MULTIVARIATE EWMA CONTROL CHART AND APPLICATION TO A SEMICONDUCTOR MANUFACTURING PROCESS

Multivariate EWMA Control Chart and Application to a Semiconductor Manufacturing Process

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A Thesis

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Abstract

The multivariate cumulative sum (MCUSUM) and the multivariate exponentially weighted moving average (MEWMA) control charts are the two leading methods to monitor a multivariate process. This thesis focuses on the MEWMA control chart. Specifically, using the Markov chain method, we study in detail several aspects of the run length distribution both for the on- and off- target cases. Regarding the on-target run length analysis, we express the probability mass function of the run length distribution, the average run length *(ARL),* the variance of run length *(V RL)* and higher moments of the run length distribution in mathematically closed forms. In previous studies, with respect to the off-target performance for the MEWMA control chart, the process mean shift was usually assumed to take place at the beginning of the process. We extend the classical off-target case and introduce a generalization of the probability mass function of the run length distribution, the *ARL* and the *V RL.* What Prabhu and Runger (1996) proposed can be derived from our new model. By evaluating the off-target *ARL* values for the MEWMA control chart, we determine the optimal smoothing parameters by using the partition method that provides an easy algorithm to find the optimal smoothing parameters and study how they respond as the process mean shift time changes. We compare the *ARL* performance of the MEWMA control chart with that of the multivariate Shewhart control chart to see whether the MEWMA chart is still effective in detecting a small mean shift as the process mean shift time changes. In order to apply the model to semiconductor manufacturing processes, we use a bivariate normal distribution to generate sample data and compare the MEWMA control chart with the multivariate Shewhart control chart to evaluate how the MEWMA control chart behaves when a delayed mean shift happens. We also apply the variation transmission model introduced by Lawless et al. (1999) to the semiconductor manufacturing process and show an

extension of the model to make our application to semiconductor manufacturing processes more realistic. All the programming and calculations were done in \boldsymbol{R}

Key words: *Multivariate Exponentially Weighted Moving Average Control Chart; Multivariate Shewhart Control Chart; Average Run Length; Markov Chain; Optimal Smoothing Parameter; Semiconductor Manufacturing.*

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Chapter 1

Introduction

1.1 Control charts and the mutivariate exponentially weighted moving average (MEWMA)

A multivariate control chart is an important tool for monitoring and improvement of the quality of products. In recent years, the importance of multivariate control charts has increased because more quality features are measured in mass production than ever before. These quality measures often exhibit substantial cross-correlations. For example, in semiconductor manufacturing, manufacturers make semiconductor devices around the clock through hundreds of processes. In this case, it would be more efficient to maintain a multivariate control chart than several univariate control charts because it is possible that individual control charts might not detect an assignable cause when quality characteristics are dependent. Several multivariate quality control charts have been proposed to monitor the mean vector of quality characteristics. The three most common multivariate control charts are the multivariate cumulative sum (MCUSUM) control chart, the multivariate exponentially weighted moving average (MEWMA) control chart and the multivariate Shewhart control chart. The latter is also known as Hotelling's χ^2 control chart. As the number of process variables grows, traditional multivariate control charts such as the multivariate Shewhart chart lose efficiency with respect to shift detection (Montgomery, 2005, pp. 486). The Shewhart control chart is poor at detecting small and moderate shifts in the mean vector. However, the MEWMA and the MCUSUM control charts are known to respond to small mean shifts very quickly. In this thesis, several aspects of the MEWMA control chart will be in detail studied.

1.2 Average run length (ARL)

The average run length *(ARL)* is a good tool to evaluate the performance of a statistical process control chart. The *ARL* is the average number of points that must be plotted before a point indicates an out-of-control condition (Montgomery, 2005, pp. 160). When a process control chart is set up, it is desirable that it produces a large *ARL* when the process is incontrol while smaller *ARL* values are preferred when the process is out-of-control (Pham, 2006, pp. 337). A large in-control *ARL* reduces the false alarms while a small out-of-control *ARL* indicates quick detection of a change. Since evaluating *ARL* values is not elementary, let us consider the univariate Shewhart control chart for the purpose of illustrating how the *ARL* is calculated. In this case, it is well-known that the run length follows a geometric distribution. Thus, its expected value is

$$
ARL = \frac{1}{p}
$$

where *p* is the probability that any point exceeds the control limits.

For instance, when the process is in-control with $p = 0.005$, then the in-control ARL (called ARL_0) equals $\frac{1}{0.005} = 200$, which means that the control chart signals a false (outof-control) alarm on average every 200 plotted points even though the process is in-control.

When the process is out-of-control, it is expected that more chart points will go out of

the control limits. Thus) the out-of-control *ARL* (called *ARL*¹) will be smaller than *ARLo.*

1.3 Semiconductor manufacturing

Materials used in electronics are classified into three types in terms of conductivity: conductors) insulators and semiconductors. Conductors are materials that can carry electrons easily thanks to the availability of free electrons such as copper and aluminum. Most metals are considered to be conductors. Insulators are materials that refuse to carry an electric current due to lack of free electorns such as glass and wood. Semiconductors are substances that are neither conductors nor insulators but they can have electrical properties by applying a certain voltage and doping impurity content (Bakshi and Godse) 2008) pp. 8). The two widely used simiconductor materials are silicon and germanium. Semicondutor devices are manufactured electronic components or integrated circuits by using semiconductor materials. Nowadays, semiconductor devices are considered as the cornerstone of electronics because most of our modern conveniences such as computers, cell phones, digital cameras) medical diagnostic equipment and all kind of domestic electric appliances are made of semicoductors. The reason that semiconductors are important is that we can alter their conductivity.

In semiconductor device fabrication, all the processing steps fall into one of the following categories: Deposition, ion-implantation, diffusion, photolithography and etching. Deposition is used to put down either a metal layer or an oxide (non-metal) layer on a wafer. Ion-implantation and diffusion are the operations that introduce dopants inside the wafer and grow a silicon oxide layer. Photolithography is the process that a light-sensitive material) called *photoresist* is applied in the wafer which is then exposed to ultraviolet light through an optical mask. Then the area of the photoresist exposed to light becomes soluble and is stripped off with solvents. Etching operation is used to create a circuit pattern that has been defined during the photolithography process by removing a thin film.

They form a process cycle and are employed on the wafer numerous times to make a semiconductor device. As a result, multiple layers are created and stacked directly on the wafer. Figures 1.1 and 1.2 are the cross-section of a semiconductor device. Specifically, Figure 1.2 is the cross-section of SRAM (Static Random Access Memory) which is taken by SEM (Scanning Electron Microscope). In this study, our focus is on the layer on which polysilicon gates (transistors) are patterned. In semiconductor manufacturing, the critical dimension (CD) of the gate width is the most critical parameter since the gate CD decides the overall speed of the integrated circuit and it has continued to shrink since the integrated circuit was introduced (Orshansky et al., 1999). The following website shows how quickly design rules for gate patterns have changed. Refer to http: / / en. wikipedia. org/wiki/ Semiconductor_device_fabrication at wikipedia.

Figure 1.1: Cross-section of a semiconductor device.

The design rule of silicon chips was 10 μ m in 1971 but chipmakers are now making 32 nm devices. That is, today's transistors are more than 300 times smaller than the ones made in 1971. Shrinkage in the gate width brings us difficulties to control it. Thus, a tighter control over the gate width has to be made to maximize process yield and throughput. Even a small amount of mean shift in the silicon gate width has to be detected. Therefore, the MEWMA control scheme which is very efficient at issuing a warning signal on a small amount of mean shift is the right choice and suitable for the semiconductor industry facing increasing quality demands. Figure 1.3 shows a finished product of semiconductor device.

As an application of the MEWMA control chart, we construct a simple bivariate normal distribution model, apply it to semiconductor manufacturing operations and provide simulation results. The main reason for the application to a semiconductor manufacturing process is that semiconductor manufacturing operations need a control chart that provides a high sensitivity in detecting a small mean shift.

Figure 1.2: Cross-section of SRAM taken by SEM.

1.4 Propagation of variability in a process

One of the main goals of statistical process control is to effectively reduce the variability in a process. In order to do that, it is important to identify at which stages variation is

Figure 1.3: 4Gb DDR DRAM chip.

added substantially and how much variation is transmitted from previous stages. Lawless et al. (1999) introduced the variation transmission model and showed how variation in key product characteristics could be built across the production stages. However, the model is constructed based on that only one machine runs at final stage. In this thesis, we will extend the model and apply it to semiconductor manufacturing.

1.5 Thesis objectives and organization

Prabhu and Runger (1996) developed a Markov chain algorithm to evaluate the performance of the MEWMA control charts. The Markov chain algorithm provides an acceptable approximation for the average run length *(ARL)* of the MEWMA control chart. The onand off-target *ARL* values can be computed by using the algorithm. However, when the performance of the off-target case is evaluated, the off-target case has to be extended in terms of the process transition time since the past studies only cover the off-target case where the process mean shifts instantaneously to a new value once manufacturing operations start; that is, the mean shift was assumed to take place at the very beginning of the process (the zero-state case). In real life, the process goes out-of-control after staying in-control for a while from the beginning and the change sustains until human intervention

(the steady-state case). The process mean shift could take place at any time in process operation, not just at the beginning. For example, in the Markov chain model, when the process mean changes at transition time τ , we consider a transition matrix P_0 until time $\tau - 1$ and a new transition matrix P_1 afterwards.

The main objectives of this thesis are as follows:

1. To calculate analytically and numerically the run length distribution and the average run length for the off-target case.

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- 2. To compare the MEWMA control with the multivariate Shewhart control chart for the off-target case.
- 3. To identify optimal smoothing parameter values for the off-target case.
- 4. To apply the MEWMA control chart to a bivariate semiconductor manufacturing process.
- 5. To develop a model for variation propagation with application to the semiconductor manufacturing process.

The study is arranged as follows. In Chapter 2, the general off-target case is discussed and we show derivations of the *ARL* and the variance for the general off-target case. Additionally, the optimal smoothing parameter and the comparison of the MEWMA control chart and the multivariate Shewhart control chart are discussed for different values of transition time. In Chapter 3, a bivariate normal distribution model for the MEWMA control chart is applied to a semiconductor fabrication process and the method is illustrated with simulated data. An extension of the variation transmission model is introduced in Chapter 4. Finally, Chapter 5 presents some conclusions.

Chapter 2

Analysis of MEWMA control chart

2.1 Overview of MEWMA control chart

The conventional Shewhart-type control charts such as the *T2* charts are pretty effective for detecting mean shifts. However, they are slow in reacting to small and moderate shifts in the process mean. In that regard, the MEWMA control chart was developed to provide more sensitivity to small mean shifts (Montgomery, 2005, pp. 504). Suppose that $X_t = (X_1, X_2, \cdots, X_p)'$ is a *p*-dimensional random vector whose components are random variables at time *t.* Lowry et al. (1992) proposed a multivariate version of the univariate exponentially weighted moving average (EWMA) control chart. As for the MEWMA control chart, it is defined by

$$
Z_t = rX_t + (1 - r)Z_{t-1}
$$
\n(2.1)

where, *r* is a smoothing parameter $(0 < r \le 1)$ and it is assumed that $Z_0 = 0_p$. The MEWMA control chart issues a warning signal when

$$
Q_t = \mathbf{Z}_t' \Sigma_{\mathbf{Z}_t}^{-1} \mathbf{Z}_t > H \tag{2.2}
$$

where *H* is a specified control limit and the covariance matrix, $\Sigma_{\mathbf{Z}_t}$ is given as $\left\{ \frac{r[1-(1-r)^{2t}]}{(2-r)} \right\} \Sigma_{\mathbf{X}}$. However, in this thesis we use the following asymptotic covariance matrix:

$$
\Sigma_{Z_t} = \left(\frac{r}{2-r}\right) \Sigma_X.
$$

Note from Equation (2.1) that when we expand Z_t recursively, we get

$$
Z_t = rX_t + r(1-r)X_{t-1} + r(1-r)^2X_{t-2} + \cdots + r(1-r)^{t-1}X_1 + (1-r)^tZ_0.
$$

Thus, *Zt* is a weighted average of the *t* quality measurements available with weights following a geometric form. However, in the literature the chart is known as *exponentially weighted.*

An important special case of the MEWMA control chart is the case that $r = 1$ leads to $Z_t = X_t$ and $Q_t = X_t' \Sigma_X^{-1} X_t$. This is precisely the multivariate Shewhart control chart also known as the chi-squared control chart. Let us assume that

$$
E(\boldsymbol{X}) = \mu = \begin{cases} \mu_0 & \text{when the process is on-target} \\ \mu_1 & \text{when the process is off-target} \end{cases}
$$

and $Var(X) = \Sigma_X$.

Consider the following transformation and let the transformed variable be $\Sigma_{\boldsymbol{X}}^{-1/2}(\boldsymbol{X}$. μ_0). By the transformation, we obtain

$$
E\left(\Sigma_{\mathbf{X}}^{-1/2}(\mathbf{X}-\boldsymbol{\mu_0})\right) = \begin{cases} \Sigma_{\mathbf{X}}^{-1/2}E(\mathbf{X}-\boldsymbol{\mu_0}) = \Sigma_{\mathbf{X}}^{-1/2}(\boldsymbol{\mu_0}-\boldsymbol{\mu_0}) = 0 & \text{when the process is on-target} \\ \Sigma_{\mathbf{X}}^{-1/2}E(\mathbf{X}-\boldsymbol{\mu_0}) = \Sigma_{\mathbf{X}}^{-1/2}(\boldsymbol{\mu_1}-\boldsymbol{\mu_0}) & \text{when the process is off-target} \end{cases}
$$

and $Var(\Sigma_X^{-1/2}(X - \mu_0)) = \Sigma_X^{-1/2} \Sigma_X (\Sigma_X^{-1/2})' = \Sigma_X^{-1/2} \Sigma_X^{1/2} \Sigma_X^{1/2} (\Sigma_X^{-1/2})' = I$. The noncentrality parameter c is defined as follows.

$$
c = (\mu - \mu_0)' \Sigma_X^{-1} (\mu - \mu_0).
$$
 (2.3)

Then, the noncentrality parameter of the transformed variable $\Sigma_X^{-1/2}(X - \mu_0)$ is

$$
c = \left(\Sigma_{\mathbf{X}}^{-1/2}(\mu - \mu_0) - 0\right)'(I)^{-1}\left(\Sigma_{\mathbf{X}}^{-1/2}(\mu - \mu_0) - 0\right)
$$

= $({\mu} - {\mu}_0)' \Sigma_{\mathbf{X}}^{-1/2} \Sigma_{\mathbf{X}}^{-1/2}({\mu} - {\mu}_0)$
= $({\mu} - {\mu}_0)' \Sigma_{\mathbf{X}}^{-1}({\mu} - {\mu}_0).$

The result is equivalent to the noncentrality parameter of X (Equation (2.3)). By this transformation, we can assume that *X* has mean zero and an identity covariance matrix since the performance of a MEWMA control chart is a function of μ only through the noncentrality parameter (Lowry, 1992). Using that, Q_t in Equation (2.2) can be rewritten as $Q_t = \left(\frac{2-r}{r}\right) ||Z_t||^2$. Thus, $Q_t > H$ is equivalent to $||Z_t|| > \sqrt{\frac{r}{2-r}H}$. That is, $||Z_t|| > H'$ where $H' = \sqrt{\frac{r}{2-r}H}$. In this thesis, we will use

$$
q_t = ||\bm{Z_t}||
$$

as the control chart statistic.

2.2 The Markov chain approximation algorithm

The main objective of statistical process control charts is to provide a way to detect process shifts as quickly as possible when the process is out-of-control. One way is through the average run length (ARL) of the control chart. Several attempts by using simulation have been made to determine on- and off-target average run length for multivariate control charts, such as MEWMA and multivariate cumulative sum (MCUSUM) control charts (Crosier, 1988; Hawkins, 1992; Pignatiello and Runger, 1990; Woodall and Ncube, 1985). However, the simulation method has the downside that we have to go through a long and tiresome process to obtain an upper control limit and a large number of simulated process runs are required to get an acceptable variance. Brooks and Evans (1972) used a Markov chain approximation for the *ARL* of a univariate CUSUM control chart and Lucas and Saccucci (1990) applied this method for the EWMA chart. Rigdon (1995a, 1995b) used integral equations to obtain *ARL* values for a MEWMA. Prabhu and Runger (1996) used the Markov chain model to determine the run length performance of a MEWMA control chart. There is a conceptual difference between the two approaches. To analyze a shift of the observed *p* dimensional mean vector (when the process becomes out-of-control), the Rigdon's method uses a change in the mean of two dependent random variables while the Markov chain approach uses a one-dimensional random variable and a $p-1$ dimensional random vector. However, the main drawback of the Rigdon's integration equation is that the equation can not be applied for the off-target setting. In this section, we review the Markov chain model that Prabhu and Runger (1996) proposed for the MEWMA control chart, which is the foundation for this study.

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The control statistic *qt* is non-negative and large values of it are indicative of out-ofcontrol. Thus, an upper control limit (UCL) is used. In the Markov chain approach, the in-control range [0, UCL] is divided into subintervals which form the states of the chain. Let

 $g_1 =$ width of the on-target states

 g_2 = width of the off-target states

 $UCL = \sqrt{H \times r/(2-r)}$

 $p =$ number of variables.

2.2.1 On-target performance

Figure 2.1 illustrates the states when the process is in-control. Dividing the range [0, UCL] into $m_1 + 1$ subintervals, m_1 of them have the same length g_1 and one of them has the length $\frac{g_1}{2}$. Thus,

$$
\frac{g_1}{2} + m_1 g_1 = \text{UCL}
$$

$$
g_1 = \frac{2\text{UCL}}{2m_1 + 1}.
$$

Figure 2.1: A illustration of the Partitioning the Control Region of a MEWMA (On-Target).

