

“Using Linear Regression Analysis and the Gibbs Sampler to Estimate the Probability of a Part Being Within Specification”

Brenda Cantell, Unitrode Corporation, Merrimack, NH

ABSTRACT

“In-line” or “process” specification limits are used in semiconductor processes to provide some level of assurance for product conformance that is measured at the end of wafer fabrication. However, these limits are not always set in a rigorous manner and may not prove to be an adequate in-line screening method for good and bad circuits.

In this paper, an alternative way for engineers to release equipment or product for production will be explored. This approach uses a probability measure to predict how likely it is that the device will be good at functional testing based upon its in-line measured characteristic. This probability is obtained using the predictions from a linear regression equation. The Gibbs sampler is then used to construct a $100(1-\alpha)\%$ credible band around the predicted probabilities.

These techniques will be demonstrated using data from a semiconductor wafer anneal process. Also, it will be shown how the SAS® system for the personal computer can be used to implement this technique.

INTRODUCTION

Semiconductor or integrated circuit manufacturing consists of hundreds of complex processing steps. At the end of wafer fabrication, the integrated circuits are electrically tested for functional problems before moving on to be assembled and packaged. It can be expensive to allow bad devices to make it to this stage of manufacturing. It is preferable to detect such anomalies as they are occurring during wafer fabrication.

Tight process controls are instituted throughout all critical steps of wafer fabrication. Critical process parameters are selected at each step and “in-line” or “unit process” specification limits are defined for each parameter and used to provide some level of assurance for product conformance measured at functional test. These in-line specification limits

are often set heuristically, and therefore, should be validated in a rigorous manner whenever possible.

One way to validate these limits is to establish the empirical relationship between the unit process parameter and a critical measurement taken at functional testing. This information can be used to develop an alternative strategy for releasing equipment or product to production. This approach is based upon the examination of a conditional probabilistic measurement, i.e., the probability that product will pass functional test given its in-line performance.

This application was motivated by the practices of a semiconductor company to release a base anneal furnace to production after maintenance. The current practice is to process one lot of material and hold the tube “down” while the “send ahead” wafers complete subsequent processing and testing. This can add an additional two week delay in getting the equipment back on line. If the test results are bad and another test run is needed the delay can be three weeks or more. The new procedure will be used to release base anneal furnace(s) to production without the need to process “send ahead” wafers and, to highlight the need for additional “fine tuning” of the furnace; thus avoiding the time and expense of processing “send aheads” which may have a high probability of failure.

The details of this new procedure are provided in the remainder of this paper. The next section describes the data collection used in this example. The following section goes into the statistical derivation of the technique, including the application of the Gibbs sampler. The use of the SAS system for the personal computer is presented next. Finally, an application is shown using data from a base anneal process.

DATA COLLECTION SCHEME

For this application, happenstance data were collected in a semiconductor manufacturing process that consisted of 131 paired observations of the

form (x_i, y_i) , $i = 1, 2, \dots, 131$. The x_i were measurements that were taken during in-line processing and, after wafer fabrication was complete, the corresponding y_i were recorded at functional testing. Both factors are measured on a continuous scale. The data were extracted from various sources and then condensed in an ASCII file that could be read into a SAS data set.

STATISTICAL DERIVATION

The first objective is to establish the relationship between the unit process parameter and a critical measurement taken at functional testing. Therefore, the procedure begins by specifying a model for the data. For this application, the empirical model is:

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i,$$

where $\varepsilon_i \sim N(0, \sigma^2)$ and are independent and identically distributed, x_i are the observed in-line measurements, and Y_i are the observed functional test parameter. Least squares estimation is used to obtain the parameter estimates for the model.

