Process adjustment with an asymmetric quality loss function

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\textbf{Abstract}

Controlling an engineering process usually focuses on maintaining the process output on-target with minimum variation. Conventionally, the quality loss incurred by the deviation from the nominal values is assumed symmetric. However, in some engineering processes, the penalties incurred by positive and negative deviations of the quality variables are different. In such cases, we need to redesign the controller so that the overall quality loss is minimized. In this work, motivated by a real ingot growing process, a new controller is proposed for an asymmetric quality loss function. Its performance and stability are studied via numerical simulation. The effectiveness of the method is also demonstrated in the real engineering process.

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1. Introduction

Process adjustment is an important quality control method used in semiconductor manufacturing to maintain process output on-target with minimum variation. The control algorithm usually takes the output obtained at the previous step or time point, and derives the optimal set-point for the next step. In this way, the expected output of the next step is driven to a desired target value. The set-point contains another automatic control loop guided by engineering controllers. Such a framework is implemented to learn process dynamics and gradually move the process on target with reduced variation \cite{1}.

Process control has been widely used in the industry with repeated discrete production runs, due to its effectiveness in improving quality and yield, and reducing cost. Examples include chemical vapor deposition \cite{2}, plasma etching \cite{3}, chemical mechanical polishing \cite{4–6}, photolithography \cite{7} and ploy silicon gate etching \cite{8}. Card et al. \cite{9} studied a plasma etch process for 8-in. silicon wafers by maintaining targeted values of post-etch metrology variables. Sachs et al. \cite{10} combined the Statistical Process Control (SPC) and the feedback control. Bode et al. \cite{11} developed a control scheme for overlay control based on linear models in semiconductor processes, and successfully implemented it in a commercial facility. All the existing work has reported the effectiveness of the controllers in reducing process variation and improving product quality.

To design such an adjustment algorithm, quality loss is the key performance index. Taguchi et al. \cite{12} established a number of ways to measure quality loss in different scenarios. He proposed three functions for measuring quality for different quality characteristic: nominal-the-best, smaller-the-better or larger-the-better.

In the nominal-the-best case, the output has a clear target. Any deviation from the target incurs penalty, and the penalty is symmetric and increases quadratically with the amount of deviation. Let $y$ be the process output and $T$ the target value, the quality loss is then defined as follows:

$$L = k(y - T)^2$$   \tag{1}

Fig. 1(a) shows this quality loss function. For this type of processes, the output $y$ should stay close to the target value such that the mean square deviation can be minimized. In practice, the nominal-the-best type of quality variables are widely used.

Taguchi et al. \cite{12} also introduced smaller-the-better and larger-the-better loss functions for cases in which the quality characteristic is expected to be as small as possible, or as large as possible. Sharma et al. \cite{13} studied the quality loss functions, and compare these three cases to devise a common methodology to represent these three loss functions. Their quality loss functions are shown in Fig. 1(b) and (c).

The different types of quality loss functions are widely seen in different manufacturing processes. For example, in a wafer preparation process \cite{see Han and Wang [14] and Wang and Han [15] for more details}, the thickness of the wafers after the lapping
operation has a target values; all wafers are expected to stay as close as possible to the target thickness value. On the other hand, the uniformity of the wafers, which is measured by the total thickness variation (TTV), is a smaller-the-better type of quality indicator; a smaller TTV value means better uniformity condition and is always the pursuit of the industry. In a footwear manufacturing process (see Jiang et al. [16] for more illustration), the inner sole, middle sole and outer sole are bounded together using a certain type of adhesive; the adhesive force between the different layers is a larger-the-better type of quality metric.

These quality loss functions, especially the nominal-the-best type function, are widely used in process adjustment. Most existing literature developed the algorithm by minimizing the expected mean sum of squared error, which is consistent with the nominal-the-best loss function, see, e.g. Wang and Tsung [17], Wang and Tsung [1], Lin and Wang [18], and Lin and Wang [19]. Many run-to-run (R2R) controllers have been introduced to reduce the impact of drift, shift and noise disturbance. These include the exponentially weighted moving average (EWMA) controller [20,10], PID controller [21], age-based double EWMA controller [4], and self-tuning controller [22]. However, the traditional definition of quality loss cannot satisfy the real engineering requirement in some manufacturing processes. For example, in silicon ingot growth, the ingot diameter is a “smaller-the-better but no-less-than” type of quality variable. That is, the diameter has a design target. The true diameter is expected to stay as close as possible to the target value, but not smaller than the target. More engineering background of this process will be introduced in the next section.