When the process is in-control $(\mu = 0)$ from the beginning, the on-target distribution of $q_t = ||Z_t||$ can be approximated by using a Markov chain.

$$
p(i,j) = P(q_t \text{ in state } j|q_{t-1} \text{ in state } i)
$$

= $P\{(j-0.5)g_1 < ||rX_t + (1-r)Z_{t-1}|| < (j+0.5)g_1|q_{t-1} = g_1 i\}$

Let us denote $S(r)$ the p - dimensional sphere of radius $r > 0$. Since Z_t has a spherical distribution, the conditional distribution of Z_t given $||Z_t||$ is the same as $||Z_t||U$, where U is the uniform random variable on the p - dimensional sphere with radius 1 (Eaton, 1983). Thus, given that $q_{t-1} = g_1 i$, the distribution of $Z_{t-1} | (q_{t-1} = g_1 i)$ follows $ig_1 U$. We get

$$
p(i,j) = P\{(j-0.5)g_1/r < ||\mathbf{X}_t + (1-r)ig_1\mathbf{U}/r|| < (j+0.5)g_1/r\} \tag{2.4}
$$

where $X_t \sim N_p(0, I)$ and $U \sim S(1)$. Assume that X_t is independent of *U*. Then Equation

(2.4) can be rewritten as

$$
p(i,j) = \int \cdots \int f(u)P\{(j-0.5)g_1/r < ||\mathbf{X_t} + (1-r)ig_1\mathbf{u}/r|| < (j+0.5)g_1/r|U = \mathbf{u}\}d\mathbf{u}.
$$

Conditioning on $U = u$,

$$
\boldsymbol{X_t} + (1-r)ig_1\boldsymbol{u}/r \sim N_p((1-r)ig_1\boldsymbol{u}/r, \boldsymbol{I}).
$$

à.

Hence, conditioning on $U = u$,

 $||X_t + (1 - r)ig_1u/r||^2 \sim \chi^2(p, c)$ where c is the noncentrality parameter.

The noncentrality parameter c can be calculated as follows.

$$
c = \left(\frac{1-r}{r}ig_1u'\right)I\left(\frac{1-r}{r}ig_1u\right) = \left(\frac{1-r}{r}ig_1\right)^2u'u = \left(\frac{1-r}{r}ig_1\right)^2||u||^2 = \left(\frac{1-r}{r}ig_1\right)^2
$$

where u represents any vector in the p - dimensional sphere of radius 1, that is $||u|| = 1$.

Thus,

$$
p(i,j) = \int \cdots \int f(u)P\left\{\frac{(j-0.5)^2 g_1^2}{r^2} < ||X_t + (1-r)i g_1 u/r||^2 < \frac{(j+0.5)^2 g_1^2}{r^2} \middle| U = u\right\} du
$$
\n
$$
= \int \cdots \int f(u)P\{(j-0.5)^2 g_1^2/r^2 < \chi^2(p,c) < (j+0.5)^2 g_1^2/r^2\} du
$$
\n
$$
= P\{(j-0.5)^2 g_1^2/r^2 < \chi^2(p,c) < (j+0.5)^2 g_1^2/r^2\} \int \cdots \int f(u) du
$$
\n
$$
= P\{(j-0.5)^2 g_1^2/r^2 < \chi^2(p,c) < (j+0.5)^2 g_1^2/r^2\}. \quad \text{(since } \int \cdots \int f(u) du = 1)
$$
\n
$$
S(1)
$$

Therefore, for $i, j = 0, 1, 2, \ldots, m_1$, the probability of a transition from state i to state

j is denoted $p(i, j)$ and defined as follows.

$$
p(i,j) = \begin{cases} P\{(j-0.5)^2 g_1^2/r^2 < \chi^2(p,c) < (j+0.5)^2 g_1^2/r^2 \} & \text{if } j \neq 0\\ P\{\chi^2(p,c) < (0.5)^2 g_1^2/r^2 \} & \text{if } j = 0 \end{cases}
$$

where $\chi^2(p, c)$ is a noncentral chi-squared random variable with *p* degrees of freeedom, noncentrality parameter $c = [(1 - r)ig_1/r]^2$ and $g_1 = \frac{2UCL}{2m_1 + 1}$. Using the transitional probabilities, the $(m_1 + 1) \times (m_1 + 1)$ transition matrix P_0 of the transient states of the chain can be constructed.

By using the above algorithm, the on-target average run length is given by

$$
ARL_0 = \lim_{m_1 \to +\infty} s'(I - P_0)^{-1} \mathbf{1} \quad \text{(Prabhu and Runger, 1996)} \tag{2.5}
$$

where s is the starting probability vector and 1 denotes a vector of 1s of the dimension $m_1 + 1$. Derivation of Equation (2.5) is provided in section 2.3.

2.2.2 Off-target performance (zero-state case)

Figure 2.2 represents the two-dimensional range of $(Z_{t1}, ||Z_{t2}||)$ with the axes Z_1 and $||Z_2||$. For the Markov chain approximation of Z_{t1} , the number of states between -UCL and UCL is $2m_2 + 1$. States are 1, 2, ..., $2m_2 + 1$. Thus, the width of each state, g_2 is $\frac{2UCL}{2m_2+1}$. For the Markov chain approximation of $||Z_{t2}||$, the number of states are $m_1 + 1$, labelled as 0, $1, \ldots, m_1$. Thus, $g_1 = \frac{2 \text{UCL}}{2m_1+1}$

Suppose that the process is out-of-control (μ_0 changes to μ_1) from the beginning and let $\delta = ||\mu_1||$. Then $\delta = ||\mu_1|| = \sqrt{(\mu_1 - 0)'I(\mu_1 - 0)} = \sqrt{\mu_1'\mu_1}$ which is the noncentrality parameter. Since the MEWMA is a function of the off-target mean $(=\mu_1)$ only through the noncentrality parameter, we can assume that $\mu_1 = \delta e$ where e is the p component unit vector $e' = (1,0,0,\ldots,0)$. Thus, Z_t can be partitioned into a one-dimensional random variable Z_{t1} with non zero mean δ and $p - 1$ dimensional random vector Z_{t2} with zero

Figure 2.2: States in the Markov Chain Used for the Off-Target Case of a MEWMA (Prabhu and Runger, 1996).

mean, where $\delta = (\mu' \Sigma_X^{-1} \mu)^{1/2}$. That is, $q_t = ||Z_t|| = (Z_{t1}^2 + Z_{t2}Z_{t2})^{1/2}$. The transitional probability of Z_{t1} from state i_x to state j_x , denoted by $h(i_x, j_x)$ is used to analyze the off-target control component. For $i_x, j_x = 1, 2, \ldots, 2m_2 + 1$,

$$
h(i_x, j_x) = P(Z_{t1} \text{ in state } j_x | Z_{t-1} \text{ in state } i_x)
$$

= $P[(-\text{UCL} + (j_x - 1)g_2 - (1 - r)c_{i_x})/r - \delta) < X_{t1} - \delta < (-\text{UCL} + j_x g_2 - (1 - r)c_{i_x})/r - \delta)]$
= $\Phi\left((- \text{UCL} + j_x g_2 - (1 - r)c_{i_x})/r - \delta\right) - \Phi\left((- \text{UCL} + (j_x - 1)g_2 - (1 - r)c_{i_x})/r - \delta\right)$
where Φ is the cumulative standard normal distribution function and $c_{i_x} = -\text{UCL} + (i_x - 0.5)g_2$.

Let *A* denote the $(2m_2+1) \times (2m_2+1)$ transition matrix of Z_{t1} . The transitional probability of $||Z_{t2}||$ from state i_y to state j_y , denoted by $v(i_y, j_y)$ is used to analyze the on-target control components. For $i_y, j_y = 0, 1, 2, ..., m_1$,

$$
v(i_y, j_y) = \begin{cases} P\{(j_y - 0.5)^2 g_1^2 / r^2 < \chi^2(p - 1, c) < (j_y + 0.5)^2 g_1^2 / r^2\} & \text{if } j_y \neq 0\\ P\{\chi^2(p - 1, c) < (0.5)^2 g_1^2 / r^2\} & \text{if } j_y = 0 \end{cases}
$$

where $c = [(1 - r)i_y g_1/r]^2$. Let *B* denote the $(m_1 + 1) \times (m_1 + 1)$ transition matrix of $||Z_{t2}||$. Since Z_{t1} is independent of Z_{t2} , the transitional probability of the bivariate chain $\{Z_{t1}, ||Z_{t2}||\}$ from state (i_x, i_y) to state (j_x, j_y) is

$$
p[(i_x, i_y), (j_x, j_y)] = h(i_x, j_x)v(i_y, j_y).
$$

Let P_1 be the transition matrix of the transient states of the bivariate chain. Using the condition $(i_x - (m_2 + 1))^2 g_2^2 + i_y^2 g_1^2 < UCL^2$ and calculating the Kronecker product of A and B (Lee, 2009), P_1 can be calculated. See Appendix A.1 for the definition of Kronecker product and Appendix B.1 for the R code for the Markov chain algorithm.

As a result, the off-target average run length is given by

$$
ARL_1 = \lim_{m_1, m_2 \to +\infty} s'(I - P_1)^{-1} 1.
$$
 (2.6)

2.3 On-target run length analysis

Assume that the process is operating on-target. Following Prabhu and Runger (1996), the Markov chain methods for the MEWMA control chart leads to

$$
P(N > n) = \lim_{m_1 \to +\infty} s' P_0^{n} 1, \ n = 0, 1, 2, \dots
$$
 (2.7)

where N is the run length of the scheme, that is the number of runs until the false signals for the first time. Here s is the starting probability vector. P_0 is the $(m_1 + 1) \times (m_1 + 1)$ transition matrix for the Markov chain, and 1 denotes a vector of Is of the dimension

 $m_1 + 1$. It turns out that the convergence is quite fast with values of 10 to 15 for m_1 , giving satisfactory results. In this thesis, we used $m_1 = 25$. Then, the probability mass function for the run length N is

$$
f(n) = P(N = n) = P(N > n - 1) - P(N > n)
$$

= $s'P_0^{n-1}1 - s'P_0^{n}1$
= $s'P_0^{n-1}(I - P_0)1$, $n = 1, 2, ...$

where $P_0^0 = I$ and *I* is the $(m_1 + 1) \times (m_1 + 1)$ identity matrix. The on-target run length distributions are provided in Figure 2.3. It is observed that the on-target run length distribution is skewed to the right (positively skewed).

Figure 2.3: On-Target Run Length Distribution for MEWMA with *ARLo* = 200,300,500 and (a) $r = 0.1$ and (b) $r = 0.3$.

Let us consider the situation that the process is operating on-target and the process mean is $\mu = \mu_0$. Since Equation (2.7) is the survival function of N, we can use it to derive $E(N)$. Thus, the on-target average run length (ARL_0) is

$$
ARL_0 = E(N) = \sum_{n=1}^{\infty} nf(n)
$$

= $1f(1) + 2f(2) + 3f(3) + 4f(4) + \cdots$
= $[f(1) + f(2) + f(3) + f(4) + \cdots] + [f(2) + f(3) + f(4) + \cdots] + [f(3) + f(4) + \cdots] + \cdots$
= $\sum_{n=1}^{\infty} f(n) + \sum_{n=2}^{\infty} f(n) + \sum_{n=3}^{\infty} f(n) + \cdots = P(N \ge 1) + P(N \ge 2) + P(N \ge 3) + \cdots$
= $\sum_{n=1}^{\infty} P(N \ge n) = \sum_{n=1}^{\infty} s' P_0^{n-1} 1 = s' \left(\sum_{n=1}^{\infty} P_0^{n-1} \right) 1 = s'(I + P_0 + P_0^2 + \cdots) 1$
= $s'(I - P_0)^{-1} 1$.

j

An alternative way to derive $E(N)$ is presented in Appendix A.2.4.1.

The variance of run length $(=VRL_0)$ when the process is operating on-target also can be derived as a closed form (See Appendix A.2.4.2).

$$
VRL_0 = Var(N) = E(N^2) - [E(N)]^2
$$

= $2s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1 - [s'(I - P_0)^{-1}1]^2$
= $2s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1[1 - s'(I - P_0)^{-1}1].$ (2.8)

2.3.1 Moments of on-target **run** length

In the previous section, we derived the first and second moments of the distribution of run length. The higher moments also can be derived by the same approach. In particular, the third and fourth moments are used to measure skewness and kurtosis of the run length distribution respectively. The third moment of N is

$$
E(N^3) = 6s'P_0^2(I - P_0)^{-3}1 + 6s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1
$$

(See Appendix A.2.4.3).

Skewness is the degree of asymmetry of a distribution and it is the standardized *3rd* central moment of run length *N.* It is defined as

$$
\gamma_1 = \frac{E[(N-\mu)^3]}{\sigma^3}
$$
, where σ is the standard deviation.

We compute

$$
E[(N-\mu)^3] = E(N^3) - 3\mu E(N^2) + 2\mu^3
$$

= $s'[6 \cdot P_0^2 (I - P_0)^{-3} + 6P_0 (I - P_0)^{-2} + (I - P_0)^{-1}]1$
- $3(s'(I - P_0)^{-1}1)[2s'P_0 (I - P_0)^{-2}1 + s'(I - P_0)^{-1}1]$
+ $2(s'(I - P_0)^{-1}1)^3$.

Thus, the skewness of the on-target run length distribution is

$$
\gamma_1 = \left\{ s' [6P_0^2 (I - P_0)^{-3} + 6P_0 (I - P_0)^{-2} + (I - P_0)^{-1}]1 - [s'(I - P_0)^{-1}1] \right\}
$$

\n
$$
[6s'P_0 (I - P_0)^{-2}1 + 3s'(I - P_0)^{-1}1 - 2(s'(I - P_0)^{-1}1)^2] \}
$$

\n
$$
/(2s'P_0 (I - P_0)^{-2}1 + s'(I - P_0)^{-1}1[1 - s'(I - P_0)^{-1}])^{3/2}.
$$

The fourth moment of N is

$$
E(N^4) = 24s'P_0^3(I - P_0)^{-4}1 + 36s'P_0^2(I - P_0)^{-3}1 + 14s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1
$$

(See Appendix A.2.4.4).

Kurtosis is a measure of the flatness of a distribution and it is the standardized *4th* central moment of run length *N.* It is defined as

$$
\kappa = \frac{E[(N-\mu)^4]}{\sigma^4}.
$$

We compute

$$
E[(N - \mu)^4] = E(N^4) - 4 \cdot \mu E(N^3) + 6 \cdot \mu^2 E(N^2) - 3 \cdot \mu^4
$$

= $\mu_4 - \mu(4 \cdot \mu_3 - 6 \cdot \mu_2 + 3 \cdot \mu^3)$

where, $\mu_4 = E(N^4)$, $\mu_3 = E(N^3)$, and $\mu_2 = E(N^2)$.

Thus, the kurtosis of the on-target run length distribution is

$$
\kappa = \frac{\mu_4 - \mu(4 \cdot \mu_3 - 6 \cdot \mu_2 + 3 \cdot \mu^3)}{(\mu_2 - \mu^2)^2}.
$$

Additionally, excess kurtosis is $\kappa - 3 = \frac{\mu_4 - \mu(4\cdot\mu_3 - 6\cdot\mu_2 + 3\cdot\mu^3)}{(\mu_2 - \mu^2)^2} - 3$. All the moments derived above can be verified numerically by using the probability mass function. For example, given the condition that $H = 12.7378, ARL_0 = 200, r = 0.1$ and $p = 4, E(N^2) =$ 76,432.59, $E(N^3) = 43,757,943$, and $E(N^4) = 33,401,107,743$ are obtained respectively. Table 2.1 shows the approximation of the moments.

| m | $\sum_{n=1}^m nf(n)$ | $\sum_{n=1}^m n^2 f(n)$ | $\sum_{n=1}^m n^3 f(n)$ | $\sum_{n=1}^m n^4 f(n)$ |
|--------|----------------------|-------------------------|-------------------------|--------------------------------|
| 100 | 19.43 | 1,257.93 | 92,355.41 | 7,290,654.00 |
| 500 | 147.33 | 37,242.22 | 11,769,166.00 | 4202406879.00 |
| 1,000 | 193.39 | 68,358.97 | 33,581,291.00 | 20075724754.00 |
| 5,000 | 200.00 | 76,432.59 | 43,757,942.00 | 33,401,104,540.00 |
| 10,000 | 200.00 | 76,432.59 | 43,757,943.00 | 33,401,107,743.00 |
| 20,000 | 200.00 | 76,432.59 | 43,757,943.00 | $\overline{33,401,107,743.00}$ |

Table 2.1: Approximation of moments of on-target run length.

2.4 Off-target run length analysis

In section 2.3, we studied the on-target run length distribution. In this section, we will see the off-target run length distribution. As mentioned earlier, Prabhu and Runger (1997) evaluated the off-target performance by assuming that the process was out-of-control at the beginning of operation (the zero-state case). The analysis in this thesis extends the above method to the steady-state case that is where it is possible for a delayed shift to take place; that is, it is not necessary to happen at the beginning. Thus, we will generalize the notion of the off-target case.

 $\frac{1}{4}$

Consider the situation where the process goes off-target from $\mu = \mu_0$ to $\mu = \mu_1$ at the time $t = \tau$ and the change sustains. Thus,

$$
\mu = \begin{cases} \mu_0, & t = 1, 2, \dots, \tau - 1, \\ \mu_1, & t = \tau, \tau + 1, \dots \end{cases}
$$

Thus, the transition matrix P changes as well according to

$$
P = \left\{ \begin{array}{ll} P_0, & t = 1, 2, \ldots, \tau - 1, \\ P_1, & t = \tau, \tau + 1, \ldots \end{array} \right.
$$

Now, let us consider the situation where the process mean stays in-control until $t = \tau - 1$ and it shifts out-of-control from $t = \tau$ on.

As a result, the survivor function of run length N becomes

$$
f_S(n) = P(N > n) = \begin{cases} s' P_0^{n} 1, & n = 1, 2, ..., \tau - 1, \\ s' P_0^{r-1} P_1^{n-\tau+1} 1, & n = \tau, \tau + 1, ... \end{cases}
$$

This leads to the following probability mass function for *N.*

For $n = 1, 2, ..., \tau - 1$,

$$
f(n) = P(N = n) = P(N > n - 1) - P(N > n) = s'P_0^{n-1}1 - s'P_0^{n}1
$$

= $s'P_0^{n-1}(I - P_0)1$.