The prediction equation can be assessed for its accuracy after the assumptions of the model have been validated and corrected if needed. If it is deemed acceptable, then the prediction equation can be used to obtain the predicted value of the response for a specific value of the independent factor, i.e., for a given $x_i = x_0$,

$$\hat{y} = \hat{\beta}_0 + \hat{\beta}_1 x_0.$$

A $100(1-\alpha)\%$ prediction interval for a new observation at $x_i=x_0$ can be obtained using the conditional distribution of $Y_i | x_i \sim N(\beta_0 + \beta_1 x_i, \sigma^2)$. The conditional distribution implies that each value of x_i produces a random value of Y from a normal distribution with a mean of $\beta_0 + \beta_1 x_i$ and a variance σ^2 . If the errors are normally distributed, then $\hat{y} | x_i=x_0 \sim N(\beta_0 + \beta_1 x_0, \sigma^2 V^2(\mathbf{x}_0))$, where $V^2(\mathbf{x}_0) = n^{-1} + S_{xx}^{-1}(\mathbf{x}_0 - \bar{x})^2$ and $S_{xx} = \sum_i (x_i - \bar{x})^2$ (Meyers, (1990)). The prediction interval is given by:

$$\hat{y}(\mathbf{x}_0) \pm t_{\alpha/2, n-2} s(1 + V^2(\mathbf{x}_0))^{1/2}.$$

Obtaining the Probability p

For the application described in the Introduction of this paper, the engineer would like to obtain the probability that a particular value of the in-line measurement $x_i = x_0$ will produce a device that is

good at functional test. A good device at functional test is defined as a device whose functional test measurement is within specifications limits (LSL, USL). Therefore, the engineer would like to evaluate, for $x_i = x_0$,

$$\text{Prob}(\text{LSL} < Y < \text{USL}) = \pi.$$

The probability π can be estimated using the conditional distribution for $\hat{y} | x_i = x_0$,

$$p = t_{n-2}((\text{USL} - \hat{y})/(sV(\mathbf{x}_0))) - t_{n-2}((\text{LSL} - \hat{y})/(sV(\mathbf{x}_0)))$$

where $t_{n-2}(\cdot)$ is the probability that an observation from the Student's t distribution is less than or equal to (\cdot) . With this information, for a given in-line value $x_i=x_0$, the engineer can assess the probability that the functional test parameter will be within specification limits.

Confidence Interval for the Probability p

The probability p alone does not provide any indication of how well the model fits the data. Therefore, it is desirable to enclose the predicted probability with some form of confidence bands that reflect, at least partially, the fit of the model to the data. One way to do this is to determine the theoretical distribution for p and use this information to construct a confidence interval. However, this approach will not be pursued in this paper.

A simulation approach, such as Monte Carlo simulation, is another method that can be used to study the distribution of p . This technique relies upon drawing a large number of random samples from the distribution of p and obtaining the appropriate quantiles from the simulated data. However, this approach also requires the density function for p .

A Bayesian approach to this problem is facilitated by the Gibbs sampler to obtain a confidence interval for p without knowing its density function. The derivation for this approach requires a reinstatement of the model,

$$Y_i = \beta_0 + \beta_1 x_i + \varepsilon_i,$$

where $\varepsilon_i \sim N(0, \sigma^2)$ and are independent and identically distributed. The conditional distribution is $Y | \Omega \sim N(\beta_0 + \beta_1 x, \sigma^2)$, where $\Omega = (\beta_0, \beta_1, \sigma^2)$. The Bayesian approach to this problem implies that the parameters in Ω are random variables.

Once again we are interested in placing a $100(1-\alpha)\%$ credible point band about the probability,

$$\Delta_x(\Omega) = \Pr\{ (LSL < Y < USL) \mid \Omega \} \\ = \Phi[(USL - \beta_0 - \beta_1 x) / \sigma] - \Phi[(LSL - \beta_0 - \beta_1 x) / \sigma],$$

where $\Phi(\cdot)$ is the area to the left under the normal density curve corresponding to the value (\cdot) . Note the change in terminology from prediction interval to credible point band.

A form of simulation will be used to determine a $100(1-\alpha)\%$ credible band for $\Delta_x(\Omega)$, i.e., a number of random samples of $\Delta_x(\Omega)$ will be generated and the distribution will be evaluated. The joint posterior density of $(\beta_0, \beta_1, \sigma^2) \mid \mathbf{y}$ ($\mathbf{y} = y_1, y_2, \dots, y_n$) is not required to generate this random sample. Instead, the Gibbs sampler will be used to obtain the empirical posterior distribution of $\Delta_x(\Omega)$.