Harris [23] studied the control of a process with asymmetric loss functions. However, the loss functions the author considered, including two quadric functions, two constant functions and two linear functions, are inapplicable to the real process that we encountered. Similarly, the work done by Colosimo et al. [24] cannot be applied to our process, since the quality loss in our process is penalized differently. Therefore, the objective of this paper is to propose a new quality loss function that better suits certain engineering needs. Based on the new loss function, the optimal run-to-run (R2R) control action is also developed; and its performance is studied via simulation.

The rest of this paper is organized as follows. In Section 2, the quality loss function derived from a real engineering process is introduced. The optimal control action is derived in Section 3. In Sections 4 and 5, we study its control performance and stability. Finally, Section 6 concludes this work with suggestions for future research.

2. Quality loss for the smaller-the-better but no-less-than (SBN) variables

In this work, we use the silicon ingot growing process as an example for illustration. The silicon ingot growing process is the first step to transform polysilicon to single silicon in semiconductor manufacturing. Single crystal growth is mainly achieved by two methods, Czochralski (CZ) and float zone (FZ). Between these two methods, the CZ process is more commonly used to produce high-quality single crystal ingots [25], Fig. 2 shows a schematic diagram of a crystal growing furnace based on the CZ process.

A typical crystal growing furnace usually consists of the pulling thread, which holds a thin seed crystal bar, the crucible, which holds raw crystal material, and a heating system, which is used to melt the raw material and create an ideal heat field for the growth of single crystal. The CZ growing process has three major phases, namely (1) seeding and necking, (2) body growth, and (3) termination. Among these steps, the body growth is the main step and lasts the longest period of time (usually 40–50 h in our example). In this step, the main body of the ingot is growing, and diameter control is one of the most critical tasks. When growing the ingot, there is usually a desired diameter value; the ingot is expected to be smooth and consistent in diameter throughout its body growth stage (see a sample ingot in Fig. 3). The diameter is monitored and measured by a CCD camera. A feedback-control system is therefore needed to maintain the diameter on target.

In most cases, it is difficult to keep the ingot diameter exactly on target due to process variation and a lot of unobservable noises (see Fig. 4 for the plot of the diameter of one sample ingot). The diameter is affected by a number of factors. It is directly affected by the pulling speed. When the pulling speed increases, the diameter decreases, or vice versa. Besides, the pulling speed, temperature, power of heater and many other factors need to be coordinated to achieve a target diameter. Due to the large number of factors, a large variation of diameters is commonly encountered in real production. In this paper, we focus on how to set and adjust the direct factor, the pulling speed online. Once the set-point of the pulling speed is known, the realization of the speed and the coordination among other variables will be achieved by a built-in automatic control system.
Although there is a target value of the ingot diameter, the effects of being higher or lower than the target are quite different. Fig. 5 illustrates different cases of the body diameter. If the true diameter is larger than the target value, i.e. $y > T$, the extra material will be removed in downstream operations. Therefore, the diameter should be smaller-the-better to reduce material waste. However, if the true diameter is smaller than the target, the whole part has to be discarded (reworked) since this segment of ingot cannot satisfy diameter requirement. For example, to produce 8-in. wafers, the diameter of the ingot should be larger than 8 in., due to the downstream material removal process such as rounding. The segment with diameter larger than 8 in. will be preserved. If the diameter is smaller than 8 in., the segment cannot be used to produce wafers, which will be discarded with a fixed cost. In the example shown in Fig. 4, the desired ingot diameter is 206 mm. In practice, to avoid under-specification situations, the real diameter is generated with a large slack value, which may cause high material waste if the slack value is not appropriately chosen.

Therefore, the ingot diameter is a “smaller-the-better but no-less-than” quality characteristic. The quality loss corresponds to the diameter is shown in Fig. 6. When $y > T$, the loss is the same as the traditional smaller-the-better type function, which increases quadratically with the magnitude of deviation from the target; when $y < T$, a fixed cost, $c_1$, is incurred. Therefore, the overall loss function is given as follows:

$$L = \begin{cases} c_1 & \text{if } y < T \\ c_2(y - T)^2 & \text{if } y > T \end{cases}$$

(1')
It is clear that this loss function is asymmetric. Intuitively, it is safer to grow larger than the target value than smaller than the target value, since the penalty for \( y < T \) has a sharp increase near \( T \). In order to minimize the quality loss, a careful development of the optimal control set-point is needed, which will be presented in the next section.

