

Research

An Improved Run-to-Run Process Control Scheme for Categorical Observations with Misclassification Errors

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When product quality characteristics are evaluated and assigned to exclusive categories, measurement errors (misclassification of products) always exist unless a perfect measurement system is used to identify the categories. In run-to-run (R2R) process control, a categorical controller has been developed for process adjustments with categorical variables. However, if process outputs are misclassified, an adjustment bias will be introduced by the controller. In this study, an improved categorical R2R controller that utilizes the misclassification probabilities to decrease process deviation is proposed. Simulation results show that the proposed controller exhibits better performance when misclassification exists. Copyright © 2008 John Wiley & Sons, Ltd.

KEY WORDS: misclassification; categorical variable; categorical R2R controller; run-to-run process

1. INTRODUCTION

Run-to-run (R2R) control refers to the actions taken to adjust controllable variables or process inputs in a new run to maintain process outputs close to the target^{1,2}. R2R control algorithms are especially important for high-tech manufacturing industries, such as semiconductor manufacturing. Versatile R2R control algorithms have been developed^{3–10}. Among others, the EWMA controller, the double EWMA controller, the self-tuning controller and various extensions of these controllers have become prevalent in industrial practice.

The performance of R2R controllers has been studied extensively by Del Castillo and Hurwitz¹ under the assumption that process outputs can be measured on a numerical scale to make process adjustments. However, this assumption is often violated in practice when certain constraints limit the availability of numerical

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information. For instance, a high-yield process cannot be stopped but measurement procedures may take a long time; some quality characteristics are intrinsically inaccurate and cannot be expressed by numerical variables. Under such circumstances, qualitative observations (categorical data) can be alternatively collected in a fast manner by sacrificing accuracy or by accounting for intrinsic quality properties. Therefore, ordered categorical variables also called ordinal variables, can be used to characterize process status observations and be considered to assist in process adjustment. However, all traditional controllers are not applicable based on the categorical variables in R2R processes.

A categorical R2R controller for process adjustment based on categorical observations was recently proposed by Wang and Tsung¹¹. They considered the deep reactive ion etching (DRIE) process and applied their categorical R2R controller to this process. The DRIE process is a critical step in semiconductor manufacturing in forming high aspect-ratio sub-micron pillars with vertical sidewalls; the profile of the sidewall is a critical quality parameter for the process. In practice, each sidewall may be over-etched or under-etched. Accordingly, each wafer is classified by qualified operators into three categories including 'negative', 'normal' and 'positive', and the exact angle of the sidewall is not measured. A poorly adjusted DRIE process will produce wafers with unsatisfactory profiles¹²; thus, reliable product status information and effective control algorithms are the keys to improving the process performance. Although the consistency of the measurement system is assumed to be satisfactory by Wang and Tsung¹¹, it is impossible to classify all products perfectly and accurately. Classification error is the major problem that may deteriorate the performance of the categorical R2R controller.

Misclassification occurs when a product is classified into the wrong category. Misclassification can be observed in many fields that involve categorical variables, such as epidemiology and engineering applications. Broad research results show that misclassification can lead to seriously biased estimates of the relationship between response and explanatory variables^{13–15}. Birkett¹⁶ studied the effect of misclassification of polychotomous exposure variables on odds ratio estimation and pointed out that the impact of misclassification of multinomial variables is more complex than the impact of misclassification of binary variables.

Research efforts have been expended on designing methods to estimate misclassification probabilities (MP), which are necessary for correcting the bias introduced by ignoring the misclassification issue. One traditional treatment is double sampling^{17–19}, in which a perfect device or measurement system is used to obtain error-free results and an ordinary device or measurement system is used to obtain practical results. These results are then combined to estimate the MP. The Bayesian approach is another popular method used to estimate the unknown probabilities when an infallible measurement system is unavailable or too expensive²⁰. In this study, we provide concise guidelines to use the Bayesian method to estimate MP.

High misclassification rates in R2R process adjustment with categorical variables are intuitively negative. If the output truly belongs to the target category, there should be no adjustment made to the controllable variables. However, if this output is incorrectly classified into any other category, the controllable variables will be wrongly adjusted and, consequently, the process output will deviate away from the target. Little research has been performed on quantifying the impact of misclassification in R2R process adjustment.

