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Estimating the Change Point of Binary Profiles with a Linear Trend Disturbance

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ABSTRACT

Identification of a real time of a change in a process, when an out-of-control signal is present is significant. This may reduce costs of defective products as well as the time of exploring and fixing the cause of defects. Another popular topic in the Statistical Process Control (SPC) is profile monitoring, where knowing the distribution of one or more quality characteristics may not be appropriate for discussing the quality of processes or products.

One, rather, uses a relationship between a response variable and one or more explanatory variable for this purpose. In this paper, the concept of Maximum Likelihood Estimator (MLE) applied to estimate of the change point in binary profiles, when the type of change is drift. Simulation studies are provided to evaluate the effectiveness of the change point estimator.

1. Introduction

Statistical Process Control (SPC) is used to monitor and reduce the variation of a process. Control charts are the most important tools in SPC which are used to monitor quality characteristics. These charts can detect any changes or shifts in a process; however, a shift usually occurs much earlier before it is detected. When a control chart signals a special cause, quality engineers should identify and remove the cause(s) of variation and return the process to in-control state. However, knowing when a process has changed would help quality engineers to limit the time window within which they should search for assignable causes. Consequently, the assignable causes can be identified sooner and corrective action can be implemented more quickly. Identifying the real time of the process change is known as change-point estimation problem.

Change point problems are mainly classified according to change types including step, drift and isotonic shifts. To find the real time of a change, many authors have suggested several methods such as Maximum Likelihood Estimator (MLE), Cumulative Sum (CUSUM), Exponentially Weighted Moving Average (EWMA) and intelligent method, (artificial network, clustering and decision tree). For example Pignatiello and Samuel [1- 4] proposed a Maximum Likelihood Estimator in different control charts to find the real time of change point under a step shift. Perry and Pignatiello [5, 6] used this method to estimate the change point in the mean of normal and poisson distribution with a linear trend disturbance, respectively.

In the area of SPC, usually the quality of a process or a product was represented by the distribution of one (or more) quality characteristic and monitored by univariate (or multivariate) control chart. However, Kang and Albin [7] presented a popular topic with widespread application in SPC namely, profiles monitoring, in which a relationship between a response

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variable and one or more independent variables, known as profiles is monitored over time.

Scientists classify profiles based on the type of relationships into the linear (simple, multiple and polynomial), nonlinear and geometric profiles. Profiles are studied in Phases I and II. In Phase I, Mestek et al. [8] used a T^2 based control charts to monitor the regression parameters of a simple linear profiles. Mahmoud and Woodall [9] used a global F-test for monitoring the regression coefficients in conjunction with a univariate control chart to monitor the variance. Mahmoud et al. [10] applied a likelihood ratio test to monitor simple linear profiles. In Phase II, Kang and Albin [7] proposed two methods including a multivariate T^2 chart and a combination of EWMA-R chart to monitor simple linear profiles.

Kim et al. [11] recommended three independent univariate EWMA control charts to monitor shifts in parameters of a simple linear profile.

Identifying the change point in profiles has been studied by some researchers. Mahmoud et al. [10] 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. [12] proposed a method based on likelihood ratio statistics to find the change point in parameters of a simple linear profile in Phase II. Kazemzadeh et al. [13] used the same method to estimate the change point in polynomial profiles under a step shift in Phase I.

Note that the change point problem in profile data is under a different sampling framework from that of the other models. In the profile applications, multiple data sets are collected over time in a functional data sampling framework and a possible change point is take place after any data set.

Most researches in profile monitoring, assume 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 non defective) or countable (as the number of defect products or number of patients in a hospital). Yeh et al. [14] studied binary profiles in Phase I. They proposed different T^2 control charts for monitoring logistic regression profiles. Shang et al. [15] proposed a control scheme based on EWMA-GLM to monitor the relationship between the binary response and random explanatory variables in Phase II. Their approach assumes that explanatory variables are random variable and takes different values in each profile sample.