For $n = \tau$,

$$
f(n) = P(N = \tau) = P(N > \tau - 1) - P(N > \tau) = s' P_0^{\tau - 1} 1 - s' P_0^{\tau - 1} P_1 1
$$

= $s' P_0^{\tau - 1} (I - P_1) 1$.

For $n = \tau + 1, \tau + 2, \tau + 3, \ldots$

$$
f(n) = P(N = n) = P(N > n - 1) - P(N > n) = s' P_0^{\tau - 1} P_1^{(n-1) - \tau + 1} 1 - s' P_0^{\tau - 1} P_1^{n - \tau + 1} 1
$$

= $s' P_0^{\tau - 1} P_1^{n - \tau} (I - P_1) 1$.

Note that the latter formula also applies to $n = \tau$. Thus the probability mass function of run length N is

$$
f(n) = P(N = n) = \begin{cases} s' P_0^{n-1} (I - P_0) 1, & \text{if } n = 1, 2, ..., \tau - 1, \\ s' P_0^{r-1} P_1^{n-r} (I - P_1) 1, & \text{if } n = \tau, \tau + 1, \end{cases}
$$
(2.9)

Note that when $\tau = \infty$ or $\tau = 1$, then the probability mass function reduces to the following forms.

$$
f(n) = P(N = n) = \begin{cases} s' P_0^{n-1} (I - P_0) 1, & \text{if } \tau = \infty \\ s' P_1^{n-1} (I - P_1) 1, & \text{if } \tau = 1. \end{cases}
$$

This result is consistent with what Prabhu and Runger (1996) proposed. Thus, Equation (2.9) is the general form of the probability mass function of run length *N.* Using Equation (2.9), the distribution of run length N can be plotted for different values of τ . Figures 2.4 and 2.5 show how the distribution of the off-target run length moves as τ value changes given the condition that $ARL₀ = 200$ and 500 respectively.

Figures 2.6 and 2.7 show the off-target run length distributions for the MEWMA when the process mean has shifted at $\tau = 50$ and $\tau = 100$ for varying values of smoothing parameter *r* given that *ARLo* = 200 and 500 respectively. Notice that the distribution shows a higher peak as a smaller smoothing parameter r is used.

Figures 2.8 and 2.9 show the off-target run length distributions for the MEWMA when the process mean has shifted at $\tau = 50$ and $\tau = 100$ for different values of mean shift δ given the condition that *ARLo* = 200 and 500 respectively. Notice that the distribution shows a higher peak as the amount of shift (δ) increases.

 $\begin{array}{c} \mathbf{1} \end{array}$

Figure 2.4: Off-Target Run Length Distribution for MEWMA when Process Mean has shifted by $\delta = 0.5$ with $ARL_0 = 200$, $r = 0.1$ and (a) $p = 2$ and (b) $p = 4$.

Figure 2.5: Off-Target Run Length Distribution for MEWMA when Process Mean has shifted by $\delta = 0.5$ with $ARL_0 = 500$, $r = 0.1$ and (a) $p = 2$ and (b) $p = 4$.

Figure 2.6: Off-Target Run Length Distribution for MEWMA when Process Mean has shifted by $\delta = 0.5$ at $\tau = 50$ with $ARL_0 = 200$ and (a) $p = 2$ and (b) $p = 4$.

Figure 2.7: Off-Target Run Length Distribution for MEWMA when Process Mean has shifted by $\delta = 0.5$ at $\tau = 100$ with $ARL_0 = 500$ and (a) $p = 2$ and (b) $p = 4$.

Figure 2.8: Off-Target Run Length Distribution for MEWMA when Process Mean has shifted at $\tau = 50$ with $ARL_0 = 200$, $r = 0.1$ and (a) $p = 2$ and (b) $p = 4$.

Figure 2.9: Off-Target Run Length Distribution for MEWMA when Process Mean has shifted at $\tau = 100$ with $ARL_0 = 500$, $r = 0.1$ and (a) $p = 2$ and (b) $p = 4$.

Table 2.2 shows the computed values of the off-target average run length (ARL_1) and the probability of false alarm for various τ values, where the probability of false alarm is defined as

Probability of false alarm =
$$
\sum_{n=1}^{\tau-1} f(n).
$$

It also contains the effective average run length, $ARL_1 - \tau$ which is the average number

of runs needed to detect a change in the mean vector after it has occurred. Table 2.2 is constructed given the condition that $ARL_0 = 500, p = 4, r = 0.1$ and $\delta = 0.5$.

Table 2.2: Probability of false alarm, *ARL1* and effective *ARL1* for each transition point $(\tau).$

 $\frac{1}{2}$

Furthermore, the off-target average run length *ARL1* can be expressed as a closed form.

$$
ARL_1 = E(N) = \sum_{n=1}^{\infty} nf(n) = \sum_{n=1}^{\tau-1} nf(n) + \sum_{n=\tau}^{\infty} nf(n)
$$

=
$$
\sum_{n=1}^{\tau-1} ns' P_0^{n-1} (I - P_0) 1 + \sum_{n=\tau}^{\infty} ns' P_0^{r-1} P_1^{n-\tau} (I - P_1) 1
$$

=
$$
s' \left\{ \left(\sum_{n=1}^{\tau-1} n P_0^{n-1} \right) (I - P_0) + P_0^{r-1} \left(\sum_{n=\tau}^{\infty} n P_1^{n-\tau} \right) (I - P_1) \right\} 1
$$

=
$$
\left\{ s'[I - P_0^{r-1}](I - P_0)^{-1} 1 + P_0^{r-1} (I - P_1)^{-1} \right\} 1 \text{ (Appendix A.2.5.1). (2.10)}
$$

Alternatively, we can derive the off-target average run length *ARL1* by using the *law of total probability.* That is, *E(N)* can be written as follows.

$$
E(N) = E(N|N < \tau)P(N < \tau) + E(N|N \ge \tau)P(N \ge \tau).
$$

 $\frac{1}{2}$

 $\frac{1}{4}$ $\begin{array}{c} 1 \\ 1 \\ 1 \end{array}$

We know that $P(N \ge \tau) = P(N > \tau - 1) = s' P_0^{\tau-1} 1$ and $P(N < \tau) = 1 - s' P_0^{\tau-1} 1$. The conditional distribution of $N,$ given that $N<\tau$ is defined as

$$
f(n|N < \tau) = \frac{f(n)}{P(N < \tau)}
$$
 $n = 1, 2, \dots, \tau - 1$ provided that $P(N < \tau) > 0$
=
$$
\frac{1}{1 - s' P_0^{\tau - 1} 1} s'[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau - 1}](I - P_0)^{-1} 1
$$
 (See Appendix A.2.6).

Thus,

$$
E(N|N < \tau)P(N < \tau) = \frac{1}{1 - s'P_0^{\tau - 1}1} s'[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau - 1}](I - P_0)^{-1}1(1 - s'P_0^{\tau - 1}1)
$$

= $s'[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau - 1}](I - P_0)^{-1}1$.

Now, the conditional distribution of $N,$ given that $N \geq \tau$ is defined as

$$
f(n|N \ge \tau) = \frac{f(n)}{P(N \ge \tau)} \quad n = \tau, \tau + 1, \cdots \quad \text{provided that } P(N \ge \tau) > 0
$$
\n
$$
= \frac{1}{s' P_0^{\tau - 1} 1} s' [P_0^{\tau - 1} (I - P_1)^{-1} + (\tau - 1) P_0^{\tau - 1}] \quad \text{(See Appendix A.2.6)}.
$$

Thus,

$$
E(N|N \ge \tau)P(N \ge \tau) = \frac{1}{s'P_0^{\tau-1}1} s'[P_0^{\tau-1}(I-P_1)^{-1} + (\tau-1)P_0^{\tau-1}]1(s'P_0^{\tau-1}1)
$$

= $s'[P_0^{\tau-1}(I-P_1)^{-1} + (\tau-1)P_0^{\tau-1}]1.$

Therefore,

$$
ARL_1 = E(N) = E(N|N < \tau)P(N < \tau) + E(N|N \ge \tau)P(N \ge \tau)
$$

= $s'[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau - 1}](I - P_0)^{-1}1 + s'[P_0^{\tau - 1}(I - P_1)^{-1} + (\tau - 1)P_0^{\tau - 1}]1$
= $s'[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau - 1} + (\tau - 1)P_0^{\tau - 1}(I - P_0)](I - P_0)^{-1}1 + s'P_0^{\tau - 1}(I - P_1)^{-1}1$
= $s'[I - P_0^{\tau - 1}](I - P_0)^{-1}1 + s'P_0^{\tau - 1}(I - P_1)^{-1}1$.

 $\frac{1}{4}$ ł

We obtain the same result as Equation (2.10).

As a special case, Equation (2.10) reduces to the following forms.

$$
ARL_1 = \begin{cases} s'(I - P_1)^{-1}1, & \text{if } \tau = 1\\ s'(I - P_0)^{-1}1 = ARL_0, & \text{if } \tau = \infty, \text{ since } P^{\infty} = 0. \end{cases}
$$

Note that above results agree with past studies by Runger and Prabhu (1996). Hence, Equation (2.10) is a generalization of of the on- and off-target ARL.

The off-target variance $(VRL₁)$ of N is

$$
VRL_1 = Var(N) = E(N^2) - [E(N)]^2
$$

= $s'\{P_0[2I - (\tau - 1)\tau P_0^{\tau - 2} + 2(\tau - 2)\tau P_0^{\tau - 1} - (\tau - 1)(\tau - 2)P_0^{\tau}](I - P_0)^{-2}$
+ $P_0^{\tau - 1}[2P_1(I - P_1)^{-2} + 2(\tau - 1)P_1(I - P_1)^{-1} + \tau(\tau - 1)I] + [I - P_0^{\tau - 1}](I - P_0)^{-1}$
+ $P_0^{\tau - 1}(I - P_1)^{-1}\}1 - \{s'[I - P_0^{\tau - 1}](I - P_0)^{-1}1 + s'P_0^{\tau - 1}(I - P_1)^{-1}1\}^2$
(See Appendix A 2.5.2)

(See Appendix A.2.5.2).

As a special case, when $\tau = \infty$,

$$
VRL_1 = Var(N)
$$

= $2s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1[I - s'(I - P_0)^{-1}1]$
= $2s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1 - [s'(I - P_0)^{-1}1]^2$
= VRL_0 .

Note that the result is equivalent to the on-target variance (See Equation (2.8)).

$$
\text{when }\tau=1,
$$

$$
VRL_1 = Var(N)
$$

= $s'\{P_0(2I - 2I)(I - P_0)^{-2} + 2P_1(I - P_1)^{-2} + I + (I - P_1)^{-1} - I\}1$
- $[s'\{(I - P_0)(I - P_0)^{-1} + (I - P_1)^{-1} - I\}1]^2$
= $2s'P_1(I - P_1)^{-2}1 + s'(I - P_1)^{-1}1 - [s'(I - P_1)^{-1}1]^2$.

2.5 Comparison of MEWMA and Shewhart control chart

Suppose that *X* is a random variable and is the number of *Bernoulli* trials until the first success is observed, supported on the set $\{1, 2, 3, \ldots\}$. Then the probability mass function of a *geometric random variable X* with success probability α is defined as

 $P(X = x) = (1 - \alpha)^{x-1}\alpha$, $x = 1, 2, 3, \dots$. As we discussed earilier, the probability mass function of the on-target run length and the average run length for the MEWMA control chart are defined as

$$
f(n) = P(N = n) = s'(I - P_0)P_0^{n-1}1, \ n = 1, 2, ...
$$

$$
ARL_0 = E(N) = s'(I - P_0)^{-1}1
$$
 respectively.

The mean, variance, skewness and excess kurtosis of a geometric distribution with probability α are given in Table 2.3.

Table 2.3: Mean, variance, skewness and excess kurtosis of geometric distribution.

Comparing the two distributions (i.e., the geometric distribution and the distribution of run length N) by matching the means leads to interesting results. For a given starting vector *s*, a transition matrix P_0 and a control limit H, then determine the α such that $E(X) = ARL_0$. As a result, we have $\alpha = \frac{1}{ARL_0} = \frac{1}{s'(I-P_0)^{-1}1}$.

Table 2.4: Comparison of MEWMA run length distribution and geometric distribution with $ARL_0 = 200.$

| $p = 4, ARL_0 = 200, prob = 0.005$ | | | | | | | | | |
|------------------------------------|----------|----------|----------|----------|----------|----------------|--|--|--|
| | 0.1 | 0.5 | 0.7 | 0.99 | | geometric dist | | | |
| Variance | 36432.61 | 39284.82 | 39593.28 | 39799.74 | 39800 | 39800 | | | |
| Skewness | 1.998662 | 1.999953 | 1.999969 | 1.999979 | 2.000006 | 2.000006 | | | |
| Excess Kurtosis | 5.994399 | 5.999810 | 5.999917 | 5.999963 | 6.000025 | 6.000025 | | | |

Table 2.5: Comparison of MEWMA run length distribution and geometric distribution with $ARL_0 = 500.$

| $p = 4, ARL_0 = 500, prob = 0.002$ | | | | | | | | | |
|------------------------------------|----------|----------|----------|----------|----------|----------------|--|--|--|
| | 0.1 | 0.5 | 0.7 | 0.99 | | geometric dist | | | |
| Variance | 239636.3 | 248085.6 | 248916.5 | 249499.2 | 249500 | 249500 | | | |
| Skewness | 1.99973 | 1.999992 | 1.999996 | 2.000001 | 2.000001 | 2.000001 | | | |
| Excess Kurtosis | 5.998916 | 5.999968 | 5.999986 | 6.000004 | 6.000004 | 6.000004 | | | |

Figures 2.10 and 2.11 illustrate that there is not much difference between the on-target run length distribution of a MEWMA and a geometric distribution by matching the mean

Figure 2.10: Comparison of on-target run length distribution with *ARLo* = 200 and geometric distribution with $prob = 0.005$ and (a) $p = 2$ and (b) $p = 4$.

Figure 2.11: Comparison of on-target run length distribution with *ARLo* = 500 and geometric distribution with $prob = 0.002$ and (a) $p = 2$ and (b) $p = 4$.

unless the smoothing parameter r is very small. It is also observed that as the smoothing parameter r gets closer to 1, the on-target run length distribution for the MEWMA is becoming the geometric distribution. That is, as $r \to 1$, then $Z_t = r(X_t - \mu_0) + (1$ $r)Z_{t-1} \rightarrow X_t - \mu_0$, which is the multivariate Shewhart control chart. On the other hand, as $r \to 0$, then $Z_t \to Z_{t-1}$, which means that all information used is past information. Thus, when *r* is 1, the on-target run length distribution for the MEWMA is equivalent to the geometric distribution. The variance, skewness and kurtosis of the two distributions are also computed in the Tables 2.4 and 2.5.

Now, let us consider the off-target distribution of the two control charts (i.e., the MEWMA control chart and the Shewhart control chart) for a given smoothing parameter *r* and *ARLo.* The general form of the multivariate Shewhart statistic is defined as

$$
T_t^2 = (X_t - \mu_0)' \Sigma^{-1} (X_t - \mu_0), \text{ where } t = 1, 2, ...
$$

and follows a chi-square distribution with *P* degrees of freedom when the process is on-target and *X* follows a multivariate normal distribution (Aparisi, 2004).

Since the on-target run length distribution for the Shewhart control chart follows a geometric distribution, the off-target run length distribution for the Shewhart chart can be constructed as follows.

$$
g(n) = \begin{cases} p_0(1-p_0)^{n-1}, & n = 1, 2, \cdots, \tau - 1, \\ (1-p_0)^{\tau-1}p_1(1-p_1)^{n-\tau}, & n = \tau, \tau + 1, \ldots \end{cases}
$$

where p_0 is the probability that any point exceeds the control limits when the process is in-control while p_1 is the the same probability when the process is out-of-control. Using the probability mass function, the out-of-control $ARL₁$ when the mean shift takes place at τ is

$$
ARL_1 = \sum_{n=1}^{\infty} n g(n) = \sum_{n=1}^{\tau-1} n (p_0 (1 - p_0)^{n-1}) + \sum_{n=\tau}^{\infty} n (1 - p_0)^{\tau-1} p_1 (1 - p_1)^{n-\tau}
$$

=
$$
\frac{(1 + (\tau - 1)(1 - p_0)^{\tau} - \tau (1 - p_0)^{\tau-1})}{p_0} + (1 - p_0)^{\tau-1} \left(\tau + \frac{1 - p_1}{p_1}\right)
$$

=
$$
\frac{(1 + (\tau - 1)(1 - p_0)^{\tau} - \tau (1 - p_0)^{\tau-1} - (\tau - 1)(1 - p_0 - 1)(1 - p_0)^{\tau-1})}{p_0} + \frac{(1 - p_0)^{\tau-1}}{p_1}
$$

=
$$
\frac{(1 - \tau (1 - p_0)^{\tau-1} + (\tau - 1)(1 - p_0)^{\tau-1})}{p_0} + \frac{(1 - p_0)^{\tau-1}}{p_1}, \quad \tau = 1, 2,
$$

As a special case, $ARL₁$ reduces to the following forms.

$$
ARL_1 = \begin{cases} 1/p_0, & \text{if } \tau = \infty \\ 1/p_1, & \text{if } \tau = 1. \end{cases}
$$

which is equivalent to the mean of the geometric distribution with probability p_0 and p_1 respectively. Additionally, the off-target VRL_1 when the mean shift occurs at time τ is

$$
VRL_1 = Var(N) = E[N(N-1)] + E(N) - E(N)^2
$$

= $p_0^{-2}(1 - p_0)[2 - (\tau - 1)\tau(1 - p_0)^{\tau - 2} + 2(\tau - 2)\tau(1 - p_0)^{\tau - 1} - (\tau - 1)(\tau - 2)(1 - p_0)^{\tau}]$
+ $(1 - p_0)^{\tau - 1}[2(1 - p_1)p_1^{-2} + 2(\tau - 1)(1 - p_1)p_1^{-1} + \tau(\tau - 1)]$
+ $[(1 - (1 - p_0)^{\tau - 1})p_0^{-1} + (1 - p_0)^{\tau - 1}p_1^{-1}][1 - ((1 - (1 - p_0)^{\tau - 1})p_0^{-1} + (1 - p_0)^{\tau - 1}p_1^{-1})].$

As a special case,

$$
VRL_1 = \begin{cases} (1 - p_0)/p_0^2, & \text{if } \tau = \infty \\ (1 - p_1)/p_1^2, & \text{if } \tau = 1 \end{cases}
$$

which is equivalent to the variance of the geometric distribution with probability p_0 and p_1 respectively.