In this paper, we propose an improved categorical R2R controller to decrease the impact of misclassification of categorical observations and improve process control performance. The remainder of this paper is organized as follows. In Section 2, the process model for categorical variables is introduced. Following that, the improved categorical R2R controller is developed and the difference between the categorical R2R controller proposed by Wang and Tsung¹¹ and the improved one is demonstrated in Section 3. A design guideline is presented for the practitioners in Section 4. In Section 5, the improved categorical controller is applied to the DRIE process described by Wang and Tsung¹¹. The conclusion of this paper is given in Section 6.

2. PROCESS MODELING

According to Wang and Tsung¹¹ and the references therein, a linear model is sufficient to characterize a single-input–single-output R2R process, upon which we may further develop and test new control algorithms.

The linear model is shown as follows:

$$y_t = \alpha + \beta u_{t-1} + d_t \quad (1)$$

where y_t is the process output at time t . u_{t-1} is the process input or the setting of the controllable factor at time $t-1$. d_t , which equals $d_{t-1} + \varepsilon_t - \theta \varepsilon_{t-1}$, is process noise and follows an IMA(1, 1) model, where $\varepsilon_t \sim N(0, 1)$ is a white noise series.

The numerical output, y_t , is unavailable in this process. Therefore, we model it as a latent variable. Let Y_t be the categorical observation that is collected after a wafer is processed at step t . The relationship between Y_t and y_t is determined by the following logical function:

$$Y_t = j \quad \text{if } \gamma_{j-1} \leq y_t < \gamma_j, \quad j = 1, \dots, J \quad (2)$$

where J is the number of output categories and $\gamma_j, j = 1, \dots, J$, are dividing parameters or cutoff points that divide the output space on a numerical scale into J intervals. Therefore, each y_t will be classified into one of the categories according to the above equation.

The categorical R2R controller proposed by Wang and Tsung¹¹, which was derived based on the above model, is expressed as follows and is called the old controller in the following sections:

$$\Delta u_t = -\frac{(E(y_t | Y_t = j) - T)(1 - \theta)}{\beta} = -\frac{((\gamma_{j-1} + \gamma_j)/2 - T)(1 - \theta)}{\beta} \quad (3)$$

where $j = 1, 2, 3$ and T is the target value of the process outputs.

The details of the derivation of the control action are presented by Wang and Tsung¹¹.

3. PROCESS ADJUSTMENT WITH MISCLASSIFICATION

In the above categorical R2R controller, the observed category is assumed to be the correct category to which the output truly belongs. In practice, due to the existence of measurement errors, we can assign an observation to the correct category only with a certain probability. In the following, we model the classification in a probabilistic way and improve the old categorical controller by considering misclassification errors.

In general, the optimal control action obtained at each step is a function of the observed categorical response variable. It is expressed as follows:

$$\Delta u_t^* = f(E(y_t | Y_t^*)) \quad (4)$$

where Y_t^* is the observed category into which the operators classify the t th process output. It should be noted that Y_t^* contains measurement errors and may not exactly follow the classification rule shown above.

We define P_i as the categorical probability that the process output truly belonging to the i th category and P_i^* as the probability that the operators classify the process output into the i th category. In addition, we use R_{ij} to denote the MP with which the process output is classified into the j th category by an operator when it truly belongs to the i th category. These definitions are formally written as follows:

$$P_i = \Pr(Y_t = i) \quad (5)$$

$$P_i^* = \Pr(Y_t^* = i) \quad (6)$$

$$R_{ij} = \Pr(Y_t^* = j | Y_t = i) \quad (7)$$

The following is the MP matrix, R :

$$R = \begin{pmatrix} R_{11} & \cdots & R_{1m} \\ \vdots & \ddots & \vdots \\ R_{m1} & \cdots & R_{mm} \end{pmatrix}_{m \times m} \quad (8)$$

Therefore, the sum of the entries in each row of the above matrix equals 1. That is, $\sum_{j=1}^m R_{ij} = 1$. It also follows that $\sum_{i=1}^m P_i = 1$ and $\sum_{i=1}^m P_i^* = 1$. As was shown by Tzavidis and Lin¹⁹, the misclassification model can be expressed as follows:

$$P_j^* = \sum_{i=1}^m \Pr(Y_t^* = j / Y_t = i) \Pr(Y_t = i) = \sum_{i=1}^m R_{ij} P_i \quad (9)$$