To the best of our knowledge, Only Sharafi et al. [16] suggested a method to identify the real time of a step change in Phase II monitoring of binary profiles and there is no more researches in this area. In this paper we propose a Maximum Likelihood Estimator to find the real time of a change in Phase II monitoring of logistic regression profiles.

Here, we assumed that the type of the disturbance is drift. The rest of the 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 x changes, and we replace π by $\pi(x)$.

For n independent observations, the number of successes has the binomial distribution specified by the index n and parameter π. 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 logistic regression model, there are n independent experimental sets, with p predictor variables for each set, which is shown by $\mathbf{x}_i = (x_{i1}, x_{i2},, x_{ip})^T$ as well as corresponding Bernoulli response variables namely z_i for $i=1,2,...,n$. The probability of success in each set is denoted by π_i and each π_i is a function of $\mathbf{x}_\mathrm{i}$. In the logistic regression model this function is characterized by the link function $g\left(\pi_i\right)$, defined as:

$$g\left(\pi_i\right) = \frac{\log\left(\pi_i\right)}{1-\log\left(\pi_i\right)} = \beta_1 x_{i1} + \beta_2 x_{i2} + ... + \beta_p x_{ip} \qquad (1)$$

where $\boldsymbol{\beta} = \left(\beta_1, \beta_2, ..., \beta_p\right)^T$ is the model parameters vector. It is usual to set $x_{i1} \equiv 1$ in order that β_1 be the intercept of the model. Equation (1) simplifies to:

$$\pi_i = \frac{\exp(\mathbf{x}_\mathrm{i}^\mathrm{T}\boldsymbol{\beta})}{1+\exp(\mathbf{x}_\mathrm{i}^\mathrm{T}\boldsymbol{\beta})} = \frac{\exp(\eta_i)}{1+\exp(\eta_i)}. \qquad (2)$$

In this equation $\eta_i = \mathbf{x}_\mathrm{i}^\mathrm{T}\boldsymbol{\beta} = \sum_{k=1}^{p} \beta_k x_{ik}$. We also assume that data are grouped so that for the i th setting of the predictor variables, there are m_i observations,

$i=1,2,...,n$. $M=\sum_{i=1}^{n} m_i$ is total number of observations. The response variable is $y_i=\sum_{k=1}^{m_i} z_{ik}$, where z_{ik} is the kth observation (0 or 1) in ith predictor variable settings, y_i follows a binomial distribution with parameters m_i, π_i. Albert and Anderson [17] proposed MLE method to estimate the model parameters for this purpose. They used the following likelihood function:

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

Where $\boldsymbol{\pi}=\left(\pi_1,\pi_2,...,\pi_n\right)^T$ and $\mathbf{y}=\left(y_1,y_2,...,y_n\right)^T$ Taking the logarithm of the Equation (3) and using $\eta_i=\mathbf{x}_i^{\mathrm{T}}\boldsymbol{\beta}=\sum_{k=1}^{p}\beta_k x_{ik}=\log\frac{\pi_i}{1-\pi_i}$, one can reexpress the log-likelihood as:

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

Taking derivative of Equation (4) with respect to $\boldsymbol{\beta}$, and using iterative weighted least square estimation method suggested by McCullagh and Nelder [18], the logistic regression parameters can be estimated as follows:

$$\hat{\boldsymbol{\beta}}=\left(\mathbf{X}^T\hat{\mathbf{W}}\mathbf{X}\right)^{-1}\mathbf{X}^T\hat{\mathbf{W}}\mathbf{q} \qquad (5)$$

In the Equation (5) $\mathbf{X}=\left(\mathbf{x}_1,\mathbf{x}_2,...,\mathbf{x}_n\right)^T$, $\hat{\mathbf{W}}=diag\left[m_1\hat{\pi}_1\left(1-\hat{\pi}_1\right),m_2\hat{\pi}_2\left(1-\hat{\pi}_2\right),...,m_n\hat{\pi}_n\left(1-\hat{\pi}_n\right)\right]$, $\mathbf{q}=\hat{\boldsymbol{\beta}}+\hat{\mathbf{W}}^{-1}\left(\mathbf{y}-\hat{\boldsymbol{\mu}}\right)$ and $\hat{\boldsymbol{\mu}}=\left(m_1\hat{\pi}_1,m_2\hat{\pi}_2,...,m_n\hat{\pi}_n\right)^T$. The procedure iterations is described in the figure I.