The above asymmetric cost function is initiated from wafer production; the slicing operation applied to the ingot makes the cost accountable on individual wafers (or ingot segments). It should be noted that as wafer is the base material of many products, such as integrated circuit (IC) and solar cells; this cost function has a great impact on many processes, and is therefore worth studying.

The above quality loss is also not limited to the ingot growth process. We have seen other processes that having a similar quality requirement. As another example, a follow-up operation of the ingot is slicing, which cuts the ingot into piece of wafers [26]. To save materials and improve utility, the thickness of the wafers is the smaller the better. However, the thickness should not be smaller than a target value, thus leave space for the following lapping process. The lapping process removes surface damagers on the wafer and finally moves the remaining wafer thickness into certain specification limits.

3. Optimal control of the smaller-the-better but no-less-than quality characteristic

In the previous section, we developed the objective function for controlling the ingot diameter, which is a smaller-the-better but no-less-than type of quality characteristic. In the following, the optimal algorithm to control the diameter will be derived so that the quality loss is minimized.

As aforementioned, ingot diameter is directly affected by pulling speed. Therefore, we assume that the diameter and the controllable variable have a linear relationship as follows:

\[
y_{t+1} = \alpha + \beta u_t + \varepsilon_{t+1} \tag{2}
\]

where \( y_{t+1} \) is the finished diameter at time \( t+1 \), and \( u_t \) is the set-point of the pulling speed set at step \( t, \varepsilon_{t+1} \sim N(0, \sigma^2) \) are normally distributed disturbance that the process has. Since the diameter of ingots is measured on a discrete time horizon, the observations of the diameter is therefore discrete. In Eq. (2), the discrete subscripts of the notations are used to reflect the decision and observation time points. In practice, initial setup bias, sudden process changes and other types of disturbances may exist. The parameters \( \alpha \) and \( \beta \) cannot be estimated accurately. Therefore, feedback control is needed for the process guided by Eq. (2).

The linear function in Eq. (2) is a commonly used form in semiconductor R2R control, see, e.g. Del Castillo and Hurwitz [22], Tseng et al. [27], Wang and Tsung [17], Wang and Tsung [1], and Shang et al. [28], among others. Even if the true relationship between \( u_t \) and \( y_{t+1} \) is not linear, the function is still a close approximation to the real system within a short operational interval. Moreover, although the following method is derived on the basis of the linear model assumption, the framework can be easily extended to nonlinear processes with minor modification.

To minimize the quality loss in Eq. (1), we study the function in greater details. Let \( a \) and \( b \) are the initial estimates of \( \alpha \) and \( \beta \) obtained from historical data, respectively, and further denote \( \tau_t = T - a - bu_t \). When \( y_{t+1} < T \), which is equivalent to \( \varepsilon_{t+1} < \tau_t \), we have

\[
E(L|\varepsilon_{t+1} < \tau_t) = c_1 \tag{3}
\]

when \( y_{t+1} = T, \varepsilon_{t+1} > \tau_t, \)

\[
E(L|\varepsilon_{t+1} > \tau_t) = E(c_2(a + bu_t + \varepsilon_{t+1} - T)^2|\varepsilon_{t+1} > \tau_t)
\]

\[
= c_2(a + bu_t - T)^2 + 2c_2(a + bu_t - T)E(\varepsilon_{t+1}|\varepsilon_{t+1} > \tau_t)
\]

\[
+ c_2E(\varepsilon_{t+1}^2|\varepsilon_{t+1} > \tau_t) \tag{4}
\]

Since \( \varepsilon_{t+1} \) is normally distributed, the conditional expectation of the mean and variance of \( \varepsilon_{t+1} \) becomes the mean and variance of a truncated normal distribution, which are given by

\[
E(\varepsilon_{t+1}|\varepsilon_{t+1} > \tau_t) = \sigma \lambda(\tau_t)
\]

and

\[
E(\varepsilon_{t+1}^2|\varepsilon_{t+1} > \tau_t) = \sigma^2(1 - \delta(\tau_t))
\]

where \( \lambda(\tau_t) = \phi(\tau_t)/(1 - \Phi(\tau_t)), \delta(\tau_t) = \lambda(\tau_t)/\lambda(\tau_t - \tau_t) \). Here, \( \phi(\cdot) \) and \( \Phi(\cdot) \) are the probability density function and cumulative distribution function of the standardized normal distribution, respectively.

