_2(1-\pi_2), \cdots, m_n\pi_n(1-\pi_n)\}$.

Whenever the T_I^2 control chart signals an out-of-control state, the real time of a change can be estimated via Eq. 9.

4 Performance evaluation

4.1 The simulation settings

In this section, we present simulation results, using Monte Carlo simulation. For this simulation study, we assumed that the number of predictor variables in logistic regression profile is two (p=2). Thus, the link function is simplified as $g(\pi_i) = \beta_1 + \beta_2 x_i$, where β_1, β_2 are respectively the intercept and the slope of the regression function and is shown by the vector $\beta = (\beta_1, \beta_2)^T$. Also, we set the matrix X as:

$$X = \begin{pmatrix} 1 & 1 & \dots & 1 \\ \log(0.1) & \log(0.2) & \dots & \log(0.9) \end{pmatrix}^T.$$

It is assumed that the number of experiments in each predictor variable is constant and equal to 50, (m_i=50 for i=1,2,…,9) and the in-control π_{i0} is $(0.04, 0.06, 0.13, 0.27, 0.48, 0.68, 0.82, 0.89, 0.91)^T$. The initial β is estimated as $(2.5,\ 3.46)^T$ from historical dataset in phase I. The covariance matrix of the logistic regression parameters ($\sum$) in phase II is computed by Eq. 11 as follows:

$$\sum = (\mathrm{X}^T\mathrm{WX})^{-1} = \begin{pmatrix} 0.06627 & 0.07693 \\ 0.07693 & 0.1179 \end{pmatrix}.$$

The upper control limit for the T_I^2 control chart is equal to $\chi^2_{2,0.05} = 5.99$.

A Monte Carlo simulation study is accomplished to examine the performance of the estimator. In this study, the process change point was considered at τ=50. During the formation of profiles j=1,2,…,50, the process parameter is equal to its known in-control value of π_{i0}. Therefore, for these profiles, the independent observations were randomly generated from a binomial distribution with parameters 50 and π_{i0}. Starting at profile 51, observations are simulated from the out-of-control process with π_{i1} until the T_I^2 control chart signals an out-of-control state. At this time, the change point estimator is used and the real time of the process change is determined. This procedure is repeated 10,000 times for each of the step changes considered in the paper.

4.2 Example 1

Suppose an out-of-control process whose parameter vector π_i changes from π_{i0} to $\pi_{i1} = \pi_{i0} + \alpha(\pi_{i0})$, where α=0.01, 0.02, 0.03, 0.05, 0.07, and 0.09. In other words, in this example, we assume that step changes in the mean of response variables in different levels of explanatory variable are not identical and depend on the magnitude of the mean of response variables.

The results are summarized in Tables 1 and 2. Table 1 shows the expected length of each simulation run $E(L)$which is the expected value of the number of samples taken until

Table 1 Expected number of samples until the signal, the expected value, and standard deviations of the change point estimator with 10,000 simulations runs when τ=50

α	0.01	0.02	0.03	0.05	0.07	0.09
$E(L)$	60.51	57.86	56.1	53.18	51.85	51.23
$\overline{\widehat{\tau}}$	48.52	49.14	49.31	49.64	49.90	50.07
$se(\widehat{\tau})$	5.77	4.14	3.12	1.56	0.59	0.09

Table 2 Estimated precision performances over a range of π_i values with 10,000 simulations runs when τ=50

α	0.01	0.02	0.03	0.05	0.07	0.09
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert=0)$	0.21	0.40	0.57	0.78	0.89	0.96
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 1)$	0.34	0.55	0.74	0.90	0.95	099
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 2)$	0.42	0.63	0.82	0.95	0.98	1.00
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 3)$	0.48	0.70	0.87	0.97	1.00	
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 4)$	0.55	0.76	0.89	0.98		
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 5)$	0.59	0.79	0.91	1.00		
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 6)$	0.64	0.82	0.92			
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 7)$	0.68	0.84	0.93			

the first alarm is given by the control chart, i.e., $E(L)$=ARL +50. Table 1 also shows the average change point estimate ($\overline{\widehat{\tau}}$) and the standard deviation of the change point estimator ($se(\widehat{\tau})$) under different magnitude of the step changes considered. Because the actual change is at time 50, the average change point estimate, $\overline{\widehat{\tau}}$, should be close to 50.

As shown in Table 1, for step rate parameter equal to 0.03, the expected number of samples taken until the signal is 56.1, the average change point estimate is 49.31, and the standard deviation of the change point estimator is 3.12. The performance of change point estimator is acceptable when the small changes in the process parameter occur; however, as the magnitude of the step change increases, the performance of the estimator improves significantly. Figure 2 also shows that the expected number of samples taken until the signal and average change point estimator are becoming near to 51 and 50, respectively as α increases. Furthermore, the standard deviation of the change point estimator, that is shown shady, is becoming smaller.