McCullagh and Nelder [18] proved that as n becomes large or m_i is constant, $\boldsymbol{\beta}$ is distributed asymptotically as a p-dimensional normal distribution $N_p\left(\boldsymbol{\beta},\left(\mathbf{X}^T\mathbf{W}\mathbf{X}\right)^{-1}\right)$. This procedure will be used in MLE change point estimator described in Section 3.

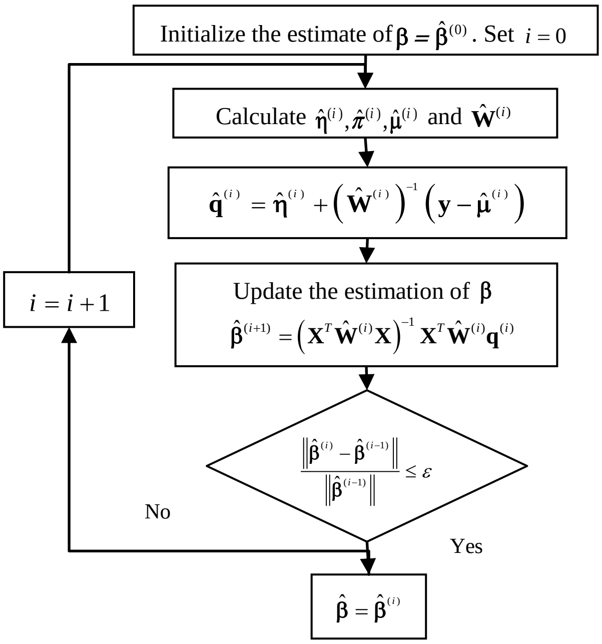

Fig. I. The procedure of estimation of logistic regression parameters

3. MLE Change Point Estimator

Here, it is assumed that the underlying process initially operates in a state of statistical control, with observations coming from a poisson distribution with the known parameters $\boldsymbol{\beta}=\boldsymbol{\beta}_0$ ($\boldsymbol{\beta}$ is a p-dimensional vector); so, the mass probability function is $f\left(y_{ij}\right)=\binom{m_i}{y_{ij}}\pi_i^{y_{ij}}\left(1-\pi_i\right)^{m_i-y_{ij}}$ where y_{ij} is the value taken by the response variable for the i th value of the predictor variable in the j th profile.

The change type is also assumed to be drift or linear trend change in the parameter π_i. Consider an in-control process with independent observations coming from a binomial distribution with parameters m_i and π_i. After elapsing an unknown amount of time, the parameter π_i changes from its in control state of π_{i0} to an unknown out-of-control state of π_{i1}, $\pi_{i1}>\pi_{i0}$, and the function of π_{i1} is given as:

$$\pi_{i1}=\pi_{i0}+b\left(j-\tau\right)\quad j=\tau+1,\tau+2,...,T, \qquad (6)$$

where b is the slope (or magnitude) of the linear trend disturbance in π_i.

During the formulation of profiles $j=1,2,...,\tau$ the process parameter π_i is equal to its known in-control value. For profiles $j=\tau+1,\tau+2,...,T$ the parameter π_i become larger with linear trend b and equal to some unknown value $\pi_{i1}=\pi_{i0}+b\left(j-\tau\right)$, where T is the last profile sampled in which the control chart signaled an out-of-control state. Two unknown parameters in model are τ and b, representing the last profile taken from an in-control process and the rate of the linear trend, respectively. To estimate these unknown parameters, this paper used a MLE approach, similar to Perry and Pignatiello [6]. We denote the MLE estimator of the change point as $\hat{\tau}$. The likelihood function is as follows:

$$L(\tau,b|\mathbf{y})=\prod_{j=1}^{\tau}\prod_{i=1}^{n}\binom{m_i}{y_{ij}}\prod_{j=1}^{\tau}\prod_{i=1}^{n}\left[\frac{\pi_{i0}}{1-\pi_{i0}}\right]\left[1-\pi_{i0}\right]^{m_i}$$
$$\prod_{j=\tau+1}^{T}\prod_{i=1}^{n}\left[\frac{\pi_{i1}+b\left(j-\tau\right)}{1-\pi_{i1}-b\left(j-\tau\right)}\right]^{y_{ij}}\left[1-\pi_{i1}-b\left(j-\tau\right)\right]^{m_i} \tag{7}$$

The MLE of τ is the value of τ that maximizes the likelihood function in Equation (7). Taking the logarithm of Equation (7).

$$Ln\ L(\tau,b|\boldsymbol{y})=\sum_{j=1}^{\tau}\sum_{i=1}^{n}Ln\binom{m_i}{y_{ij}}+\sum_{j=1}^{\tau}\sum_{i=1}^{n}y_{ij}Ln\left[\frac{\pi_{i0}}{1-\pi_{i0}}\right]+$$
$$\sum_{j=1}^{\tau}\sum_{i=1}^{n}m_iLn\left(1-\pi_{i0}\right)+\sum_{j=\tau+1}^{T}\sum_{i=1}^{n}y_{ij}Ln\left[\frac{\pi_{i1}+b\left(j-\tau\right)}{1-\pi_{i1}-b\left(j-\tau\right)}\right] \tag{8}$$
$$+\sum_{j=\tau+1}^{T}\sum_{i=1}^{n}m_iLn\left[1-\pi_{i1}-b\left(j-\tau\right)\right],$$

To determine the unknown parameters in Equation (8), (τ and b), an expression is required for b in terms of τ which maximize the log-likelihood function in Equation (8), defined as $\hat{b}_\tau$. Obtaining this expression is not a trivial task. The partial derivative of Equation (8) with respect to b is given by:

$$\frac{\partial Ln\ L(\tau,b|\boldsymbol{y})}{\partial b}=$$
$$\sum_{j=\tau+1}^{T}\sum_{i=1}^{n}y_{ij}\left[\frac{\left(j-\tau\right)}{\left[1-\pi_{i1}-\hat{b}_\tau\left(j-\tau\right)\right]\left[\pi_{i1}+\hat{b}_\tau\left(j-\tau\right)\right]}\right] \tag{9}$$
$$-\sum_{j=\tau+1}^{T}\sum_{i=1}^{n}m_i\left[\frac{\left(j-\tau\right)}{\left[1-\pi_{i1}-\hat{b}_\tau\left(j-\tau\right)\right]}\right]$$

In Equation (9) there is no closed-form solution for b. Perry and Pignatiello [6] proposed the Newton's method (also known as the Newton–Raphson method) to find the MLE of the rate parameter, b. Newton's method is one of the Numerical analysis which is used to find successively better approximations to the roots of a function. We use Newton's method to find the MLE of the rate parameter, b, and denote it as $\hat{b}_\tau$. Substituting $\hat{b}_\tau$ for b in Equation (8) and computing Equation (8) over all possible change points τ in search of the maximum log-likelihood function yields.

$$\hat{\tau}=\arg\ \max\ \{\sum_{j=1}^{\tau}\sum_{i=1}^{n}y_{ij}Ln\left[\frac{\pi_{i0}}{1-\pi_{i0}}\right]+$$
$$\sum_{j=1}^{\tau}\sum_{i=1}^{n}m_iLn\left(1-\pi_{i0}\right)$$
$$+\sum_{j=\tau+1}^{T}\sum_{i=1}^{n}y_{ij}Ln\left[\frac{\pi_{i1}+b\left(j-\tau\right)}{1-\pi_{i1}-b\left(j-\tau\right)}\right] \tag{10}$$
$$+\sum_{j=\tau+1}^{T}\sum_{i=1}^{n}m_iLn\left[1-\pi_{i1}-b\left(j-\tau\right)\right]\}$$

where $\hat{\tau}$ is the MLE for the last profile taken from the in-control process. Whenever this chart signals an out-of-control state, the real time of a change can be estimated via Equation (10).