Now, let us compare the performance of the MEWMA control chart with that of the multivariate Shewhart control chart when the mean shift happens. For example, we pick $r = 0.1$ (since 0.1 is the value most often used) and determine the MEWMA control limit that satisfies $ARL_0 = 200$. Then consider the geometric distribution matching with the same mean $ARL_0 = 200$. This is the geometric distribution with parameter $p_0 = \frac{1}{ARL_0}$ 0.005. Determine the control limit for the Shewhart control chart with $ARL_0 = 200$. Notice that the noncentrality parameter of the multivariate Shewhart control chart is defined as $c = (\mu - \mu_0)' \Sigma_X^{-1} (\mu - \mu_0)$ while the noncentrality of the MEWMA is defined as $\delta =$ $((\mu - \mu_0)' \Sigma_X^{-1} (\mu - \mu_0))^{1/2}$. That is $c = \delta^2$.

Figures $2.12 - 2.14$ show the comparison of the out-of-control $ARL₁$ values for the two distributions for different values for δ and different values of τ . It is well known that the MEWMA control chart is effective in detecting small shifts when the shift happens at $\tau = 1$ (Lowry et al., 1992). Just as in the case $\tau = 1$, the MEWMA control chart outperforms the Shewhart control chart as τ increases until the mean shift δ is 1.5. However, when the large mean shift takes place (i.e., δ is greater than 1.5), the Shewhart control chart is as good as the MEWMA at detecting large shifts in the mean or performs slightly better. Additionally, as τ increases (i.e., the mean shift is delayed more steps), the MEWMA control chart loses its sensitivity to a small mean shift.

Figure 2.12: Off-Target *ARL* Comparision of MEWMA and Shewhart with *ARLo* = 200 (a) $\delta = 0.5$ and (b) $\delta = 1.0$.

Figure 2.13: Off-Target *ARL* Comparision of MEWMA and Shewhart with $ARL₀ = 200$ (a) $\delta = 1.5$ and (b) $\delta = 2.0$.

Figure 2.14: Off-Target *ARL* Comparision of MEWMA and Shewhart with $ARL_0 = 200$ (a) $\delta = 2.5$ and (b) $\delta = 3.0$.

2.6 Analysis of optimal smoothing parameter *r*

When a shift has taken place in the process mean, it is very important to detect the occurrence of the change as early as possible. In the MEWMA control charts, smaller values of r are more effective in detecting small shifts in the mean (Lowry et al., 1992). Thus, for a given *ARLo,* we need to find the smoothing parameter that is associated with the smallest *ARL*1. First, let us consider the case that the process goes off-target at the beginning of operation $(\tau = 1)$. Tables C.5 - C.7 in Appendix C present optimum MEWMA control charts for various shifts (δ) and in-control values of ARL_0 (from 200 to 1,000). The smoothing parameter corresponding to a minimum *ARLI* for a given *ARLo* can be obtained by using the Markov chain algorithm and the partition method (The \bm{R} code is provided in Appendix B.4).

The partition method generates a combination of a smoothing parameter r and a control limit H satisfying a given *ARLo* and find the optimal smoothing parameter. The basic idea of the method is as follows. For a fixed smoothing parameter r , the method inspects the middle point of a lower control limit H_{low} and a upper control limit H_{up} such that $ARL_{H_{low}} \leq ARL_0$ and $ARL_{H_{up}} \geq ARL_0$. Once H_{mid} , the middle point of two control limits is obtained, *ARL* can be calculated by using the Markov chain algorithm. If the difference of *ARLo* and the newly computed *ARL* is less than a very small number (i.e., $\epsilon < 10^{-3}$), the smoothing parameter r and the control limit H_{mid} is a pair that can satisfy the given *ARLo.* Otherwise, keep doing the previous procedures until a sought pair is found. If this task is carried out until the method covers a whole range of smoothing parameter r $(0 < r \leq 1)$, a number of combinations of r and H can be obtained. With the combinations obtained, $ARL₁$ values can be calculated for a given shift δ . Then, the smoothing parameter r for which ARL_1 is the smallest can be identified.

Now we are interested in how the optimal value of r behaves as transition point τ changes. Figures 2.15 and 2.16 show that the optimal values of r increases as τ increases in

each case. It is observed that the optimal parameter *T* changes more slowly when the *ARLo* value gets bigger or p increases. That is, when we have smaller *ARLo* and p, the change of transition time gives a huge impact on deciding the optimal smoothing parameter r . For instance, when we have $ARL_0 = 500$ and $p = 10$, the smoothing parameter changes very little (from 0.10 to 0.13) as τ changes from 1 to 200 while it changes from 0.14 to 0.26 in case we have $ARL_0 = 200$ and $p = 2$. Notice that the usual practice is to pick the optimal value for $\tau = 1$. However, this is unrealistic since most process starts operating well for a while and later on out-of-control slippage occurs.

 $\overline{}$ \sim \sim

 $\ddot{}$

 $\hat{\mathbf{r}}$

Figure 2.15: Comparison of optimal smoothing parameter as τ increases with (a) $p = 2$ and (b) $p = 4$.

Figure 2.16: Comparison of optimal smoothing parameter as τ increases with (a) $p = 6$ and (b) $p = 10$.

Chapter 3

Application to semiconductor manufacturing

Figure 3.1: Semiconductor fabrication process.

Figure 3.1 illustrates the process steps involved in patterning of the transistor gate. A polysilicon layer is formed on a silicon wafer (2). The wafer is coated with a photoresist which is sensitive to ultraviolet light (3) . A mask pattern is exposed and the photoresist is developed (4 and 5). By using gases in a plasma through the resist pattern and removing unwanted areas of film (etching), a circuit pattern is made (6 and 7) (Quirk and Serda, 2000). Among a number of semiconductor manufacturing processes, the patterning of polisilicon gates has been the most important and challenging process in semiconductor manufacturing since it defines the success of semiconductor manufacturing. The linewidth of a gate transistor before etching is called the developed inspection critical dimension (DI CD) and it is called the final inspection critical dimension (FI CD) after etching (Joung et al., 2004). As mentioned before, the tighter control for the DI CD and FI CD is required since the degree of integration on a chip increases. Notice that since optical lenses are used in photolithography, it is impossible to have the best focus over the entire wafer area because silicon wafers have rough surfaces and they also have bow and warpage. Therefore, in this study, we assume that we have the best focus in the central area of a wafer, which is normally happening in semiconductor manufacturing. Additionally, we do not expect any process particles to happen. Then we do a simple simulation to see how the MEWMA control chart performs.

Suppose $X = (X_1, X_2)'$ is a 2 × 1 random vector representing the DI CD (X_1) and the FI CD (X_2) . The quality characteristic X_1 (DI CD) is normally distributed with mean μ_{DI} and standard deviation σ_{DI} , where both μ_{DI} and σ_{DI} are known and correspond to in-control production (Greer et al., 2003). Moreover, the statistical model between the final inspection critical dimensioin (FI CD) and the developed inspection critical dimension (DI CD) is $X_2 = \alpha + \beta X_1 + \epsilon$, where ϵ is a random variable representing noise or environmental factor affecting FI CD and $\epsilon \sim N(0, \sigma_{\epsilon}^2)$. Thus, the random vector, **X** can be expressed as $\mathbf{X} = (X_1, X_2)' = (\text{DI CD}, \text{FI CD})' = (X_1, \alpha + \beta X_1 + \epsilon)'$. Suppose that $\sigma_{\epsilon} < \sigma_{DI}$ and ϵ is independent of X_1 .

The mean and variance of X_2 and the covariance between X_1 and X_2 can be calculated

as follows.

$$
E(X_2) = E(\alpha + \beta X_1 + \epsilon) = \alpha + \beta E(X_1) + E(\epsilon) = \alpha + \beta \mu_{DI}
$$

$$
Var(X_2) = Var(\alpha + \beta X_1 + \epsilon) = \beta^2 Var(X_1) + Var(\epsilon) = \beta^2 \sigma_{DI}^2 + \sigma_{\epsilon}^2.
$$

The covariance between X_1 and X_2 is

$$
\sigma_{X_1, X_2}^2 = \sigma_{DI, FI}^2 = Cov(X_1, X_2) = Cov(X_1, \alpha + \beta X_1 + \epsilon)
$$

= $Cov(X_1, \alpha) + Cov(X_1, \beta X_1) + Cov(X_1, \epsilon)$
= $0 + \beta Var(X_1) + 0 = \beta \sigma_{DI}^2$. (since X_1 is independent of ϵ)

Therefore, the random vector, *X* is distributed as a bivariate normal distribution as follows.

$$
\mathbf{X} \sim N\left(\mu_0, \Sigma_{\mathbf{X}}\right), \text{ where } \Sigma_{\mathbf{X}} = \begin{pmatrix} \sigma_{DI}^2 & \sigma_{DI,FI}^2 \\ \sigma_{DI,FI}^2 & \sigma_{FI}^2 \end{pmatrix} \text{ and } \mu_0 = \begin{pmatrix} \mu_{DI} \\ \mu_{FI} \end{pmatrix}.
$$

Furthermore, the covariance matrix, Σ_X is

$$
\Sigma_X = \begin{pmatrix} \sigma_{DI}^2 & \beta \sigma_{DI}^2 \\ \beta \sigma_{DI}^2 & \beta^2 \sigma_{DI}^2 + \sigma_{\epsilon}^2 \end{pmatrix}.
$$

Let n be the sample size. In semiconductor manufacturing, normally several wafers are selected from a run to measure **DI** CD and **FI** CD at regular time intervals when the process is thought to be in-control. For the purpose of simulation, we assume that five wafers are selected from a run $(n = 5)$ and the mean of five measurements is used. We also make use of experimental results from the U.S patent (7,541,286 B2) suggesting parameters values $\alpha = -0.03$ and $\beta = 0.98$. Suppose that X_1 is distributed as $N(130, 14.78)$ and ϵ is distributed as $N(0, 1)$, then the distribution of the sample mean X is

$$
\bar{X} = \frac{\Sigma_{j=1}^{5} X_j}{5} \sim N\left(\mu_0 = \begin{pmatrix} 130.00 \\ 127.37 \end{pmatrix}, \Sigma_{\bar{X}} = \begin{pmatrix} 2.956 & 2.897 \\ 2.897 & 3.100 \end{pmatrix}\right).
$$

Figures 3.2 - 3.5 show the results of simulation to compare the performance of the MEWMA chart and the multivariate Shewhart control chart with the condition that the on-target $ARL = 200$ with $p = 2$ and $r = 0.1$. The control limits for a MEWMA and a multivariate Shewhart control chart are 8.66 and 10.6 respectively. That is, the multivariate Shewhart control chart issues an out-of-control signal when $T_t^2 = (\bar{X}_t - \mu_0)' \Sigma_{\bar{X}}^{-1} (\bar{X}_t - \mu_0) >$ 10.6, whereas the MEWMA chart procedure signals when $Z_t' \Sigma_Z^{-1} Z_t > 8.66$, where $\Sigma_{Z_t} =$ $\frac{r}{2-r}\sum_{\bar{X}}$. Suppose that the process is initially in-control and a shift in the mean happens at $\tau = 20$. When a small shift happens, it is observed that the MEWMA chart is superior to the multivariate Shewhart control chart. Otherwise, both control charts perform well. For example, when $\delta = 0.5$ (Figure 3.2), the MEWMA issued a signal at 53th run while no indication of an out-of-control condition was observed for the multivariate Shewhart control chart. When $\delta = 1.0$ (Figure 3.3), an out-of-control signal was generated at 30th run for the MEWMA while the multivariate Shewhart chart detected the shift at 43th run.

Now, when a relatively big shift happens ($\delta = 2.0$ and 3.0), both control chart issued a out-of-signal as quickly as possible (Figures 3.4 and 3.5). The above simulation results show good agreement with previously obtained results in Chapter 2 section 5.

Figure 3.2: Comparision MEWMA and Hotelling control chart with $\delta = 0.5$ (a) MEWMA control chart and (b) Hotelling control chart.

Figure 3.3: Comparision MEWMA and Hotelling control chart with $\delta = 1.0$ (a) MEWMA control chart and (b) Hotelling control chart.

Figure 3.4: Comparision MEWMA and Hotelling control chart with $\delta = 2.0$ (a) MEWMA control chart and (b) Hotelling control chart.

Figure 3.5: Comparision MEWMA and Hotelling control chart with $\delta = 3.0$ (a) MEWMA control chart and (b) Hotelling control chart.

Chapter 4

Propagation of variability

4.1 Introduction

So far, we have discussed a shift in the mean for the process monitoring. Additionally, throughout the manufacturing processes, it is also important to know which stage contributes most to variation. In terms of analysis of variation transmission in manufacturing processes, Lawless et al. (1999) discussed methodology for understanding how variation is added and transmitted across the manufacturing process. Let us assume we have discrete manufacturing stages as follows.

Figure 4.1: Manufacturing processes.

Let X be a quality characteristic of the output and X_k be the measurement at stage k . We have a target value for the quality characteristic but there is variation in the product. That is, there is variation in the quality characteristic, X . As the measurement of interest X passes through the above processes, each step makes a contribution to the variance of *X.* The objective of this chapter is to understand the amount of variation attributable to different stages of a manufacturing process and to introduce an extension of the variation transmission model suggested by Lawless et al. (1999) by using a simple linear regression model.

4.2 Variation transmission model

Figure 4.2 illustrates how the variation transmission model is applied to semiconductor manufacturing. For simplicity, we use two steppers and one etcher. *Y*1 denotes the DI CD while *Y2* denotes the FI CD. The random variable *Y2* is a linear function of an independent variable *Y*1 such that

$$
Y_2 = \alpha + \beta Y_1 + e \tag{4.1}
$$

where α and β are parameters and the random variable $e \sim N(0,\sigma_A^2)$. We assume that the

Figure 4.2: Photo and etch stages in a gate patterning process in model I.

DI CD is measured right after photo processing as *Y*1 while the FI CD is measured after etching process as Y_2 . By defining $\sigma_i^2 = Var(Y_i)$, we can obtain from Equation (4.1)

$$
\sigma_2^2 = \beta^2 \sigma_1^2 + \sigma_A^2
$$

where $\beta^2 \sigma_1^2$ is the variance transmitted through the etcher and σ_A^2 is the variance added by the etching process. Let us define $Y_{1j} = Y_1 | Z_1 = j$ where Z_1 is a random variable such that $Z_1 = j$ if a wafer is processed by a stepper j. μ_1 and σ_1^2 are the mean and variance of the first measurement Y_1 and it can be expressed as

$$
\mu_1 = \frac{1}{2} \sum_{i=1}^{2} \mu_{1j} \tag{4.2}
$$

$$
\sigma_1^2 = \frac{1}{2} \sum_{j=1}^2 \sigma_{1j}^2 + \frac{1}{2} \sum_{j=1}^2 (\mu_{1j} - \mu_1)^2
$$
\n(4.3)

where $\mu_{1j} = E(Y_1|Z_1 = j)$ and $\sigma_{1j}^2 = Var(Y_1|Z_1 = j)$ (See section A.2.1 in Appendix).

In addition, using Equations (4.2) and (4.3), the mean and variance of Y_2 (=FI CD) are

$$
\mu_2 = E(Y_2) = \alpha + \beta \left(\frac{1}{2} \sum_{j=1}^2 \mu_{1j}\right)
$$

$$
Var(Y_2) = \beta^2 \left(\frac{1}{2} \sum_{j=1}^2 \sigma_{1j}^2 + \frac{1}{2} \sum_{j=1}^2 (\mu_{1j} - \mu_1)^2\right) + \underbrace{\sigma_A^2}_{\text{Variance added}}
$$

$$
Variance transmitted
$$

In this simple case, the variance added by the etch operation is determined completely by one etcher. The downside of this model is that possibly the etcher will be overloaded since it is the only machine running. Since many etchers and steppers are involved for mass production in semiconductor manufacturing, the model can be extended with the addition of etchers. Intuitively, it would be more complicated if more etchers were involved in the etching process. For simplicity, we have two steppers and two etchers (See Figure 4.3).

Let us define $Y_{2jk} = Y_2 | (Z_1 = j, Z_2 = k)$ and Z_2 is a random variable such that $Z_2 = k$ if a wafer is etched by etcher *k*. Thus, $Y_{2_{jk}}$ is the measurement of polysilicon gate line width (FI CD) processed by stepper *j* and etcher k ($j = 1, 2; k = 1, 2$). Since we have four possible combinations of steppers and etchers working in a pair, we can think of four linear equations as follows.