Since \( E(L) = E(E(L|\varepsilon_{t+1})) \), it is easy to obtain that

\[
E(L) = E(L|\varepsilon_{t+1} < \tau_t)\Phi\left(\frac{\tau_t}{\sigma}\right) + E(L|\varepsilon_{t+1} > \tau_t)\left(1 - \Phi\left(\frac{\tau_t}{\sigma}\right)\right) \tag{5}
\]

By plugging Eqs. (3) and (4) into Eq. (5), we have the final objective function. Then, the optimal control action can be obtained as follows:

\[
u_t = \arg \min_{u} E(L)
\]

To minimize Eq. (5), a common way used in designing R2R controllers is to take the derivative of \( E(L) \) with respective to \( u_t \) and set it to zero, then solve for \( u_t \). However, the complex form of the objective function makes the close form hard to trace. Therefore, we first investigate the property of the function, then suggest a way to minimize the expected loss function in the following part.

Without loss of generality, we first assume the following parameter settings: \( T = 600, \alpha = 100, \beta = 10, \sigma = 1 \). Two scenarios have different fixed cost values \((c_1 = 20, c_2 = 1) \) and \((c_1 = 30, c_2 = 1) \), are studied. The expected loss functions are shown in Fig. 7.
It is learned from Fig. 7 that the expected quality loss is first flat with respect to $u$, and then drop and increase with $u$ after a certain threshold value. The lowest $L$ on each graph is identified and labeled in Fig. 7. It is easily known that if the expected loss function is symmetric and all parameters known exactly, the optimal control $u$ should be

$$u_0 = \frac{T - \alpha}{\beta}$$

which is $u = 50$ in the above settings. This value that corresponds to the symmetric loss function is also shown in the graph for comparison. We also plot $u_0$ in Fig. 7 for comparison purpose.

Fig. 7 suggests that under this asymmetric loss function, the optimal control action moves rightward. This is reasonable since the penalty in Fig. 6 increases quickly if $u$ is too small. Therefore, the algorithm automatically chooses a more conservative control action and uses the expected quality loss curve on the right of the target to reduce the risk of being overly punished. Moreover, if the fixed cost, $c_1$, increases from 20 to 30, the optimal control action moves further larger, from 50.14 to 50.16, to reduce the overall expected loss. Further investigation shows that the choice of the optimal control action is quite robust to the change of $c_1$.

Therefore, with the quality loss function in Fig. 6, the optimal control action $u$ is always larger than $u_0$ in Eq. (6). Within the range $u > u_0$, the expected loss $E(L)$ decreases first, then increases. Therefore, a single global minimum exists in this range. With this information, the traditional numerical search algorithms, such as the damped Newton’s method, can be used to locate the optima easily. The optimize function in R, or the FindRoot function in Mathematica, can help find the solution easily.

In practice, the true values of $\alpha$ and $\beta$ are never known; these parameters usually need to be estimated from historical data first, and be updated continuously when new observations arrive. Let $a_0$ and $b$ be the initial estimates of $\alpha$ and $\beta$, respectively. Following the treatment of the traditional EWMA controller, we update the estimates of $\alpha$ in the following way:

$$a_t = \lambda(y_t - bu_{t-1}) + (1 - \lambda)a_{t-1}$$

Then, the updated parameters $a_t$ and $b$ are used to replace $\alpha$ and $\beta$ in Eqs. (4) and (5) to calculate the optimal set-point for the next step.
that is, the controller tries to move the process output to a value that is different from the target T (which is usually the center of LSL and USL). The exact location is affected by the penalty cost. If $c_1 > c_2$, that is, the lower side incurs a higher penalty, the process mean should be driven upward and stay closer to the upper specification limit. The authors also derived a policy for estimating and updating the setup bias and generating optimal control actions. The details control law is referred to the original work of Colosimo et al. [24].