Yeh et al. [14] introducted five Hotelling T^2 control charts to monitor binary profiles in Phase I. The plotting statistic for profile j is defined as:

$$T_j^2=\left(\hat{\boldsymbol{\beta}}_j-\boldsymbol{\beta}\right)^T\boldsymbol{S}^{-1}\left(\hat{\boldsymbol{\beta}}_j-\boldsymbol{\beta}\right)\ , \tag{11}$$

where $\hat{\boldsymbol{\beta}}_j$ is estimator of the logistic regression parameters in j th profile and $\boldsymbol{S}$ is the variance covariance matrix of $\hat{\boldsymbol{\beta}}_j$. Any of these T^2 charts uses a different method to estimate the mean vector and covariance matrix. They showed T_I^2 control chart which estimate the covariance matrix by averaging the covariance estimates of each given sample, provides more effective way to detect step shifts and drift. These control charts 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. Covariance matrix in Phase II is computed using the following equation:

$$\Sigma=(\mathbf{X}^T\mathbf{W}\mathbf{X})^{-1}\ , \tag{12}$$

where $\mathbf{W}$ is equal to $diag\{m\pi_1(1-\pi_1),m\pi_2(1-\pi_2),\cdots,m\pi_n(1-\pi_n)\}$. The upper control limit for the proposed control chart is also equal to $\chi^2_{2,\alpha}$,the α percentile points on the chi-square distribution with 2 degrees of freedom.

4. Performance of the MLE Estimator

To estimate the performance of the MLE estimator, an example is given. In this example, number of explanatory variables is equal to 2, (*p*=2). Thus the link function is simplified as $g(\pi_i) = \beta_1 + \beta_2 x_i$, where β_1 and β_2 are the intercept and the slope of the regression function respectively and is shown by the vector $\boldsymbol{\beta} = (\beta_1, \beta_2)^T$ We set the matrix $\boldsymbol{X}$ as:

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

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 $\boldsymbol{\beta}$ is estimated as $(2.5, 3.46)^T$ from historical dataset in Phase I. The upper control limit for the T_I^2 control chart is equal to $\chi^2_{2,0.005} = 10.59$. The covariance matrix of the logistic regression parameters (Σ) in Phase II is computed by Equation (12) as follows:

$$\Sigma = (X^T W X)^{-1} = \begin{pmatrix} 0.06627 & 0.07693 \\ 0.07693 & 0.1179 \end{pmatrix}$$

Now, suppose an out-of-control process whose parameter vector π_i shifts from π_{i0} to $\pi_{i1} = \pi_{i0} + b(j - \tau)$. A Monte Carlo simulation study is accomplished to examine the performance of the estimator. The change point is simulated at profile 50 ($\tau = 50$). For profiles $j = 1, 2, ..., 50$ the independent observations is produced by binomial distribution with parameters 50 and π_{i0}. Starting at profile 51, observations are simulated from the out-of-control process with $\pi_{i1} = \pi_{i0} + b(j - 50)$ until the T_I^2 chart signals an out-of-control.

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 magnitude of the change under study, which is described in the figure 2.

The results are summarized in Tables 1 and 2 and Figure III. Table I shows the expected length of each simulation run $E(T)$ which is the expected value of the number of samples taken until the first alarm is given by the control chart, i.e. $E(T) = ARL + 50$. Table I also shows the average change point estimate and the standard deviation of the change point estimator under different magnitude of the shifts considered. Because the actual change is at time 50, the average change point estimate, $\bar{\hat{\tau}}$, should be close to 50.