According to the Bayes theorem, the calibration probability can be denoted as C_{ji} with which the process output truly belongs to the i th category when it is classified into the j th category¹⁹:

$$C_{ji} = \Pr(Y_t = i / Y_t^* = j) = \Pr(Y_t^* = j / Y_t = i) \frac{\Pr(Y_t = i)}{\Pr(Y_t^* = j)} = \frac{R_{ij} P_i}{P_j^*} \quad (10)$$

Based on the calibration probability equation, the item $E(y_t | Y_t^*)$ in Equation (4) can be expressed as:

$$E(y_t | Y_t^* = j) = \sum_{i=1}^J \Pr(Y_t = i / Y_t^* = j) E(y_t / Y_t = i) = \sum_{i=1}^J C_{ji} \frac{\gamma_{i-1} + \gamma_i}{2} \quad (11)$$

where $j = 1, \dots, J$.

Therefore, we modify the old R2R categorical controller based on the newly defined Y_t^* as follows:

$$\begin{aligned} \Delta u_t^* &= - \frac{(E(y_t / Y_t^* = j) - T)(1 - \theta)}{\beta} \\ &= \pi E(y_t | Y_t^* = j) - \eta \end{aligned} \quad (12)$$

where $\pi = -1 - \theta/\beta$, $\eta = \pi T$.

The improved controller takes misclassification into consideration and models real scenarios that suffer from misclassification in handling categorical observations. It is also clear that when the misclassification probability is zero, Equation (12) reduces to Equation (3). Therefore, when there is no misclassification error, the new controller is equivalent to the old one. In the following sections, we study the performance of the improved categorical controller and compare it with the old one.

4. DESIGN GUIDELINES

In the above section, we described the new categorical controller. In this section, we implement the new controller with the DRIE process presented by Wang and Tsung¹¹ via simulation studies. The output space is divided into three zones. The values of the model and cutoff parameters, $\Theta = (\alpha, \beta, \theta, \gamma_0, \gamma_1, \gamma_2, \gamma_3)$, are taken from Wang and Tsung¹¹. The estimation procedure for these parameters is described in that paper. Specifically, $\Theta = (91.7, -1.8, 0.6, 87, 89.14, 90.59, 93)$. In addition, the initial setting of the controllable factor, u_0 , is set to 1.

Apart from the above parameters, the categorical probabilities and MP are also necessary for the new controller. For the DRIE process example, the standard deviation, σ , is known and equal to 1, and the mean

is the target, $T = 90$. Therefore, those probabilities are obtained and integrated into the new controller as follows:

Step 1: The categorical probabilities are calculated based on Equations (2) and (5). In this example, we have $P = \{0.195, 0.527, 0.278\}$.

Step 2: According to the definition of MP, we assume that the probability that any product is wrongly classified into non-adjacent categories is zero. This assumption is reasonable for ordered categorical observations because the output is less likely to be classified into the category that is not adjacent to the true category. The misclassification matrix R can be simplified as follows:

$$R = \begin{pmatrix} R_{11} & 1 - R_{11} & 0 \\ R_{21} & R_{22} & R_{23} \\ 0 & 1 - R_{33} & R_{33} \end{pmatrix}$$

Based on the known standard deviation, the ratio between R_{21} and R_{23} can be computed approximately for this example as follows:

$$\frac{R_{21}}{R_{23}} = \frac{\Pr(\gamma_1 \leq y \leq T)}{\Pr(T \leq y \leq \gamma_2)} \approx 3/2$$

Therefore, the misclassification matrix, R , can be further simplified to

$$R = \begin{pmatrix} R_{11} & 1 - R_{11} & 0 \\ 3(1 - R_{22})/5 & R_{22} & 2(1 - R_{22})/5 \\ 0 & 1 - R_{33} & R_{33} \end{pmatrix} \quad (13)$$

When the main diagonal probabilities are known, the above misclassification matrix is also known. In the following simulation, the MP are assumed to be known:

Step 3: Calculate the calibration probabilities based on Equation (10).

Step 4: Calculate the adjustment magnitude based on Equations (11) and (12).

Step 5: Adjust the controllable variables according to the new controller result from Step 4.