In the following, we name this method the Asymmetric Constant-Cost (ACC) controller, and compare with the proposed method in this paper. The parameter settings used by the ACC controller are: $c_1 = 20$, $c_2 = 200$, $LSL = 205$, $USL = 207$.

The initial estimates of $\alpha$ and $\beta$ are set to $\alpha = 190$ and $b = 0.1$. For each instance, the process is simulated for 200 steps and mean squared errors (MSE) between the true output and the target value is calculated. 1000 instances are repeated and the mean of all MSEs (MMSE) and the quality loss based on Eq. (1) are recorded and shown in Table 1.

In Table 1, it is clearly seen that the EWMA Controller has the smallest MMSE among all. However, MMSE loss function cannot represent the overall quality loss. The ACC controller has a moderate MMSE, but the largest quality loss. The overall quality loss of the proposed controller is much smaller than the other two controllers. Fig. 9 further shows one instance of the simulated output from each controller. It is seen that all controllers are capable of moving the output to the target after compensating the initial bias. Differently, the EWMA moves the output to the target value exactly and allows it varies around it, the ACC controller suffers from an overshoot in the beginning, then gradually moves the output back to the target. Based on the above parameter settings, we obtain that the target value, defined on Eq. (8), is in fact $T_c = 206.1835$. For he ACC controller, since the under-specification cost is higher than the over-specification cost, the controller tries to move the output higher than the process target, which is $T_c = 206$. Instead, the proposed controller moves the output to a value that is higher than the target value and tries to reduce the number of occurrence that the output goes below the target. It clearly shows that the different cost function would result in rather different output trajectories. Therefore, selecting a cost function that fits the real engineering situation is of great importance.

---

**Table 1**

<table>
<thead>
<tr>
<th></th>
<th>EWMA controller</th>
<th>ACC controller</th>
<th>Proposed controller</th>
</tr>
</thead>
<tbody>
<tr>
<td>MMSE loss</td>
<td>13.0 (0.4)</td>
<td>42.8 (6.1)</td>
<td>224.1 (1.5)</td>
</tr>
<tr>
<td>Quality loss</td>
<td>1960.2 (86.3)</td>
<td>3133.9 (125.2)</td>
<td>449.3 (29.9)</td>
</tr>
</tbody>
</table>

**Fig. 10.** Comparison of the stability if the slope parameter is incorrectly specified.

**Fig. 11.** Comparison of the quality loss if the slope parameter is incorrectly specified.
5. Stability study

Ingolfsson and Sachs [20] and Sachs et al. [10] presented the stability region of the EWMA controller and concludes that the process is only stable if

\[ 0 < \frac{\lambda \beta}{b} < 2 \]  

(9)

which means that \( \beta \) and \( \beta \) should have the same sign, and \( \beta \) should be no smaller than \( \lambda \beta/2 \).

For the proposed controller, since the close form of the control action \( u_t \) is difficult to obtain, the stability range also becomes hard to be obtained accurately. However, through an analysis of the behavior of the controller, it is possible for us to learn more about the controller.

Following the settings used in Section 4, we simulate the cases with different \( b \) values. The MSE of the process is shown in Fig. 10. It is clear that when \( b \) is larger than a certain threshold value, the MSE of the proposed controller is always smaller than the EWMA controller. It has already been known from the literature that the EWMA controller is stable as long as \( b \) is not too small (compared to its true value). Similar trend is also concluded for the proposed controller. That is, an overly estimated \( b \) would make the controller more stable, higher quality loss is paid as the price.

6. Conclusions

In some engineering processes, the quality losses for over- and under-target values are different, which lead to an asymmetric loss function. However, most conventional process adjustment algorithms are developed for symmetric loss functions, which cannot be applied directly.

In this case, based on a real single crystal silicon ingot growing process, we propose a new controller for diameter control. The optimal control action that minimizes the overall asymmetric quality loss is derived. Simulation results show that under the asymmetric quality loss function, the controller tends to push the output further away from the side which has higher penalty. The controller tends to be more stable if the slope parameter \( \beta \) is over-estimated than it is under-estimated.

It should be noted that the output of the controller is a set-point; the controller is not used to control the true physical variable (the pulling speed in this example) directly. The real physical variable is usually guarded by other engineering control algorithms, such as the PID controller. Since the true process involves both set-point determination and physical variable control, the integrated consideration of the engineering control loop and the process adjustment algorithm is an interesting topic for future research.

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