Simply stated, the Gibbs sampler is a technique for generating random variables from a distribution indirectly without having to calculate its density (see Casella and George (1992)). This is accomplished by iteratively drawing random samples from the conditional posterior distributions of $\beta \mid \sigma^2, \mathbf{y}$ and $\sigma^2 \mid \beta, \mathbf{y}$. If no prior information about the joint distribution for $(\beta_0, \beta_1, \sigma^2)$ is assumed, i.e., $P(\beta_0, \beta_1, \sigma^2) \propto (\sigma^2)^{-1}$ has an improper prior, then the conditional posterior distributions are easily determined (Tanner (1993)).

The iterative procedure begins by drawing the first random sample of the parameters β_0 and β_1 from a bivariate normal distribution,

$$\beta \mid \sigma^2, \mathbf{x}, \mathbf{y} \sim N(\hat{\beta}, \sigma^2 \Sigma),$$

where $\hat{\beta}$ is the least squares estimates of β , Σ is taken to be $(\mathbf{x}'\mathbf{x})^{-1}$, and σ^2 is estimated by the mean square error from the least squares fit.

The first random sample for the variable σ^2 is then drawn using the following conditional distribution,

$$(\sum_i (y_i - \beta_0 - \beta_1 x_i)^2) / \sigma^2 \mid \beta_0, \beta_1, \mathbf{x}, \mathbf{y} \sim \chi^2_{n-1},$$

where β_0 and β_1 is the random sample that were previously drawn. Therefore, by generating a random sample of chi-square values we can obtain an estimate of $\sigma^2 = \sum_i (y_i - \beta_0 - \beta_1 x_i)^2 / \chi^2_{n-1}$.

The procedure continues by using this value of σ^2 to draw another random sample for β . Then these values for β are used to draw another random sample for σ^2 and so forth and so on.

Finally, the credible band is obtained by generating a large sample of size k for $\beta_0, \beta_1, \sigma^2$. Using the last $(k - 200)$ iterates we calculate $\Delta_x(\Omega)$ for a grid of points x in (x_1, x_n) . For each value in x , we obtain the 2.5, 50, and 97.5th percentiles for the empirical distribution of $\Delta_x(\Omega)$. It should be noted that there are several methods to check for convergence of the Gibbs sequence (Casella and George (1992)). For the approach that is used here, an autocorrelation function plot can be used to make sure there is no autocorrelation present in the series.

SAS CODE

The SAS System for the personal computer was used to implement this algorithm. The code is set up as a SAS MACRO with 5 parameters: `%Gibbs(data, resp, indep, usl, lsl)` where *data* is the name of the SAS data set, *resp* in the name of the response variable, *indep* is the name of the independent factor, *usl* is the value of the upper specification limit, and *lsl* is the value of the lower specification limit. The basic structure of the SAS code, along with some examples of actual code, are given next.

1. Fit the model using the REG procedure in SAS/STAT[®] and output the parameter estimates, covariance matrix, and MSE. Make these variables available for the next procedure.
 - ```
/*Fit model and output necessary parameters*/
proc reg data=&data outest=temp covout mse;
 model &resp = &indep / covb;
run;
```
  - The CALL SYMPUT function can be used to set the macro variables for the next step. For example, the following code will set a macro variable named MSE with the MSE from the regression model:
 

```
data _null_;
 set temp(firstobs=1 obs=1);
 call symput('mse', _mse_);
run;
```
2. Using the IML procedure in SAS/IML<sup>®</sup>, create the design matrix, response vector, parameter

estimates vector, and the covariance matrix for the parameter estimates.