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Figure 4.3: Photo and etch stages in a gate patterning process in model **II.**

Let us assume that

$$
Y_{2_{11}} = Y_2|(Z_1 = 1, Z_2 = 1) = \alpha_1 + \beta_1 Y_{11} + e_1, \text{ where } e_1 \sim N(0, \sigma_{A_1}^2)
$$

\n
$$
Y_{2_{12}} = Y_2|(Z_1 = 1, Z_2 = 2) = \alpha_2 + \beta_2 Y_{11} + e_2, \text{ where } e_2 \sim N(0, \sigma_{A_2}^2)
$$

\n
$$
Y_{2_{21}} = Y_2|(Z_1 = 2, Z_2 = 1) = \alpha_3 + \beta_3 Y_{12} + e_1, \text{ where } e_3 \sim N(0, \sigma_{A_1}^2)
$$

\n
$$
Y_{2_{22}} = Y_2|(Z_1 = 2, Z_2 = 2) = \alpha_4 + \beta_4 Y_{12} + e_2, \text{ where } e_4 \sim N(0, \sigma_{A_2}^2)
$$

where α_i and β_i are parameters, $i = 1, 2, 3, 4$ and $\sigma_{A_k}^2$ is the variance added by etcher k, $k=1,2.$ The expected value of Y_{2jk} from each combination is

$$
\mu_{211} = E(Y_{211}) = E[Y_2|(Z_1 = 1, Z_2 = 1)] = \alpha_1 + \beta_1 \mu_{11}
$$

\n
$$
\mu_{212} = E(Y_{212}) = E[Y_2|(Z_1 = 1, Z_2 = 2)] = \alpha_2 + \beta_2 \mu_{11}
$$

\n
$$
\mu_{221} = E(Y_{221}) = E[Y_2|(Z_1 = 2, Z_2 = 1)] = \alpha_3 + \beta_3 \mu_{12}
$$

\n
$$
\mu_{222} = E(Y_{222}) = E[Y_2|(Z_1 = 2, Z_2 = 2)] = \alpha_4 + \beta_4 \mu_{12}.
$$

The variance of $Y_{2_{jk}}$ from each combination is

$$
\sigma_{2_{11}}^2 = Var(Y_{2_{11}}) = Var[Y_2|(Z_1 = 1, Z_2 = 1)] = \beta_1^2 \sigma_{11}^2 + \sigma_{A_1}^2
$$

\n
$$
\sigma_{2_{12}}^2 = Var(Y_{2_{12}}) = Var[Y_2|(Z_1 = 1, Z_2 = 2)] = \beta_2^2 \sigma_{11}^2 + \sigma_{A_2}^2
$$

\n
$$
\sigma_{2_{21}}^2 = Var(Y_{2_{21}}) = Var[Y_2|(Z_1 = 2, Z_2 = 1)] = \beta_3^2 \sigma_{12}^2 + \sigma_{A_1}^2
$$

\n
$$
\sigma_{2_{22}}^2 = Var(Y_{2_{22}}) = Var[Y_2|(Z_1 = 2, Z_2 = 2)] = \beta_4^2 \sigma_{12}^2 + \sigma_{A_2}^2.
$$

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We assume that workload is evenly distributed through the combinations mentioned above and each stepper (etcher) is independent of the others, respectively. Thus, the expected value of *Y*2 (FI CD) is

$$
E(Y_2) = \frac{1}{4} \Big(\sum_{i=1}^{4} \alpha_i + \mu_{11}(\beta_1 + \beta_2) + \mu_{12}(\beta_3 + \beta_4) \Big) = \mu_2 \quad \text{(See section A.2.2 in Appendix)}.
$$

Thus, the variance of Y_2 is

$$
Var(Y_2) = E(Y_2^2) - [E(Y_2)]^2
$$

= $\frac{1}{4} \Big\{ \sigma_{11}^2 (\beta_1^2 + \beta_2^2) + \sigma_{12}^2 (\beta_3^2 + \beta_4^2) + 2 \sum_{k=1}^2 \sigma_{A_k}^2 + (\alpha_1 + \beta_1 \mu_{11})^2 + (\alpha_2 + \beta_2 \mu_{11})^2 + (\alpha_3 + \beta_3 \mu_{12})^2 \Big\} - \frac{1}{16} \big((\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4) + \mu_{11} (\beta_1 + \beta_2) + \mu_{12} (\beta_3 + \beta_4) \big)^2$
(See section A.2.2 in Appendix).

Furthermore, we can compute the overall variance added by the etching operation as well. The overall variance added by the etching operation can be obtained by subtracting the variance transmitted through the etching operation.

$$
\sigma_A^2 = Var(Y_2) - \beta^2 \sigma_1^2
$$

= $\frac{1}{4} \Big\{ \sigma_{11}^2 (\beta_1^2 + \beta_2^2) + \sigma_{12}^2 (\beta_3^2 + \beta_4^2) + 2 \sum_{k=1}^2 \sigma_{A_k}^2 + (\alpha_1 + \beta_1 \mu_{11})^2 + (\alpha_2 + \beta_2 \mu_{11})^2 + (\alpha_3 + \beta_3 \mu_{12})^2$
+ $(\alpha_4 + \beta_4 \mu_{12})^2 \Big\} - \frac{1}{16} \big((\alpha_1 + \alpha_2 + \alpha_3 + \alpha_4) + \mu_{11} (\beta_1 + \beta_2) + \mu_{12} (\beta_3 + \beta_4) \big)^2 - \beta^2 \sigma_1^2$
where $\sigma_1^2 = \frac{1}{2} \Big(\sum_{j=1}^2 \sigma_{1j}^2 + (\mu_{1j} - \mu_1)^2 \Big).$

The result shows that the variance of the random variable Y_2 becomes more complicated and cumbersome as the number of etchers in operation increases.

As a special case, if a stepper is paired with a specific etcher (for instance, stepper $\#1(2)$) only works with etcher $\#1(2)$), more simplified model can be constructed (See Figure 4.4). Denote that Y_{2k} is the measurement of line width (FI CD) processed by etcher k ($k = 1, 2$). Suppose that

$$
Y_{21} = Y_2 | Z_2 = 1 = \alpha_1 + \beta_1 Y_{11} + e_1, \text{where } e_1 \sim N(0, \sigma_{A_1}^2)
$$

$$
Y_{22} = Y_2 | Z_2 = 2 = \alpha_2 + \beta_2 Y_{12} + e_2, \text{where } e_2 \sim N(0, \sigma_{A_2}^2)
$$

where α_i and β_i are parameters, $i = 1, 2$ and $\sigma_{A_k}^2$ is the variance added by etcher k, $k = 1, 2$.

We see that

$$
\mu_{21} = E(Y_2|Z_2 = 1) = \alpha_1 + \beta_1 \mu_{11}
$$

$$
\mu_{22} = E(Y_2|Z_2 = 2) = \alpha_2 + \beta_2 \mu_{12}
$$

$$
\sigma_{21}^2 = Var(Y_2|Z_2 = 1) = \beta_1^2 \sigma_{11}^2 + \sigma_{A_1}^2
$$

$$
\sigma_{22}^2 = Var(Y_2|Z_2 = 2) = \beta_2^2 \sigma_{12}^2 + \sigma_{A_2}^2.
$$

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Figure 4.4: Photo and etch stages in a gate patterning process in model III.

If the workload is processed at equal proportion, $E(Y_2)$, $Var(Y_2)$ and σ_A^2 are

$$
E(Y_2) = \frac{\alpha_1 + \alpha_2 + \beta_1 \mu_{11} + \beta_2 \mu_{12}}{2}
$$

\n
$$
Var(Y_2) = \frac{\sum_{k=1}^2 \beta_k^2 \sigma_{1k}^2 + \sum_{k=1}^2 \sigma_{Ak}^2 + \sum_{k=1}^2 (\alpha_k + \beta_k \mu_{1k})^2}{2}
$$

\n
$$
-\frac{\sum_{k=1}^2 (\alpha_k + \beta_k \mu_{1k})^2}{4}
$$

\n
$$
\sigma_A^2 = \frac{\sum_{k=1}^2 \beta_k^2 \sigma_{1k}^2 + \sum_{k=1}^2 \sigma_{Ak}^2 + \sum_{k=1}^2 (\alpha_k + \beta_k \mu_{1k})^2}{2} - \frac{\sum_{k=1}^2 (\alpha_k + \beta_k \mu_{1k})^2}{4} - \beta^2 \sigma_1^2
$$

\nwhere $\sigma_1^2 = \frac{1}{2} \Big(\sum_{j=1}^2 \sigma_{1j}^2 + (\mu_{1j} - \mu_1)^2 \Big).$ (4.4)

4.3 Numerical example

The following is a simple numerical example for the second case introduced in the previous section. Suppose that we have

$$
Y_1|(Z_1 = 1) = Y_{11} \sim N(130.2, 14.5)
$$

$$
Y_1|(Z_1 = 2) = Y_{12} \sim N(129.8, 15.0)
$$

and each stepper has capability of processing 1,000 wafers on a daily basis and move them to a specific etcher and one measurement is captured from each wafer. We use the following straight line equations to estimate parameters $\alpha_1, \alpha_2, \beta_1$ and β_2 in equation.

$$
\widehat{y}_{21} = \widehat{\alpha}_1 + \widehat{\beta}_1 y_{11}
$$

$$
\widehat{y}_{22} = \widehat{\alpha}_2 + \widehat{\beta}_2 y_{12}.
$$

j.

For the purpose of simulation, we use the following equations but we pretend not to know them.

$$
Y_{21} = -0.02 + 0.97Y_{11} + e_1, \text{ where } e_1 \sim N(0, 1.5)
$$

$$
Y_{22} = -0.03 + 0.98Y_{12} + e_2, \text{ where } e_2 \sim N(0, 1.2).
$$

Let us denote that Y_{1jk} is the measurement of Y_1 from stepper j for wafer k and Y_{2jk} is the measurement of Y_2 from etcher j for wafer k $(k = 1, 2, \dots, 1000; j = 1, 2)$.

Here are the estimates for parameters.

$$
\begin{aligned}\n\hat{\sigma}_{11}^{2} &= \sum_{k=1}^{1000} (y_{11k} - \bar{y}_{11})^{2} / 1000 = 15.6328 \\
\hat{\sigma}_{12}^{2} &= \sum_{k=1}^{1000} (y_{12k} - \bar{y}_{12})^{2} / 1000 = 15.1519 \\
\hat{\sigma}_{1}^{2} &= \sum_{j=1}^{1000} \sum_{k=1}^{1000} (y_{1jk} - \bar{y}_{1})^{2} / 2000 = 15.4634 \\
\hat{\sigma}_{2}^{2} &= \sum_{j=1}^{2} \sum_{k=1}^{1000} (y_{2jk} - \bar{y}_{2})^{2} / 2000 = 16.3839 \\
\hat{\beta}_{1} &= \begin{cases}\n1000 \sum_{k=1}^{1000} y_{11k}y_{21k} - \sum_{k=1}^{1000} y_{11k} \sum_{k=1}^{1000} y_{21k} \end{cases} / \begin{cases}\n1000 \sum_{k=1}^{1000} y_{11k}^{2} - \left(\sum_{k=1}^{1000} y_{11k}\right)^{2}\right) = 0.9692 \\
\hat{\alpha}_{1} &= \bar{y}_{21} - \hat{\beta}_{1}\bar{y}_{11} = 0.0422 \\
\hat{\beta}_{2} &= \begin{cases}\n1000 \sum_{k=1}^{1000} y_{12k}y_{22k} - \sum_{k=1}^{1000} y_{12k} \sum_{k=1}^{1000} y_{22k} \end{cases} / \begin{cases}\n1000 \sum_{k=1}^{1000} y_{12k}^{2} - \left(\sum_{k=1}^{1000} y_{12k}\right)^{2}\right) = 0.9960 \\
\hat{\alpha}_{2} &= \bar{y}_{22} - \hat{\beta}_{2}\bar{y}_{12} = -2.1300 \\
\hat{\beta} &= \begin{cases}\n2000 \sum_{j=1}^{2} \sum_{k=1}^{1000} y_{1jk}y_{2jk} - \sum_{j=1}^{2} \sum_{k=1}^{1000} y
$$

į.

Now, by using Equation (4.4) and replacing the parameters by the estimates calculated above, we obtain the estimate of $Var(Y_2) = 16.3622$, which provides good agreement with the result (4.5). The estimate of variation transmitted $(\widehat{\beta}^2 \widehat{\sigma}_1^2)$ is 14.5825 and the estimate of variation added $(\hat{\sigma}_A^2)$ by etching operation is 1.7798. Thus, in our numerical example, the variance added by etching operation accounts for about 11% of the total variance of Y_2 . It is observed that most contribution comes from Y_1 (DI CD).

Chapter 5

Conclusions

The multivariate exponentially weighted moving average (MEWMA) control chart is an extension of the well-known univariate EWMA chart applicable where product quality is characterized by two or more variables. It contains the well-known Shewhart chi-squared chart as a particular case. Several aspects of the run length distribution not studied before are discussed in detail in this thesis. The methods are applied to the problem of monitoring a semiconductor manufacturing process where bivariate quality is measured. The thesis also discusses methods to model and quantify variability built in a manufacturing process.

The previous study for the MEWMA by Runger and Prabhu (1997) was concentrated on two areas: the on-target run length analysis and the off-target run length analysis. For the on-target analysis, we derive the probability mass function, the second, third and fourth moment of the run length distribution as closed forms respectively. When the off-target case was analyzed before, it was assumed that the process mean shift happened at the beginning of the operation (the zero-state case). We introduce a general off-target form such that the mean shift can happen at any time, including the beginning of the operation (the steady-state case). Here is a generalization of the probability mass function of the run length distribution for the MEWMA control chart.

$$
f(n) = P(N = n) = \begin{cases} s' P_0^{n-1} (I - P_0) 1 & \text{if } n = 1, 2, ..., \tau - 1, \\ s' P_0^{n-1} P_1^{n-r} (I - P_1) 1 & \text{if } n = \tau, \tau + 1, ... \end{cases}
$$

where P_0 is an in-control transition matrix and P_1 is an out-of-control transition matrix. With the general probability mass function, more derivations are made and all the results are consistent with those of past studies.

The MEWMA scheme is well-known for detecting a small shift and a good way to improve the ability to detect a small shift is to find an optimum smoothing parameter. In the general off-target case ($\tau \geq 1$), the smoothing parameter shows the optimum parameter value increases as transition time (τ) increases. Moreover, as either the in-control average run length $(ARL₀)$ or the number of variables (p) increases, the optimum parameter value increases slowly to the change of transition time τ .

When a small shift happens at the beginning $(\tau = 1)$, the MEWMA control chart is very effective in detecting the change. Our interest is how the control chart behaves in case that a process change happens at a different transition time. Even though the transition time changes, just as in the previous case, the MEWMA control chart still outperforms the multivariate Shewhart control chart in performance when the shift is small. Otherwise both control charts perform well.

As an application, we suggest a bivariate normal distribution model for the MEWMA control chart and apply the model to the main semiconductor manufacturing processes. Since the critical dimension of polysilicon gate has been continued to shrink, the impact of environment errors can not be negligible any more and the tighter control over the DI CD and FI CD is required. The model is defined as follows.

$$
\mathbf{X}=(X_1,\alpha+\beta X_1+\epsilon)'\sim N(\boldsymbol{\mu_0},\boldsymbol{\Sigma_X}), \text{ where } \boldsymbol{\mu_0} \text{ is the process mean in control.}
$$

The variation transmission model suggested by Lawless et al. (1999) is based on that products processed by a multiple of machines, move from one operation to the next stage and are processed by a machine. Since semiconductor manufacturing is composed of hundreds of processes, it is more realistic to consider the case that products are processed by a multiple of machines from one stage to another. We suggest an extension for the original variation transmission model. By using the extended model, the total variance transmitted can be calculated.

 \mathbb{T} $\hat{\boldsymbol{\beta}}$ $\frac{1}{4}$

 $\frac{1}{4}$

Appendix A

Derivations

A.I Kronecker product

Let *A* be an $n \times p$ matrix and *B* be an $m \times q$ matrix . The $mn \times pq$ matrix

$$
A \otimes B = \begin{pmatrix} a_{1,1}B & \cdots & a_{1,p}B \\ a_{2,1}B & \cdots & a_{2,p}B \\ \vdots & \ddots & \vdots \\ a_{n,1}B & \cdots & a_{n,p}B \end{pmatrix}
$$

 \mathbf{r}

is called the Kronecker product of \boldsymbol{A} and \boldsymbol{B} .

For example, let
$$
A = \begin{pmatrix} 2 & 1 & 3 \\ 4 & 2 & 5 \end{pmatrix}
$$
 and $B = \begin{pmatrix} 1 & 2 \\ 3 & 4 \end{pmatrix}$.

\n $A \otimes B = \begin{pmatrix} 2 & 4 & 1 & 2 & 3 & 6 \\ 6 & 8 & 3 & 4 & 9 & 12 \\ 4 & 8 & 2 & 4 & 5 & 10 \\ 12 & 16 & 6 & 8 & 15 & 20 \end{pmatrix}$

 $\ddot{}$

A.2 Derivations

A.2.1 Derivation of the mean and variance in the transmission model I

Let $\mu_{1j} = E(Y_1|Z_1 = j)$ and $\sigma_{1j}^2 = Var(Y_1|Z_1 = j)$ where $j = 1, 2$. Given that the stepper j is in operation, μ_{1j} and σ_{1j}^2 are the expected value and variance of the measurement Y_1 respectively. Since each stepper processes the parts at equal proportion, it is assumed that $P(Z_1 = 1) = P(Z_1 = 2) = \frac{1}{2}$. The expected value of Y_1 is

$$
E(Y_1) = \sum_{j=1}^{2} \{ E(Y_1 | Z_1 = j) P(Z_1 = j) \} = \frac{1}{2} \sum_{j=1}^{2} E(Y_1 | Z_1 = j)
$$

since $P(Z_1 = j) = \frac{1}{2}$.