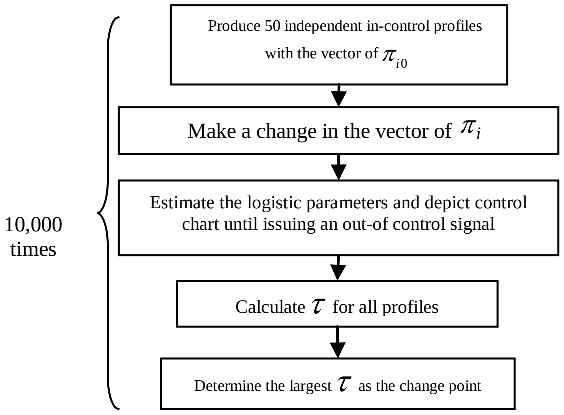

Fig. 2. The flowchart of the simulation procedure

Tab. 1. Expected number of samples until the signal and standard deviations of the change point estimators with 10,000 simulations runs when $\tau = 50$

b	$E(T)$	$\bar{\hat{\tau}}$	$se(\hat{\tau})$
0.003	56.13	51.82	2.39
0.005	55.01	51.21	1.73
0.007	53.86	50.86	1.32
0.01	53.02	50.58	1.01
0.015	52.43	50.44	0.74
0.02	52.04	50.29	0.51
0.025	51.72	50.21	0.41

As shown in Table I, for drift rate parameter equal to 0.003 the expected number of samples taken until the signal is 56.13, the average change point estimate is 51.82 and the standard deviation of the change point estimator is 2.39. Moreover, the performance of the estimator improves significantly with increases in magnitude of the drift rate parameter (b). Figure III also indicates this issue. As perceived from this figure, with increasing b, the expected number of samples taken until the signal and average change point estimator are becoming near to 51 and 50, respectively. Furthermore, the standard deviation of the change point estimator, that is shown shady, is becoming smaller.

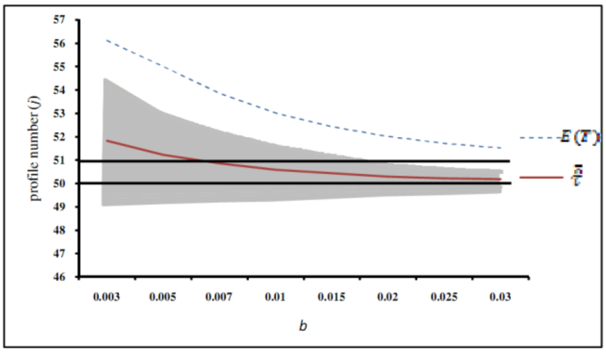

Fig. 3. The performance of the MLE estimator

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. For example if $b = 0.01$, the estimated probability that $\hat{\tau}$ lies within 1 or less from the real change point is 0.81. Also in this case, in 46% 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 shift in the slope, b .

Tab. 2. Estimated precision performances over a range of π_i with 10,000 simulations runs when $\tau = 50$

b	0.003	0.005	0.007	0.01	0.015	0.02	0.025
$\hat{p}(\lvert\hat{\tau}-\tau\rvert = 0)$	0.21	0.30	0.36	0.46	0.57	0.72	0.83
$\hat{p}(\lvert\hat{\tau}-\tau\rvert \le 1)$	0.47	0.59	0.70	0.81	0.85	0.97	0.99
$\hat{p}(\lvert\hat{\tau}-\tau\rvert \le 2)$	0.64	0.81	0.89	0.94	0.99	1.00	1.00
$\hat{p}(\lvert\hat{\tau}-\tau\rvert \le 3)$	0.79	0.92	0.98	1.00	1.00		
$\hat{p}(\lvert\hat{\tau}-\tau\rvert \le 4)$	0.90	0.98	1.00				
$\hat{p}(\lvert\hat{\tau}-\tau\rvert \le 5)$	0.97	1.00					
$\hat{p}(\lvert\hat{\tau}-\tau\rvert \le 6)$	1.00						

5. Conclusions

In this paper, we provided the MLE method to estimate the change point in phase II monitoring of logistic regression profiles, when the type of change is drift. The results of this study showed that the performance of the proposed estimator is fine to identify the real time of change point under different magnitude of drift rate.

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

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