Although the following simulation is implemented according to the above steps, in real processes, the procedure is not applicable because these probabilities are usually unknown. Swartz *et al.*¹⁴ developed the Bayesian model combined with Gibbs sampling to estimate the probability parameters. A brief introduction of the method is given to demonstrate the estimation of the probabilities in this example.

First, we consider that N products are drawn and classified by operators randomly, and we let $P = (P_1, P_2, P_3)$ and $R_i = (R_{i1}, R_{i2}, R_{i3}), i = 1, 2, 3$. Let $Y^* = (Y_1^*, \dots, Y_N^*)$ and $Y = (Y_1, \dots, Y_N)$ be two vectors of observed and true values, respectively. In addition, the true category, Y_i , is also unknown, which can be treated as a latent categorical variable.

4.1. Prior distributions

It is reasonable to assume that prior distributions for probabilities are Dirichlet distributions, which are conjugate to multinomial distribution. The prior distributions are described as follows:

$$P = (P_1, P_2, P_3) \sim \text{Dir}(a)$$

$$R_i = (R_{i1}, R_{i2}, R_{i3}) \sim \text{Dir}(b_i)$$

$$a = (a_1, a_2, a_3), \quad b_i = (b_{i1}, b_{i2}, b_{i3})$$

where $a_i > 0$ and $b_{ij} > 0, i, j = 1, 2, 3$. Under practical situations, it is less likely that one product will be classified into one category that is far away from the true category using the good but imperfect measurement system for the ordered categorical variable. Therefore, for any $i, R_{i1} < \dots < R_{i,i-1} < R_{ii} > R_{i,i+1} > \dots > R_{i3}$.

4.2. Full conditional distributions

The conditional probability function of the latent categorical variable is the same as the calibration probability (Equation (10)). The conditional distributions for P and R_i are also Dirichlet distributions. Therefore,

$$\begin{aligned}
 f(P/R_1, R_2, R_3, Y, Y^*) &= f(P/Y) \sim \text{Dir}(a^*) \\
 f(R_i/P, Y, Y^*) &= f(R_i/Y, Y^*) \\
 &\sim \text{Dir}(b_i^*) I(R_{i1} <, \dots, < R_{i,i-1} < R_{ii} > R_{i,i+1} >, \dots, > R_{i3}) \\
 a^* &= \left(a_1 + \sum_{t=1}^N I(Y_t = 1), \dots, a_3 + \sum_{t=1}^N I(Y_t = 3) \right) \\
 b_i^* &= \left(b_{i1} + \sum_{t=1}^N I(Y_t = i) I(Y_t^* = 1), \dots, b_{i3} + \sum_{t=1}^N I(Y_t = i) I(Y_t^* = 3) \right)
 \end{aligned} \tag{14}$$

where the function $I(A)$ equals 1 if A is true, otherwise 0. The full conditional distribution for R_i is a truncated Dirichlet distribution for $i = 1, 2, 3$.

4.3. Gibbs sampling

Given the prior distributions that can be determined by the experience and knowledge about the process, a value for each unknown parameter is sampled from its full conditional distribution at one time. The steps for implementing Gibbs sampling with the latent categorical variable are outlined as follows:

- Sample $Y^{(t)}$ from Equation (10);
- Sample $P^{(t)}$ from $f(P/R_1^{(t-1)}, R_2^{(t-1)}, R_3^{(t-1)}, Y^t, Y^*)$;
- Sample $R_i^{(t)}$ from $f(R_i/P^{(t)}, Y^t, Y^*)$;

where the superscript (t) indicates the t th estimate based on other parameters and observations up to step t .

According to these steps, all parameters can be updated recursively. After the convergence is reached, estimates of the mean and standard deviation of these parameters can be obtained. Then, we can return to Steps 3 and 4 to implement the new categorical controller.

5. SIMULATION STUDY

In this section, we investigate the performance of the proposed controller by calculating the mean square error (MSE) of the process outputs to evaluate the deviations from the target. The MSE is defined as follows:

$$MSE = E((y_t - T)^2) \tag{15}$$

In reality, due to the practical constraints discussed in Section 1, it is infeasible for us to run a real process to test the performance of this new controller and compare its MSE with the old controller, nor can we apply these two controllers to one process simultaneously. For example, the devices exactly measuring the wafers that are etched during the DRIE process are kept in a clean room and the whole measurement process is time consuming. We cannot waste many wafers to determine the controller's performance. Therefore, we use Monte Carlo simulations to generate samples based on the real context and the process model to study the performance of the new categorical controller.