Thus,
$$
E(Y_1) = (1/2) \sum_{j=1}^{2} \mu_{1j} = \mu_1.
$$
 (A.1)

The conditional expectation of Y_1^2 is

$$
E(Y_1^2|Z_1=j) = Var(Y_1|Z_1=j) + [E(Y_1|Z_1=j)]^2 = \sigma_{1j}^2 + \mu_{1j}^2.
$$

Thus, the second moment of Y_1 can be expressed as follows.

$$
E(Y_1^2) = \sum_{j=1}^2 \{ E(Y_1^2 | Z_1 = j) P(Z_1 = j) \}
$$

=
$$
\sum_{j=1}^2 \{ (\sigma_{1j}^2 + \mu_{1j}^2) P(Z_1 = j) \} = \frac{1}{2} \sum_{j=1}^2 (\sigma_{1j}^2 + \mu_{1j}^2)
$$

=
$$
\frac{1}{2} \sum_{j=1}^2 \sigma_{1j}^2 + \frac{1}{2} \sum_{j=1}^2 \mu_{1j}^2.
$$

Thus, for the variance of Y_1 , $\sigma_1^2 = Var(Y_1) = E(Y_1^2) - [E(Y_1)]^2 = \frac{1}{2} \sum_{i=1}^{3} \sigma_{1j}^2 + \frac{1}{2} \sum_{i=1}^{3} \mu_{1j}^2 - \mu_1^2$. $j=1$ $j=1$
Since it is known that

$$
\sum_{j=1}^{2} (\mu_{1j} - \mu_1)^2 = \sum_{j=1}^{2} (\mu_{1j}^2 - 2\mu_1 \mu_{1j} + \mu_1^2)
$$

=
$$
\sum_{j=1}^{2} \mu_{1j}^2 - 2\mu_1 \sum_{j=1}^{2} \mu_{1j} + 2\mu_1^2 = \sum_{j=1}^{2} \mu_{1j}^2 - 2\mu_1 (2\mu_1) + 2\mu_1^2
$$

=
$$
\sum_{j=1}^{2} \mu_{1j}^2 - 4\mu_1^2 + 2\mu_1^2 = \sum_{j=1}^{2} \mu_{1j}^2 - 2\mu_1^2
$$

$$
\frac{1}{2} \sum_{j=1}^{2} \mu_{1j}^2 - 2\mu_1^2 = \frac{1}{2} \sum_{j=1}^{2} \mu_{1j}^2 - \mu_1^2 = \frac{1}{2} \sum_{j=1}^{2} (\mu_{1j} - \mu_1)^2.
$$

 \bar{z}

we obtain

$$
\frac{1}{2}\sum_{j=1}^{2}\mu_{1j}^{2}-2\mu_{1}^{2}=\frac{1}{2}\sum_{j=1}^{2}\mu_{1j}^{2}-\mu_{1}^{2}=\frac{1}{2}\sum_{j=1}^{2}(\mu_{1j}-\mu_{1})^{2}.
$$

Hence, the variance of Y*1* is

$$
\sigma_1^2 = Var(Y_1) = E(Y_1^2) - [E(Y_1)]^2
$$

= $\frac{1}{2} \sum_{j=1}^{2} \sigma_{1j}^2 + \frac{1}{2} \sum_{j=1}^{2} (\mu_{1j} - \mu_1)^2$.

A.2.2 Derivation of the mean and variance in the transmission model II

$$
E(Y_2) = \sum_{j=1}^{2} \sum_{k=1}^{2} \{ E(Y_2 | Z_1 = j, Z_2 = k) P(Z_1 = j) P(Z_2 = k | Z_1 = j) \}.
$$

For simplicity, we assume that $P(Z_1 = j)P(Z_2 = k | Z_1 = j) = \frac{1}{4}$ where $j, k = 1, 2$. Thus, we obtain

$$
E(Y_2) = \frac{1}{4} \sum_{j=1}^{2} \sum_{k=1}^{2} E(Y_2 | Z_1 = j, Z_2 = k)
$$

=
$$
\frac{1}{4} \left(\sum_{i=1}^{4} \alpha_i + \mu_{11}(\beta_1 + \beta_2) + \mu_{12}(\beta_3 + \beta_4) \right) = \mu_2.
$$

The conditional expectation of Y_2^2 is

$$
E(Y_2^2|Z_1=j, Z_2=k)=Var(Y_2|Z_1=j, Z_2=k)+[E(Y_2|Z_1=j, Z_2=k)]^2=\sigma_{2jk}^2+\mu_{2jk}^2.
$$

 $\bar{\Sigma}$

Thus, the second moment of \mathcal{Y}_2 is

$$
E(Y_2^2) = \sum_{j=1}^2 \sum_{k=1}^2 \{ E(Y_2^2 | Z_1 = j, Z_2 = k) P(Z_1 = j) P(Z_2 = k | Z_1 = j) \}
$$

\n
$$
= \sum_{j=1}^2 \sum_{k=1}^2 \{ (\sigma_{2jk}^2 + (\mu_{2jk})^2 P(Z_1 = j) P(Z_2 = k | Z_1 = j) \}
$$

\n
$$
= \frac{1}{4} \sum_{j=1}^2 \sum_{k=1}^2 (\sigma_{2jk}^2 + \mu_{2jk}^2)
$$

\n
$$
= \frac{1}{4} \{ \sigma_{11}^2 (\beta_1^2 + \beta_2^2) + \sigma_{12}^2 (\beta_3^2 + \beta_4^2) + 2 \sum_{k=1}^2 \sigma_{A_k}^2 + (\alpha_1 + \beta_1 \mu_{11})^2 + (\alpha_2 + \beta_2 \mu_{11})^2 + (\alpha_3 + \beta_3 \mu_{12})^2
$$

\n
$$
+ (\alpha_4 + \beta_4 \mu_{12})^2 \}.
$$

A.2.3 Identities

Identity 1. *For every positive integer a,*

$$
I + P + P2 + \cdots Pa-1 = (I - Pa)(I - P)-1 = (I - P)-1(I - Pa). \qquad (A.2)
$$

Proof·

$$
(I + P + P2 + \dots + Pa-2 + Pa-1)(I - P)
$$

= $(I + P + P2 + \dots + Pa-2 + Pa-1) - (I + P + P2 + \dots + Pa-2 + Pa-1 + Pa)$
= $I - Pa$.

Thus, $(I + P + P^2 + \cdots + P^{a-2} + P^{a-1})(I - P) = I - P^a$. Multiplying on the right on both sides by $(I - P)^{-1}$ yields

$$
(I + P + P2 + \cdots + Pa-2 + Pa-1) = (I - Pa)(I - P)-1.
$$

Identity 2. For every positive integer a,

$$
I+2P+3P^{2}+\cdots+aP^{a-1}=[I+(aP-(a+1)I)P^{a}](I-P)^{-2}=(I-P)^{-2}[I+(aP-(a+1)I)P^{a}].
$$
\n(A.3)

 $\bar{1}$

Proof.

$$
[I + 2P + 3P^{2} + 4P^{3} + \dots + (a - 2)P^{a-3} + (a - 1)P^{a-2} + aP^{a-1}](I - P)^{-2}
$$
\n
$$
= [I + 2P + 3P^{2} + 4P^{3} + \dots + (a - 2)P^{a-3} + (a - 1)P^{a-2} + aP^{a-1}](I - 2P + P^{2})
$$
\n
$$
= I + 2P + 3P^{2} + 4P^{3} + \dots + aP^{a-1} - (2P + 4P^{2} + 6P^{3} + \dots + 2(a - 1)P^{a-1} + 2aP^{a})
$$
\n
$$
+ P^{2} + 2P^{3} + \dots + (a - 2)P^{a-1} + (a - 1)P^{a} + aP^{a+1}
$$
\n
$$
= I - 2aP^{a} + (a - 1)P^{a} + aP^{a+1}
$$
\n
$$
= I - (a + 1)P^{a} + aP^{a+1}
$$
\n
$$
= I + [aP - (a + 1)I]P^{a}.
$$
\nThus [I + 3P + 3P^{2} + 4P^{3}] = |aP^{a-1}|(I - P)^{2} = I + [aP - (a + 1)I]P^{a}

Thus, $[I + 2P + 3P^2 + 4P^3 + \cdots + aP^{a-1}](I - P)^2 = I + [aP - (a+1)I]P^a$. Multiplying on the right both sides by $(I - P)^{-2}$ yields $I + 2P + 3P^2 + 4P^3 + \cdots + aP^{a-1} = [I + (aP - (a+1)I)P^a](I - P)^{-2}$. Similarly, we can show that

$$
I + 2P + 3P^{2} + 4P^{3} + \cdots + aP^{a-1} = (I - P)^{-2}[I + (aP - (a+1)I)P^{a}].
$$

Identity 3. *For every positive integer a,*

$$
(2 \cdot 1)I + (3 \cdot 2)P + (4 \cdot 3)P^{2} + \dots + a(a-1)P^{a-2}
$$

=
$$
[2I - a(a+1)P^{a-1} + 2(a-1)(a+1)P^{a} - a(a-1)P^{a+1}](I - P)^{-3}
$$

=
$$
(I - P)^{-3}[2I - a(a+1)P^{a-1} + 2(a-1)(a+1)P^{a} - a(a-1)P^{a+1}].
$$
 (A.4)

 $\label{eq:3} \begin{split} \mathcal{L}_{\text{in}}(\mathcal{L}_{\text{in}}) = \mathcal{L}_{\text{in}}(\mathcal{L}_{\text{out}}) = \mathcal{L}_{\text{out}}(\mathcal{L}_{\text{out}}) \end{split}$

Proof·

$$
[(2 \cdot 1)I + (3 \cdot 2)P + (4 \cdot 3)P^{2} + \dots + a(a-1)P^{a-2}](I - P)^{3}
$$

=
$$
[(2 \cdot 1)I + (3 \cdot 2)P + (4 \cdot 3)P^{2} + \dots + a(a-1)P^{a-2}](I - 3P + 3P^{2} - P^{3})
$$

=
$$
2I - a(a+1)P^{a-1} + 2(a-1)(a+1)P^{a} - a(a-1)P^{a+1}.
$$
 (A.5)

Multiplying by
$$
(I - P)^{-3}
$$
 on the right-hand side of both sides yields
\n $(2 \cdot 1)I + (3 \cdot 2)P + (4 \cdot 3)P^2 + \cdots + a(a-1)P^{a-2}$
\n $= [2I - a(a+1)P^{a-1} + 2(a-1)(a+1)P^a - a(a-1)P^{a+1}](I - P)^{-3}.$
\nSimilarly, we can show that
\n $(2 \cdot 1)I + (3 \cdot 2)P + (4 \cdot 3)P^2 + \cdots + a(a-1)P^{a-2}$
\n $= (I - P)^{-3}[2I - a(a+1)P^{a-1} + 2(a-1)(a+1)P^a - a(a-1)P^{a+1}].$

Identity 4. *For every positive integer a,*

$$
(3 \cdot 2 \cdot 1) \mathbf{I} + (4 \cdot 3 \cdot 2) \mathbf{P} + (5 \cdot 4 \cdot 3) \mathbf{P}^{2} + \dots + a(a-1)(a-2) \mathbf{P}^{a-3}
$$

=
$$
[(3 \cdot 2 \cdot 1) \mathbf{I} - (a-1)a(a+1) \mathbf{P}^{a-2} + 3(a-2)a(a+1) \mathbf{P}^{a-1}
$$

$$
-3(a-2)(a-1)(a+1) \mathbf{P}^{a} + (a-2)(a-1)a \mathbf{P}^{a+1}](\mathbf{I} - \mathbf{P})^{-4}
$$

=
$$
(\mathbf{I} - \mathbf{P})^{-4}[(3 \cdot 2 \cdot 1)\mathbf{I} - (a-1)a(a+1) \mathbf{P}^{a-2} + 3(a-2)a(a+1) \mathbf{P}^{a-1}
$$

$$
-3(a-2)(a-1)(a+1) \mathbf{P}^{a} + (a-2)(a-1)a \mathbf{P}^{a+1}]. \tag{A.6}
$$

Proof·

$$
[(3 \cdot 2 \cdot 1)I + (4 \cdot 3 \cdot 2)P + (5 \cdot 4 \cdot 3)P^2 + \dots + a(a-1)(a-2)P^{a-3}]
$$

\n
$$
\times (I - P)^4 = [(3 \cdot 2 \cdot 1)I + (4 \cdot 3 \cdot 2)P + (5 \cdot 4 \cdot 3)P^2 + \dots + a(a-1)(a-2)P^{a-3}]
$$

\n
$$
\times (I - 4P + 6P^2 - 4P^3 + P^4)
$$

\n
$$
= (3 \cdot 2 \cdot 1)I - (a-1)a(a+1)P^{a-2} + 3(a-2)a(a+1)P^{a-1}
$$

\n
$$
-3(a-2)(a-1)(a+1)P^a + (a-2(a-1)aP^{a+1}).
$$

Multiplying by $(\boldsymbol{I}-\boldsymbol{P})^{-4}$ on the right both sides yields

$$
(3 \cdot 2 \cdot 1) \mathbf{I} + (4 \cdot 3 \cdot 2) \mathbf{P} + (5 \cdot 4 \cdot 3) \mathbf{P}^2 + \dots + a(a-1)(a-2) \mathbf{P}^{a-3}
$$

=
$$
[(3 \cdot 2 \cdot 1) \mathbf{I} - (a-1)a(a+1) \mathbf{P}^{a-2} + 3(a-2)a(a+1) \mathbf{P}^{a-1}
$$

$$
-3(a-2)(a-1)(a+1) \mathbf{P}^a + (a-2(a-1)a \mathbf{P}^{a+1})(\mathbf{I} - \mathbf{P})^{-4}.
$$

Similarly, we can show that

$$
(3 \cdot 2 \cdot 1) \mathbf{I} + (4 \cdot 3 \cdot 2) \mathbf{P} + (5 \cdot 4 \cdot 3) \mathbf{P}^2 + \dots + a(a-1)(a-2) \mathbf{P}^{a-3}
$$

= $(\mathbf{I} - \mathbf{P})^{-4} [(3 \cdot 2 \cdot 1) \mathbf{I} - (a-1)a(a+1) \mathbf{P}^{a-2} + 3(a-2)a(a+1) \mathbf{P}^{a-1}$
 $-3(a-2)(a-1)(a+1) \mathbf{P}^a + (a-2(a-1)a \mathbf{P}^{a+1}].$

Identity 5. For every positive integer a,

$$
(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} + (5 \cdot 4 \cdot 3 \cdot 2) \mathbf{P} + (6 \cdot 5 \cdot 4 \cdot 3) \mathbf{P}^{2} + \dots + a(a-1)(a-2)(a-3) \mathbf{P}^{a-4}
$$

\n
$$
= [(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} - (a-2)(a-1)a(a+1) \mathbf{P}^{a-3} + 4(a-3)(a-1)a(a+1) \mathbf{P}^{a-2}
$$

\n
$$
-6(a-3)(a-2)a(a+1) \mathbf{P}^{a-1} + 4(a-3)(a-2)(a+1) \mathbf{P}^{a}
$$

\n
$$
-(a-3)(a-2)(a-1)a \mathbf{P}^{a+1}[(\mathbf{I} - \mathbf{P})^{-5}]
$$

\n
$$
= (\mathbf{I} - \mathbf{P})^{-5}[(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} - (a-2)(a-1)a(a+1) \mathbf{P}^{a-3} + 4(a-3)(a-1)a(a+1) \mathbf{P}^{a-2}
$$

\n
$$
-6(a-3)(a-2)a(a+1) \mathbf{P}^{a-1} + 4(a-3)(a-2)(a+1) \mathbf{P}^{a}
$$

\n
$$
-(a-3)(a-2)(a-1)a \mathbf{P}^{a+1}]. \tag{A.7}
$$

 $\label{eq:3.1} \frac{1}{\sqrt{2\pi}}\int_{0}^{\pi} \frac{1}{\sqrt{2\pi}}\left(\frac{1}{\sqrt{2\pi}}\right)^{2\pi} \frac{1}{\sqrt{2\pi}}\int_{0}^{\pi} \frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{1}{\sqrt{2\pi}}\frac{$

Proof.

$$
[(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} + (5 \cdot 4 \cdot 3 \cdot 2) \mathbf{P} + (6 \cdot 5 \cdot 4 \cdot 3) \mathbf{P}^{2} + \dots + a(a-1)(a-2)(a-3) \mathbf{P}^{a-4}]
$$

\n
$$
\times (\mathbf{I} - \mathbf{P})^{5} = [(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} + (5 \cdot 4 \cdot 3 \cdot 2) \mathbf{P} + (6 \cdot 5 \cdot 4 \cdot 3) \mathbf{P}^{2} + \dots + a(a-1)(a-2)(a-3) \mathbf{P}^{a-4}]
$$

\n
$$
\times (\mathbf{I} - 5\mathbf{P} + 10\mathbf{P}^{2} - 10\mathbf{P}^{3} + 5\mathbf{P}^{4} - \mathbf{P}^{5})
$$

\n
$$
= (4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} - (a-2)(a-1)a(a+1) \mathbf{P}^{a-3} + 4(a-3)(a-1)a(a+1) \mathbf{P}^{a-2}
$$

\n
$$
-6(a-3)(a-2)a(a+1) \mathbf{P}^{a-1} + 4(a-3)(a-2)(a+1) \mathbf{P}^{a}
$$

\n
$$
-(a-3)(a-2)(a-1)a \mathbf{P}^{a+1}.
$$

Multiplying by $(\boldsymbol{I}-\boldsymbol{P})^{-5}$ on the right both sides yields

$$
(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} + (5 \cdot 4 \cdot 3 \cdot 2) \mathbf{P} + (6 \cdot 5 \cdot 4 \cdot 3) \mathbf{P}^2 + \dots + a(a-1)(a-2)(a-3) \mathbf{P}^{a-4}
$$

=
$$
[(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} - (a-2)(a-1)a(a+1) \mathbf{P}^{a-3} + 4(a-3)(a-1)a(a+1) \mathbf{P}^{a-2}
$$

$$
-6(a-3)(a-2)a(a+1) \mathbf{P}^{a-1} + 4(a-3)(a-2)(a+1) \mathbf{P}^a
$$

$$
-(a-3)(a-2)(a-1)a \mathbf{P}^{a+1}](\mathbf{I} - \mathbf{P})^{-5}.
$$

Similarly, we can show that

$$
(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} + (5 \cdot 4 \cdot 3 \cdot 2) \mathbf{P} + (6 \cdot 5 \cdot 4 \cdot 3) \mathbf{P}^2 + \dots + a(a-1)(a-2)(a-3) \mathbf{P}^{a-4}
$$

= $(\mathbf{I} - \mathbf{P})^{-5} [(4 \cdot 3 \cdot 2 \cdot 1) \mathbf{I} - (a-2)(a-1)a(a+1) \mathbf{P}^{a-3} + 4(a-3)(a-1)a(a+1) \mathbf{P}^{a-2}$
-6(a-3)(a-2)a(a+1) \mathbf{P}^{a-1} + 4(a-3)(a-2)(a+1) \mathbf{P}^{a} - (a-3)(a-2)(a-1)a \mathbf{P}^{a+1}].