Table 2 shows the results of proportion of 10,000 simulation runs that the estimator lies within a specified tolerance of the real change point value. The results provided in Table 2 are similar to those provided in Table 1, For example, if α=0.01, the estimated probability that $\widehat{\tau}$ lies within 1 or less from the real change point is 0.34. Also, in this case, in 21% of the simulation runs the estimator correctly identifies the real time of the change. Table 2 shows that the performance of the MLE estimator improves significantly with increases in magnitude of the step change, α.

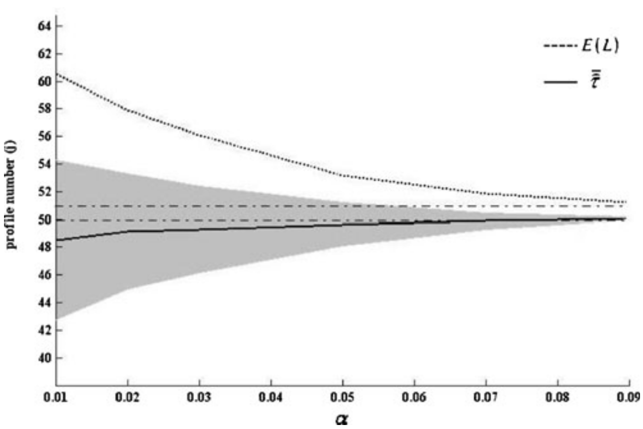

Fig. 2 The performance of the MLE estimator

Table 3 Expected number of samples until the signal, the expected value, and standard deviations of the change point estimator with 10,000 simulations runs when τ=50

δ	0.01	0.02	0.03	0.04	0.05	0.06
$E(L)$	59.42	54.81	52.83	51.69	51.30	51.11
$\overline{\widehat{\tau}}$	53.15	51.38	50.63	50.24	50.07	50.02
$se(\widehat{\tau})$	3.61	2.05	1.21	0.71	0.29	0.14

4.3 Example 2

As the second example, we set another type of step change in the former example. Suppose an out-of-control process whose parameter vector π_i changes from π_{i0} to $\pi_{i1}=\pi_{i0}+\delta$, where δ= 0.01,0.02,0.03,0.04,0.05, and 0.06. In this example, we assume that step changes in the mean of response variable in different levels of explanatory variable are identical. The results are given in Tables 3 and 4 as well as Fig. 3. Table 3 and Fig. 3 show accuracy performances of the change point estimator and Table 4 shows the results of proportion of 10,000 simulation runs that the estimator lies within a specified tolerance of the real change point value. Similar results are obtained in this example which shows the acceptable performance of the proposed change point estimator.

5 Conclusions

In many industrial applications of profiles monitoring, the response variable is discrete such as binary, which is often modeled as a logistic regression of an explanatory variable.

Table 4 Estimated precision performances over a range of π_i values with 10,000 simulations runs when τ=50

δ	0.01	0.02	0.03	0.04	0.05	0.06
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert=0)$	0.30	0.48	0.66	0.85	0.93	0.97
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 1)$	0.50	0.68	0.83	0.95	0.99	1.00
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 2)$	0.58	0.79	0.92	0.98	1.00	
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 3)$	0.66	0.87	0.96	0.99		
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 4)$	0.72	0.92	0.98	0.99		
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 5)$	0.77	0.95	0.99	1.00		
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 6)$	0.81	0.96	0.99			
$\widehat{p}(\lvert\widehat{\tau}-\tau\rvert\leq 7)$	0.86	0.97	1.00			

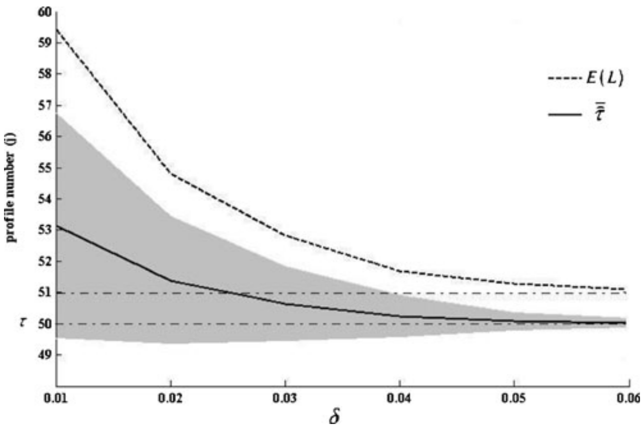

Fig. 3 The performance of the MLE estimator for example 2

The main motivation of this paper is to identify the real time of a step change to find the root cause of a problem as quick as possible and then do a corrective action. We provided an MLE method to estimate the change point in phase II monitoring of logistic regression profiles, when the type of change is step change. The results showed that the performance of the proposed estimator is fine to identify the real time of change point under different magnitude of step change.

Developing this method to the other distributions of the exponential family such as Poisson and Gamma would be future researches in this area. Furthermore, the other types of the change, including drift changes and isotonic changes could be investigated by researchers.

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