In the following simulations, each simulated process is run for 200 steps and repeated 100 times for each MP in order to use the average of the MSEs to evaluate the performance of the controllers. Without loss of generality, the seed for generating random numbers is set to 2, and the MP for each category is assumed to be equal to facilitate the calculation and comparison.

Before investigating the performance of the new improved controller (12), we first study the performance and stability of the old categorical R2R controller proposed by Wang and Tsung¹¹ in the case where the misclassification exists, because this old controller has been shown to be stable with different uncertainties including parameter estimates uncertainty, disturbance model and so on. In this section, the old controller is used as a benchmark for comparison with the new controller.

The process is simulated under different MP with the old controller. In Figure 1, we clearly see that the MSE for the process with the old controller in the case where the misclassification exists is larger than the opposite case where there is no misclassification (the dashed line). Moreover, when the misclassification probability is larger, the MSE increases quickly, and the old controller performs poorly. As shown in Table I,

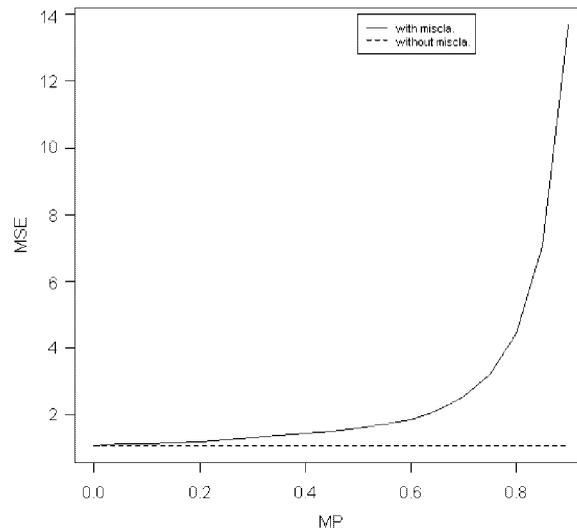


Figure 1. MSE of the old categorical controller under different misclassification probabilities

Table I. MSE comparison under different misclassification probabilities

| MP | MSE without misclassification | MSE with old controller |
|------|-------------------------------|-------------------------|
| 0.00 | 1.092 | 1.092 |
| 0.05 | 1.092 | 1.126 |
| 0.10 | 1.092 | 1.154 |
| 0.15 | 1.092 | 1.180 |
| 0.20 | 1.092 | 1.215 |
| 0.25 | 1.092 | 1.263 |
| 0.30 | 1.092 | 1.320 |
| 0.35 | 1.092 | 1.376 |
| 0.40 | 1.092 | 1.452 |
| 0.45 | 1.092 | 1.512 |
| 0.50 | 1.092 | 1.610 |
| 0.55 | 1.092 | 1.735 |
| 0.60 | 1.092 | 1.863 |
| 0.65 | 1.092 | 2.144 |
| 0.70 | 1.092 | 2.539 |
| 0.75 | 1.092 | 3.215 |
| 0.80 | 1.092 | 4.456 |
| 0.85 | 1.092 | 7.060 |
| 0.90 | 1.092 | 13.682 |