Since the matrix P is made up of transient states, $P^a \to 0$ as $a \to \infty$ (Karen, S. and Taylor, H. M., 1975, pp. 77). Taking the limit in Identities (1-5) yields the following identities.

$$
I + P + P2 + \dots = \sum_{n=1}^{\infty} P^{n-1} = (I - P)^{-1}.
$$
 (A.8)

$$
I + 2P + 3P^{2} + \dots = \sum_{n=1}^{\infty} nP^{n-1} = (I - P)^{-2}.
$$
 (A.9)

$$
(2 \cdot 1)I + (3 \cdot 2)P + (4 \cdot 3)P^{2} + \dots = \sum_{n=2}^{\infty} n(n-1)P^{n-2} = 2(I - P)^{-3}.
$$
 (A.10)

$$
(3 \cdot 2 \cdot 1) \mathbf{I} + (4 \cdot 3 \cdot 2) \mathbf{P} + (5 \cdot 4 \cdot 3) \mathbf{P}^2 + \dots = \sum_{n=3}^{\infty} n(n-1)(n-2) \mathbf{P}^{n-3} = 6(\mathbf{I} - \mathbf{P})^{-4}.
$$
 (A.11)

$$
(4\cdot3\cdot2\cdot1)I + (5\cdot4\cdot3\cdot2)P + (6\cdot5\cdot4\cdot3)P^2 + \dots = \sum_{n=4}^{\infty} n(n-1)(n-2)(n-3)P^{n-4} = 24(I-P)^{-5}.
$$
\n(A.12)

A.2.4 moments (on-target case)

Let *N* be a random variable and let *k* be a positive integer. Then the kth *moment* of *N* is defined as ${\cal E}(N^k),$ if ${\cal E}(N^k)$ exists and is finite.

A.2.4.1 The first moment

The first moment of random variable N is defined as follows.

$$
E(N) = \sum_{n=1}^{\infty} n f(n) = \sum_{n=1}^{\infty} s' P_0^{n-1} (I - P_0) 1
$$

= $s' \left(\sum_{n=1}^{\infty} n P_0^{n-1} \right) (I - P_0) 1.$

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By equation (A.9)

$$
\sum_{n=1}^{\infty} n P_0^{n-1} = I + 2P_0 + 3P_0^2 + \dots = (I - P_0)^{-2}
$$

$$
E(N) = s'(I - P_0)^{-2}(I - P_0)1 = s'(I - P_0)^{-1}1.
$$

A.2.4.2 The second moment

For the second moment, $E(N^2)$, compute $E[N(N-1)]$.

$$
E[N(N-1)] = \sum_{n=1}^{\infty} n(n-1)f(n) = \sum_{n=1}^{\infty} n(n-1)s'P_0^{n-1}(I-P_0)1
$$

= $s'\left(\sum_{n=1}^{\infty} n(n-1)P_0^{n-1}\right)(I-P_0)1.$

By equation (A.10)

$$
\sum_{n=1}^{\infty} n(n-1) P_0^{n-1} = \sum_{n=2}^{\infty} n(n-1) P_0^{n-1} = P_0 \sum_{n=2}^{\infty} n(n-1) P_0^{n-2}
$$

= $P_0 \cdot 2(I - P_0)^{-3} = 2P_0(I - P_0)^{-3}$.

Thus,

$$
E[N(N-1)] = s'(2P_0(I - P_0)^{-3})(I - P_0)1 = 2s'P_0(I - P_0)^{-2}1.
$$

Therefore, the second moment, ${\cal E}(N^2)$ is

$$
E(N^{2}) = 2s'P_{0}(I - P_{0})^{-2}1 + E(N) = 2s'P_{0}(I - P_{0})^{-2}1 + s'(I - P_{0})^{-1}1.
$$

A.2.4.3 The **third** moment

For the third moment, $E(N^3)$, consider $E[N(N-1)(N-2)]$.

$$
E[N(N-1)(N-2)] = \sum_{n=2}^{\infty} n(n-1)(n-2)f(n) = \sum_{n=2}^{\infty} n(n-1)(n-2)s'P_0^{n-1}(I-P_0)1
$$

= $s'\left(\sum_{n=2}^{\infty} n(n-1)(n-2)P_0^{n-1}\right)(I-P_0)1.$

By equation (A.II)

$$
\sum_{n=2}^{\infty} n(n-1)(n-2)P_0^{n-1} = \sum_{n=3}^{\infty} n(n-1)(n-2)P_0^{n-1} = P_0^2 \sum_{n=3}^{\infty} n(n-1)(n-2)P_0^{n-3}
$$

= $P_0^2 \cdot 6(I-P_0)^{-4} = 6P_0^2(I-P_0)^{-4}$.

Thus,

$$
E[N(N-1)(N-2)] = s'\left(6P_0^2(I-P_0)^{-4}\right)(I-P_0)1 = 6s'P_0^2(I-P_0)^{-3}1.
$$

Therefore, the third moment, $E(N^3)$ is

$$
E(N^3) = 6s'P_0^2(I - P_0)^{-3}1 + 3E(N^2) - 2E(N)
$$

= $6s'P_0^2(I - P_0)^{-3}1 + 3(2s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1) - 2s'(I - P_0)^{-1}1$
= $6s'P_0^2(I - P_0)^{-3}1 + 6s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1.$

A.2.4.4 The fourth moment

For the fourth moment, $E(N^4)$, consider $E[N(N-1)(N-2)(N-3)]$.

$$
E[N(N-1)(N-2)(N-3)] = \sum_{n=3}^{\infty} n(n-1)(n-2)(n-3)f(n)
$$

=
$$
\sum_{n=3}^{\infty} n(n-1)(n-2)(n-3)s'P_0^{n-1}(I-P_0)1
$$

=
$$
s'\left(\sum_{n=3}^{\infty} n(n-1)(n-2)(n-3)P_0^{n-1}\right)(I-P_0)1.
$$

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÷,

By equation (A.12)

$$
\sum_{n=3}^{\infty} n(n-1)(n-2)(n-3)P_0^{n-1} = \sum_{n=4}^{\infty} n(n-1)(n-2)(n-3)P_0^{n-1}
$$

= $P_0^3 \sum_{n=4}^{\infty} n(n-1)(n-2)(n-3)P_0^{n-4} = P_0^3 \cdot 24(I-P_0)^{-5} = 24P_0^3(I-P_0)^{-5}.$ (A.13)

Thus,

$$
E[N(N-1)(N-2)(N-3)] = s'\left(24P_0^3(I-P_0)^{-5}\right)(I-P_0)1 = 24s'P_0^3(I-P_0)^{-4}1.
$$

Therefore, the fourth moment, ${\cal E}(N^4)$ is

$$
E(N^4) = 24s'P_0^3(I - P_0)^{-4}1 + 6E(N^3) - 11E(N^2) + 6E(N)
$$

= $24s'P_0^3(I - P_0)^{-4}1 + 6(6s'P_0^2(I - P_0)^{-3}1 + 6s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1)$
-11 $(2s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1) + 6s'(I - P_0)^{-1}1$
= $24s'P_0^3(I - P_0)^{-4}1 + 36s'P_0^2(I - P_0)^{-3}1 + 14s'P_0(I - P_0)^{-2}1 + s'(I - P_0)^{-1}1.$

A.2.5 Moments (off-target case)

A.2.5.1 The first moment

$$
E(N) = \sum_{n=1}^{\infty} nf(n) = \sum_{n=1}^{\tau-1} nf_1(n) + \sum_{n=\tau}^{\infty} nf_2(n)
$$

=
$$
\sum_{n=1}^{\tau-1} ns' P_0^{n-1} (I - P_0) 1 + \sum_{n=\tau}^{\infty} ns' P_0^{r-1} P_1^{n-\tau} (I - P_1) 1
$$

=
$$
s' \left\{ \left(\sum_{n=1}^{\tau-1} n P_0^{n-1} \right) (I - P_0) + P_0^{r-1} \left(\sum_{n=\tau}^{\infty} n P_1^{n-\tau} \right) (I - P_1) \right\} 1.
$$

Using Identity 2 (A.3), we get

$$
\sum_{n=1}^{\tau-1} n P_0^{n-1} = I + 2P_0 + 3P_0^2 + \dots + (\tau - 1)P_0^{\tau-2}
$$

= $(I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau-1})(I - P_0)^{-2}.$

Using equations $(A.8) - (A.9)$ we also get

$$
\sum_{n=\tau}^{\infty} n P_1^{n-\tau} = \sum_{n=\tau}^{\infty} (n-\tau+1) P_1^{n-\tau} + \sum_{n=\tau}^{\infty} (\tau-1) P_1^{n-\tau}
$$

= $(I+2P_1+3P_1^2+\cdots)+(\tau-1)(I+P_1+P_2+\cdots)$
= $(I-P_1)^{-2}+(\tau-1)(I-P_1)^{-1}.$

Thus,

$$
E(N) = s'\{[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau-1}](I - P_0)^{-2}(I - P_0)
$$

+ $P_0^{\tau-1}[(I - P_1)^{-2} + (\tau - 1)(I - P_1)^{-1}](I - P_1)\}$]
= $s'\{[I + (\tau - 1)P_0^{\tau} - \tau P_0^{\tau-1}](I - P_0)^{-1} + P_0^{\tau-1}[(I - P_1)^{-1} + (\tau - 1)]\}$]
= $s'\{[I + \tau P_0^{\tau} - P_0^{\tau} - \tau P_0^{\tau-1}](I - P_0)^{-1} + P_0^{\tau-1}(I - P_1)^{-1} + (\tau - 1)P_0^{\tau-1}\}$]
= $s'\{[I - P_0^{\tau} - \tau P_0^{\tau-1}(I - P_0)](I - P_0)^{-1} + P_0^{\tau-1}(I - P_1)^{-1} + \tau P_0^{\tau-1} - P_0^{\tau-1}\}$]
= $s'\{(I - P_0^{\tau})(I - P_0)^{-1} - \tau P_0^{\tau-1} + P_0^{\tau-1}(I - P_1)^{-1} + \tau P_0^{\tau-1} - P_0^{\tau-1}\}$]
= $s'\{(I - P_0^{\tau})(I - P_0)^{-1} - P_0^{\tau-1} + P_0^{\tau-1}(I - P_1)^{-1}\}$]
= $s'\{(I - P_0)^{-1}1 - s'P_0^{\tau}(I - P_0)^{-1}1 - s'P_0^{\tau-1}1 + s'P_0^{\tau-1}(I - P_1)^{-1}1$
= $s'(I - P_0)^{-1}1 - s'P_0^{\tau}(I - P_0)^{-1}1 - s'P_0^{\tau-1}1 + s'P_0^{\tau-1}(I - P_1)^{-1}1$
= $s'(I - P_0)^{-1}1 - s'P_0^{\tau}(I - P_0)^{-1}1 - s'P_0^{\tau-1}(I - P_0)(I - P_0)^{-1}1 + s'P_0^{\tau-1}(I - P_1)^{-1}$
= $s'[I - P_0^{\tau} - P_0^{\tau-1}$

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Therefore, $E(N) = s'[I - P_0^{\tau-1}](I - P_0)^{-1}1 + s'P_0^{\tau-1}(I - P_1)^{-1}1$. $(A.14)$

A.2.5.2 The second moment

$$
E[N(N-1)] = \sum_{n=1}^{\infty} n(n-1)f(n) = \sum_{n=1}^{\tau-1} n(n-1)f(n) + \sum_{n=\tau}^{\infty} n(n-1)f(n)
$$

=
$$
\sum_{n=1}^{\tau-1} n(n-1)s'P_0^{n-1}(I-P_0)1 + \sum_{n=\tau}^{\infty} n(n-1)s'P_0^{\tau-1}P_1^{n-\tau}(I-P_1)1
$$

=
$$
s' \left\{ \left(\sum_{n=1}^{\tau-1} n(n-1)P_0^{n-1} \right) (I-P_0) + P_0^{\tau-1} \left(\sum_{n=\tau}^{\infty} n(n-1)P_1^{n-\tau}(I-P_1) \right) \right\} 1.
$$

Using Identity 3 (A.4), we get

$$
\sum_{n=1}^{\tau-1} n(n-1)P_0^{n-1} = (2 \cdot 1)P_0 + (3 \cdot 2)P_0^2 + (4 \cdot 3)P_0^3 + \dots + (\tau - 1)(\tau - 2)P_0^{\tau-2}
$$

= $P_0[(2 \cdot 1)I + (3 \cdot 2)P_0 + (4 \cdot 3)P_0^2 + \dots + (\tau - 1)(\tau - 2)P_0^{\tau-3}]$
= $P_0[(2 \cdot 1)I + (3 \cdot 2)P_0 + (4 \cdot 3)P_0^2 + \dots + (\tau - 1)(\tau - 2)P_0^{\tau-3}]$
= $P_0[2I - (\tau - 1)\tau P_0^{\tau-2} + 2(\tau - 2)\tau P_0^{\tau-1} - (\tau - 1)(\tau - 2)P_0^{\tau}](I - P_0)^{-3}.$

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While using the identities in equations (A.8) - (A.10), we get

$$
\sum_{n=\tau}^{\infty} n(n-1)P_1^{n-\tau} = \sum_{n=\tau}^{\infty} \underbrace{(n-\tau+1+\tau-1)(n-1-\tau+1+\tau-1)}_{n-\tau+1} + \tau-1} + \tau-1)P_1^{n-\tau}
$$
\n
$$
= \sum_{n=\tau}^{\infty} [(n-\tau+1)(n-\tau)+(n-\tau+1)(\tau-1)+(\tau-1)(n-\tau)+(\tau-1)^2}]P_1^{n-\tau}
$$
\n
$$
= \sum_{n=\tau}^{\infty} [(n-\tau+1)(n-\tau)+(n-\tau)(\tau-1)+\tau-1+(\tau-1)(n-\tau)+\tau^2-2\tau+1]P_1^{n-\tau}
$$
\n
$$
= \sum_{n=\tau}^{\infty} [(n-\tau+1)(n-\tau)+2(n-\tau)(\tau-1)+\tau(\tau-1)]P_1^{n-\tau}
$$
\n
$$
= \sum_{n=\tau}^{\infty} (n-\tau+1)(n-\tau)P_1^{n-\tau} + 2(\tau-1) \sum_{n=\tau}^{\infty} (n-\tau)P_1^{n-\tau} + \tau(\tau-1) \sum_{n=\tau}^{\infty} P_1^{n-\tau}
$$
\n
$$
= (1 \cdot 0)I + (2 \cdot 1)P_1 + (3 \cdot 2)P_1^2 + (4 \cdot 3)P_1^3 + (5 \cdot 4)P_1^4 + \cdots
$$
\n
$$
+2(\tau-1)[0 \cdot I + P_1 + 2P_1^2 + 3P_1^3 + \cdots] + \tau(\tau-1)[I + P_1 + P_1^2 + P_1^3 \cdots]
$$
\n
$$
= P_1[(2 \cdot 1) + (3 \cdot 2)P_1 + (4 \cdot 3)P_1^2 + \cdots] + 2(\tau-1)P_1[I + 2P_1 + 3P_1^2]
$$
\n
$$
+ \tau(\tau-1)[I + P_1 + P_1^2 + \cdots]
$$
\n
$$
= 2P_1(I - P_1)^{-3} + 2(\tau-1)P_1(I - P_1)^{-2} + \tau(\tau-1)(I - P_1)^{-1}.
$$

Thus,

$$
E[N(N-1)] = s'\{P_0[2I - (\tau - 1)\tau P_0^{\tau - 2} + 2(\tau - 2)\tau P_0^{\tau - 1} - (\tau - 1)(\tau - 2)P_0^{\tau}](I - P_0)^{-2} + P_0^{\tau - 1}[2P_1(I - P_1)^{-2} + 2(\tau - 1)P_1(I - P_1)^{-1} + \tau(\tau - 1)I]\}.
$$

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Hence,

$$
E(N^{2}) = s'\{P_{0}[2I - (\tau - 1)\tau P_{0}^{\tau - 2} + 2(\tau - 2)\tau P_{0}^{\tau - 1} - (\tau - 1)(\tau - 2)P_{0}^{\tau}](I - P_{0})^{-2}
$$

+
$$
P_{0}^{\tau - 1}[2P_{1}(I - P_{1})^{-2} + 2(\tau - 1)P_{1}(I - P_{1})^{-1} + \tau(\tau - 1)I] + [I - P_{0}^{\tau - 1}](I - P_{0})^{-1}
$$

+
$$
P_{0}^{\tau - 1}(I - P_{1})^{-1}\}1.
$$

A.2.6 Conditional probability mass function and conditional expection

The conditional distribution of N , given that $N < \tau$ is defined as

$$
f(n|N < \tau) = \frac{f(n)}{P(N < \tau)} = \frac{s' P_0^{n-1} (I - P_0) 1}{1 - s' P_0^{\tau-1} 1} \quad n = 1, 2, \ldots, \tau - 1.
$$

The conditional expectation of $N,$ given that $N<\tau$ is defined as

$$
E(N|N < \tau) = \sum_{n=1}^{\tau-1} nf(n|N < \tau) = \sum_{n=1}^{\tau-1} n \frac{s' P_0^{n-1} (I - P_0) 1}{1 - s' P_0^{\tau-1} 1}
$$

=
$$
\frac{1}{1 - s' P_0^{\tau-1} 1} \sum_{n=1}^{\tau-1} n s' P_0^{n-1} (I - P_0) 1 = \frac{1}{1 - s' P_0^{\tau-1} 1} s' \left(\sum_{n=1}^{\tau-1} n P_0^{n-1} \right) (I - P_0) 1
$$

=
$$
\frac{1}{1 - s' P_0^{\tau-1} 1} s' \{ I + 2P_0 + 3P_0^2 + \dots + (\tau - 1) P_0^{\tau-2} \} (I - P_0) 1
$$

=
$$
\frac{1}{1 - s' P_0^{\tau-1} 1} s' \{ I + ((\tau - 1)P_0 - \tau I) P_0^{\tau-1} \} (I - P_0)^{-1} 1.
$$
 (A.15)

Additionally, the conditional distribution of $N,$ given that $N \geq \tau$ is defined as

$$
f(n|N \geq \tau) = \frac{f(n)}{P(N \geq \tau)} = \frac{s' P_0^{\tau-1} P_1^{n-\tau} (I - P_1) 1}{s' P_0^{\tau-1} 1} \quad n = \tau, \tau + 1, ...
$$

The conditional expectation of $N,$ given that $N\geq \tau$ is defined as

$$
E(N|N \geq \tau) = \sum_{n=\tau}^{\infty} nf(n|N \geq \tau) = \sum_{n=\tau}^{\infty} n \frac{s' P_0^{\tau-1} P_1^{n-\tau} (I - P_1) 1}{s' P_0^{\tau-1} 1}
$$