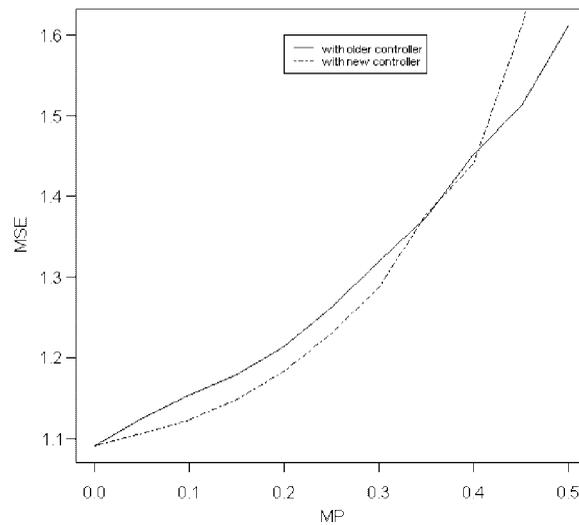


Figure 2. MSE comparison of the new controller and the old controller

Table II. MSE comparison of the new controller and the old controller

| MP | MSE without misclassification | MSE with old controller | MSE with new controller |
|------|-------------------------------|-------------------------|-------------------------|
| 0.00 | 1.092 | 1.092 | 1.092 |
| 0.05 | 1.092 | 1.126 | 1.107 |
| 0.10 | 1.092 | 1.154 | 1.124 |
| 0.15 | 1.092 | 1.180 | 1.149 |
| 0.20 | 1.092 | 1.215 | 1.184 |
| 0.25 | 1.092 | 1.263 | 1.231 |
| 0.30 | 1.092 | 1.320 | 1.288 |
| 0.35 | 1.092 | 1.376 | 1.379 |
| 0.40 | 1.092 | 1.452 | 1.440 |
| 0.45 | 1.092 | 1.512 | 1.610 |
| 0.50 | 1.092 | 1.610 | 1.830 |

the same conclusion can be reached that the old controller's performance becomes worse when there is misclassification.

As shown in Figure 2, the range of the studied MP varies from 0 to 0.5, and the dot-dashed line denotes the MSE of the improved R2R categorical controller. We can see that the average MSE in the process adjusted by the new R2R categorical controller is smaller than that with the old categorical controller under different MP unless the probability is larger than approximately 0.35. This means that when the probability that outputs are classified into their true categories is smaller than 0.65, both controllers cannot maintain outputs close to the target effectively. Careful investigation reveals that the new controller suggests more cautious adjustment when the MP is larger than 0.35. However, when the MP is smaller than 0.35, the new controller is always superior to the old one. Table II shows the complete data set corresponding to Figure 2.

The normal distribution curves in Figure 3 are generated by 500 simulated samples with the new controller and the old controller when the MP is equal to 0.2. As shown in Figure 3, the mean of the outputs with the new controller is much closer to the target 90 than that with the old controller. In addition, the probability between the two cutoff points with the new controller is larger than that of the old one. Therefore, the

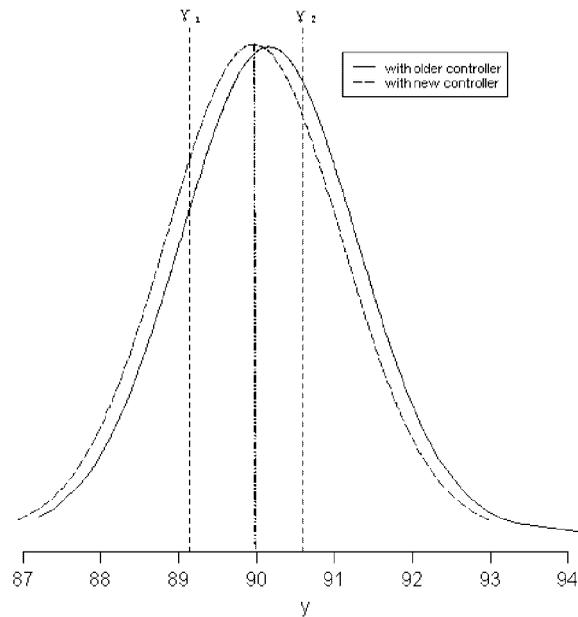


Figure 3. Normal distribution comparison

number of outputs in the second category (good outputs) with the new controller is larger than that of the old one.

6. CONCLUSION

In some practical scenarios, only categorical observations are available, and it is common that misclassification exists when the measurement system is not infallible, especially when the system classifying the outputs into certain categories relies on human operators. This paper proposes a new improved categorical R2R controller to reduce the effect of misclassification on the process and make the process output close to the target.

Simulation studies show that misclassification results in larger deviations of the process outputs from the target value when the MP increases, and the new improved categorical controller, compared with the old categorical controller, can significantly decrease the deviation when the MP is not too large (smaller than 0.35 in the case we studied). Because a measurement system with larger MP cannot be acceptable in practice, the new categorical controller should be useful in real applications.

This paper investigates the performance of the new controller based on the exactly known parameters including the categorical probabilities and the MP. However, in reality, these parameters are unknown. Although the Bayesian method to estimate these parameters has been described, we do not use the estimates to study the performance of the proposed controller. The performance and stability of the new improved R2R categorical controller with unknown parameters are interesting topics for future research.

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