\n
$$
= \frac{1}{s' P_0^{\tau-1} 1} \sum_{n=\tau}^{\infty} n s' P_0^{\tau-1} P_1^{n-\tau} (I - P_1) 1 = \frac{1}{s' P_0^{\tau-1} 1} s' P_0^{\tau-1} \left(\sum_{n=\tau}^{\infty} n P_1^{n-\tau} \right) (I - P_1) 1
$$

\n
$$
= \frac{1}{s' P_0^{\tau-1} 1} s' P_0^{\tau-1} \{ \tau I + (\tau + 1) P_1 + (\tau + 2) P_1^2 + \cdots \} (I - P_1) 1
$$

\n
$$
= \frac{1}{s' P_0^{\tau-1} 1} s' P_0^{\tau-1} \{ (I - P_1)^{-2} + (\tau - 1) (I - P)^{-1} \} (I - P_1) 1
$$

\n
$$
= \frac{1}{s' P_0^{\tau-1} 1} s' \{ P_0^{\tau-1} (I - P_1)^{-1} + (\tau - 1) P_0^{\tau-1} \} 1.
$$
 (A.16)

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Appendix B

Programming (R- code)

B.l Markov chain algorithm for the calculation of ARL

ARL_Calculator<-function(r,h,d,p){

r is a smoothing parameter

h is a control limit

d is a mean shift

p is the number of variables

S is a starting vector

 $UCL < -sqrt(h*r/(2-r))$

m1<-25

m2<-25

g1<-2*UCL/(2*m1+1)

g2<-2*UCL/(2*m2+1)

H<-matrix(data=NA,nrow=2*m1+1,ncol=2*m1+1)

#[Defining an identity matrix and a vector of 1s]

```
z < - (2*m1+1)* (m2+1)
n1 < -c(z)I \leftarrow matrix(0, nrow=n1, ncol=n1)I[row(I) == col(I)] < -1one<- matrix(1,nrow=z,ncol=1)
```

```
#[Transition Matrix of Wt1] 
range1<-2*m1+1 # range1 is the number of states of Wt1 
for (i in 1:range1){ 
c_1 <- UCL + (i-0.5) * g1for (j in 1:range1){ 
up<-(-UCL+j*g1-(1-r)*c_i)/r-deltadown<-(-UCL+(j-1)*g1-(1-r)*c_i)/r-deltaH[i,j] <-pnorm(up,mean=O,sd=1)-pnorm(down,mean=O,sd=1) 
} 
} 
#[Transition Matrix of Wt2] 
range2<-m2+1 # range2 is the number of states of Wt2 
V<-matrix(data=NA,nrow=range2,ncol=range2) 
for (i \text{ in } 0:\text{m2}) {
c < - ((1-r)*i*g2/r) ^2
for (j \text{ in } 0:\text{m2}) {
if (j==O) { 
V[i+1,1]<-pchisq((0.5*(g2)/r)^2, df=p-1,ncp=c)} 
else { 
up < -((j+0.5)*g2/r)<sup>-2</sup>
```
Ť

```
down \frac{-((j-0.5)*g^2}{r})^2V[i+1,j+1] <-pchisq(up,df=p-1,ncp=c)-pchisq(down,df=p-1 ,ncp=c) 
} 
} 
} 
E<- kronecker(H,V) # Operating kronecker product 
#[Finding transient statesJ 
counter<-1 
for (alpha in 1:range1){ 
for (beta in 0: m2) {
if ((\text{alpha}-(m1+1))^2*\text{g1}^2+(\text{beta}*\text{g2})^2) = \text{UCL}^2({}E [, counterJ <-0 
E[counter,] <-0 
} 
counter<-counter+1 
} 
} 
temp<-solve(I-E)
ternp%*%one 
S <- matrix(0, nrow=z, ncol=1)start<-m1*(m2+1)+1S[start, 1]<-1ARL<-t(S)%*% temp%*%one
ARL 
}
```

```
77
```
B.2 On-target run length distribution

```
#On-target run length distribution 
OT_Dist<-function(x) { 
RL < -xSfunc <-NULL 
Pfunc<-NULL 
Tmatrix<-I 
range<-RL+1 
for (i in 1:range){ 
Sfunc[i]<-t(S)%*% Tmatrix %*%one 
Tmatrix <- Tmatrix %*%E # E is an on-target transition matrix 
} 
for (i \text{ in } 1:n){
Pfunc[i] < -Sfunc[i] - Stunc[i+1] #f(N) = P(N > n-1) - P(N > n)} 
plot(spline(seq(1,RL,by=i),Pfunc,n=200),type="1",col="blue",ylab="probability" 
,xlab="run length") 
}
```
B.3 Off-target run length distribution

```
#Off-target run length distribution 
Off_Dist<-function(x,t){ 
RL < -xtau<-t # tau is a mean shift time 
range1<-tau-1 
Sfunc<-NULL
```

```
Pfunc <-NULL 
TmatrixO<-I 
Tmatrix1<-Q # Q is a off-target transition matrix 
Tmatrix2<-I 
range2<-RL+1 
for (i in 1:range1){ 
Tmatrix2<- Tmatrix2%*%E 
} 
for (i in 1:range2){ 
if (i \leq tan){
Sfunc[i]<-t(S)%*% TmatrixO%*%one 
TmatrixO<- TmatrixO%*%E 
} 
else 
\{ Sfunc[i] <-t(S)%*% Tmatrix2%*%Tmatrix1%*%one
Tmatrix1<- Tmatrix1%*%Q}
} 
for (i \text{ in } 1:RL) {
Pfunc[i]<- Sfunc[i]- Sfunc[i+1] #f(N) = P(N > n-1) - P(N > n)} 
plot(spline(seq(1,RL,by=1),Pfunc,n=200),type="1",col="blue",ylab="probability",
xlab="run length") 
}
```
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B.4 The partition method

```
# The partition method 
# The following code is constructed 
# based on the condition that in-control ARL = 200, p = 4delta-1.5p < -4h_max<-30 # Initial upper control limit value 
h_min<-0.01 # Initial lower control limit value 
h_tem<-O 
ARL_tem<-O 
ARL_0<-200 # In-control ARL value 
epsilon<-0.01 # Degree of precision 
k < -1R_opt<-O # Initialization of smoothing parameter 
ARL<-NULL 
H<-NULL
ARL_opt<-ARL_O 
ARLLopt<-O 
for (i in 1:100){ 
r<-i/100 
h_t = \frac{h_t - m}{h_t} + h_t = \frac{m}{n}ARL_tem<-ARL_Calculator(r,h_tem,O,p) 
while(abs(ARL_0-ARL_tem)> epsilon)
{ 
if (ARL_tem > ARL_O)
```

```
{ 
h_max<-h_tem
h_t = (h_{max} + h_{min})/2ARL_tem<- ARL_Calculator(r,h_tem,O,p) 
} 
else 
{ 
h_min<-h_tem 
h_t = \frac{1}{2} h_max + h_{min} /2
ARL_tem<- ARL_Calculator(r,h_tem,O,p) 
} 
} 
ARL[k] <-ARL_Calculator(r,h_tem,delta,p) 
if(ARL_opt > ARL[k]) #If-statement to find the optimal smoothing parameter 
{ 
ARL_opt<-ARL[k] 
R_opt<-r 
} 
H[K]<-h_tk=k+1h_max<-30
h_{\text{min}}<-0.01h_tem<-O 
} 
R_opt 
ARL_opt
```
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Appendix C

Tables

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Table C.1: Optimal MEWMA Control Charts for τ ($1 \leq \tau \leq 200$), $p = 2$.

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| $p = 4, \delta = 1, ARL_0 = 200.00$ | | | | | | | | | | | |
|-------------------------------------|--------------|--------|--------|--------|--------|---------|---------|---------|---------|---------|---------|
| $\tau =$ | 1 | 20 | 40 | 60 | 80 | 100 | 120 | 140 | 160 | 180 | 200 |
| r | 0.13 | 0.14 | 0.15 | 0.16 | 0.18 | 0.19 | 0.19 | 0.20 | 0.21 | 0.22 | 0.23 |
| H | 13.203 | 13.324 | 13.433 | 13.532 | 13.703 | 13.778 | 13.778 | 13.846 | 13.909 | 13.967 | 14.021 |
| ARL_{min} | 12.061 | 29.304 | 46.078 | 61.167 | 74.751 | 86.985 | 98.010 | 107.949 | 116.910 | 124.995 | 132.290 |
| $p = 4, \delta = 1, ARL_0 = 300.00$ | | | | | | | | | | | |
| $\tau =$ | 1 | 20 | 40 | 60 | 80 | 100 | 120 | 140 | 160 | 180 | 200 |
| r | 0.12 | 0.12 | 0.13 | 0.14 | 0.15 | 0.15 | 0.16 | 0.17 | 0.17 | 0.18 | 0.18 |
| H | 14.156 | 14.156 | 14.282 | 14.395 | 14.495 | 14.495 | 14.586 | 14.669 | 14.669 | 14.744 | 14.744 |
| ARL_{min} | 13.197 | 30.834 | 48.652 | 65.263 | 80.758 | 95.213 | 108.707 | 121.292 | 133.046 | 144.019 | 154.267 |
| $p = 4, \delta = 1, ARL_0 = 400.00$ | | | | | | | | | | | |
| $\tau =$ | 1 | 20 | 40 | 60 | 80 | 100 | 120 | 140 | 160 | 180 | 200 |
| r | 0.11 | 0.11 | 0.12 | 0.13 | 0.13 | 0.14 | 0.14 | 0.15 | 0.15 | 0.16 | 0.16 |
| H | 14.777 | 14.777 | 14.913 | 15.032 | 15.032 | 15.139 | 15.139 | 15.234 | 15.234 | 15.320 | 15.320 |
| \overline{ARL}_{min} | 14.002 | 31.837 | 50.193 | 67.619 | 84.153 | 99.856 | 114.776 | 128.928 | 142.379 | 155.157 | 167.293 |
| $p = 4, \delta = 1, ARL_0 = 500.00$ | | | | | | | | | | | |
| $\tau =$ | $\mathbf{1}$ | 20 | 40 | 60 | 80 | 100 | 120 | 140 | 160 | 180 | 200 |
| \boldsymbol{r} | 0.11 | 0.11 | 0.11 | 0.12 | 0.12 | 0.13 | 0.13 | 0.13 | 0.14 | 0.14 | 0.15 |
| \overline{H} | 15.361 | 15.361 | 15.361 | 15.491 | 15.491 | 15.606 | 15.606 | 15.606 | 15.708 | 15.708 | 15.800 |
| ARL_{min} | 14.637 | 32.585 | 51.262 | 69.188 | 86.379 | 102.879 | 118.706 | 133.902 | 148.477 | 162.471 | 175.906 |

Table C.2: Optimal MEWMA Control Charts for τ ($1 \leq \tau \leq 200$), $p = 4$.

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Table C.3: Optimal MEWMA Control Charts for τ ($1 \leq \tau \leq 200$), $p = 6$.

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Table C.4: Optimal MEWMA Control Charts for τ ($1 \leq \tau \leq 200$), $p = 10$.

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| | Condition: $p = 2, m_1 = m_2 = 25, \tau = 1$ | | | | | | | | | |
|----------|--|---------|---------|---------|---------|---------|---------|---------|---------|---------|
| δ | $\overline{A}RL_0$ | 200 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 |
| | \boldsymbol{r} | 0.05 | 0.05 | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 |
| 0.5 | $H\,$ | 7.3813 | 8.3930 | 9.1058 | 9.2427 | 9.6975 | 10.0801 | 10.4102 | 10.7003 | 10.9589 |
| | ARL_{min} | 26.7482 | 30.3318 | 33.0044 | 35.0648 | 36.7685 | 38.2371 | 39.5312 | 40.6910 | 41.7433 |
| | \boldsymbol{r} | 0.14 | 0.13 | 0.12 | 0.12 | 0.12 | 0.11 | 0.11 | 0.11 | 0.11 |
| 1 | $H\,$ | 9.1602 | 9.9887 | 10.5367 | 11.0468 | 11.4612 | 11.6952 | 11.9983 | 12.2647 | 12.5023 |
| | ARL_{min} | 9.9857 | 10.9458 | 11.6374 | 12.1734 | 12.6198 | 12.9915 | 13.3169 | 13.6073 | 13.8697 |
| | \boldsymbol{r} | 0.25 | 0.24 | 0.22 | 0.22 | 0.21 | 0.20 | 0.20 | 0.20 | 0.19 |
| 1.5 | H_{\rm} | 9.8824 | 10.7268 | 11.2672 | 11.7522 | 12.1029 | 12.3901 | 12.6793 | 12.9338 | 13.1133 |
| | ARL_{min} | 5.4381 | 5.8736 | 6.1842 | 6.4261 | 6.6237 | 6.7923 | 6.9370 | 7.0660 | 7.1814 |
| | \boldsymbol{r} | 0.38 | 0.35 | 0.34 | 0.32 | 0.32 | 0.31 | 0.30 | 0.30 | 0.30 |
| 2 | \boldsymbol{H} | 10.2466 | 11.0450 | 11.6313 | 12.0602 | 12.4436 | 12.7466 | 13.0056 | 13.2528 | 13.4736 |
| | ARL_{min} | 3.5265 | 3.7737 | 3.9496 | 4.0863 | 4.1981 | 4.2927 | 4.3751 | 4.4475 | 4.5128 |
| | \boldsymbol{r} | 0.53 | 0.49 | 0.47 | 0.45 | 0.44 | 0.43 | 0.42 | 0.41 | 0.41 |
| 2.5 | H | 10.4333 | 11.2332 | 11.8071 | 12.2477 | 12.6132 | 12.9206 | 13.1854 | 13.4176 | 13.6341 |
| | ARL_{min} | 2.5152 | 2.6842 | 2.8021 | 2.8923 | 2.9656 | 3.0271 | 3.0802 | 3.1269 | 3.1688 |
| | \boldsymbol{r} | 0.68 | 0.65 | 0.63 | 0.61 | 0.59 | 0.58 | 0.57 | 0.56 | 0.5 |
| 3 | H | 10.5147 | 11.3238 | 11.8984 | 12.3426 | 12.7042 | 13.0125 | 13.2789 | 13.5135 | 13.7230 |
| | ARL_{min} | 1.8812 | 2.0064 | 2.0962 | 2.1656 | 2.2221 | 2.2696 | 2.3104 | 2.3461 | 2.3779 |

Table C.5: Optimal MEWMA Control Chart, $p = 2$, $\tau = 1$.

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| | | | | Condition: $p = 4, m_1 = m_2 = 25, \tau = 1$ | | | | | | |
|----------------|------------------|---------|---------|--|---------|---------|---------|---------|---------|---------|
| δ | ARL ₀ | 200 | 300 | 400 | 500 | 600 | 700 | 800 | 900 | 1000 |
| | \boldsymbol{r} | 0.05 | 0.04 | 0.04 | 0.04 | 0.04 | 0.04 | 0.03 | 0.03 | 0.03 |
| 0.5 | $\,H$ | 11.2683 | 11.9742 | 12.8373 | 13.4946 | 14.0240 | 14.4667 | 14.2589 | 14.6039 | 14.9105 |
| | ARL_{min} | 32.4380 | 36.9214 | 40.0895 | 42.6254 | 44.7534 | 46.5966 | 48.1545 | 49.4744 | 50.6670 |
| | \boldsymbol{r} | 0.13 | 0.12 | 0.11 | 0.11 | 0.10 | 0.10 | 0.10 | 0.09 | 0.09 |
| 1 | H | 13.2030 | 14.1561 | 14.7776 | 15.3613 | 15.6894 | 16.0888 | 16.4322 | 16.5786 | 16.8494 |
| | ARL_{min} | 12.0608 | 13.1970 | 14.0026 | 14.6367 | 15.1436 | 15.5777 | 15.9584 | 16.2920 | 16.5843 |
| | \boldsymbol{r} | 0.22 | 0.21 | 0.20 | 0.19 | 0.19 | 0.18 | 0.18 | 0.17 | 0.17 |
| 1.5 | H | 13.9672 | 14.9324 | 15.5921 | 16.0856 | 16.5332 | 16.8515 | 17.1768 | 17.4021 | 17.6579 |
| | ARL_{min} | 6.5072 | 7.0104 | 7.3673 | 7.6436 | 7.8705 | 8.0599 | 8.2255 | 8.3715 | 8.5006 |
| $\overline{2}$ | \boldsymbol{r} | 0.33 | 0.31 | 0.30 | 0.29 | 0.28 | 0.28 | 0.27 | 0.27 | 0.26 |
| | H | 14.3900 | 15.3181 | 15.9808 | 16.4855 | 16.8908 | 17.2546 | 17.5420 | 17.8186 | 18.0381 |
| | ARL_{min} | 4.1790 | 4.4617 | 4.6620 | 4.8172 | 4.9439 | 5.0512 | 5.1434 | 5.2252 | 5.2980 |
| 2.5 | r | 0.45 | 0.42 | 0.41 | 0.39 | 0.38 | 0.38 | 0.37 | 0.37 | 0.36 |
| | H | 14.6098 | 15.5253 | 16.1841 | 16.6766 | 17.0855 | 17.4413 | 17.7356 | 18.0061 | 18.2347 |
| | ARL_{min} | 2.9739 | 3.1563 | 3.2842 | 3.3827 | 3.4632 | 3.5311 | 3.5898 | 3.6419 | 3.6881 |
| | r | 0.61 | 0.57 | 0.55 | 0.52 | 0.51 | 0.50 | 0.49 | 0.48 | 0.47 |
| 3 | H | 14.7408 | 15.6532 | 16.3008 | 16.7933 | 17.2023 | 17.5464 | 17.8431 | 18.1036 | 18.3356 |
| | ARL_{min} | 2.2343 | 2.3749 | 2.4720 | 2.5453 | 2.6041 | 2.6532 | 2.6953 | 2.7319 | 2.7645 |

Table C.6: Optimal MEWMA Control Chart, $p = 4$, $\tau = 1$.

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Table C.7: Optimal MEWMA Control Chart, $p = 10, \tau = 1$.

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