- `/*Set up matrices in PROC IML*/`  

```
proc iml;
 use &data;
 read all var{&resp} into y;
 read all var{&indep} into x1;
 nrow=nrow(x1);
 x = J(nrow,1,1) || x1;
 s = {&varb0, &cov, &cov, &varb1}#&mse**-1;
 var=&mse;
 seed=0;
 z=J(1, 2,.);
 newbeta=J(2,1,.);
 finbeta=J(1500, 4, .);
```
- 3. Using the Cholesky decomposition, draw the first random sample for the parameter estimates from the stated bivariate normal distribution. Then compute the first estimate of  $\sigma^2$  by drawing a random chi-square value and computing the residual sums of squares using the parameter estimates that you just drew and taking the ratio of the two. This is done iteratively k times. Save the results into a SAS data set and exit PROC IML.

- `/*Continuation of PROC IML code*/`  

```
do j=1 to k;
 sigma=s#var;
 chol=half(sigma);
 z[1,1]=rannor(seed);
 z[1,2]=rannor(seed);
 newbeta[1,1] = &b0+chol[1,1]#z[1,1];
 newbeta[2,1] = &b1 + chol[1,2]#z[1,1] +
 chol[2,2]#z[1,2];
 yhat=x*newbeta;
 resid = y - yhat;
 sse = resid`*resid;
 chi = 2*rangam(seed, 65);
 var = sse / chi;
 finbeta[j,1]=newbeta[1,1];
 finbeta[j,2]=newbeta[2,1];
 finbeta[j,3]=sse;
 finbeta[j,4]=var;
end;
create finbeta from finbeta[colname={'b0' 'b1'
 'sse' 'var'}];
append from finbeta;
quit;
```

- 4. With the outputted data set from (3), using the last k-200 observations, check for

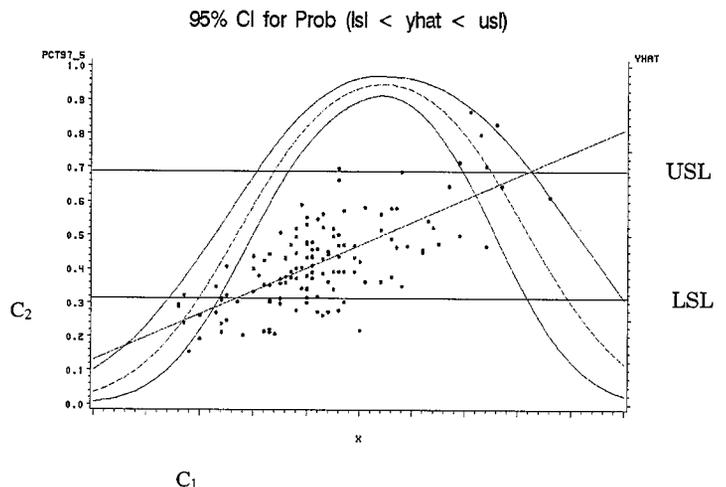
autocorrelation in the random samples with the ARIMA procedure in SAS/ETS®.

- 5. Through a SAS DATA step, calculate the desired probabilities that the prediction is within specification limits.
- 6. Obtain the stated quantiles for the credible band using the CAPABILITY procedure in SAS/QC®.
- `proc capability data=pred noprint;`  

```
var prob;
by x;
output out=predci mean=pmean pctlpts=2.5
 97.5 pctlpre=pct;
run;
```
- 7. Generate the final graph using the GPLOT procedure in SAS/GRAPH®.

### APPLICATION TO WAFER ANNEAL DATA

The major output from this procedure is shown in the graph below. There are two y-axes shown on this graph. The y-axis shown on the right hand side depicts the values for the response which are measured post fabrication. The x-axis shows the values for the independent variable which are observed during fabrication. The actual readings are shown by the dots on the graph. The dashed line represents the predicted equation for Y. The prediction equation is  $\hat{Y} = -3117.585 + 27.245 x$ .



The y-axis on the left hand side of the graph represents the area under the normal density function that is bounded by the specification values of LSL and USL for Y. In other words, it is the probability for a given value of X producing a value

of Y that is within specification. This probability curve is surrounded by a 95% credible band that was obtained from the Gibbs sampler.

In theory, the information in this graph could be used to determine if product associated with given values for x should be allowed to continue on in the wafer fabrication process or if it should be scrapped/held/etc. For example, for  $x_1 = C_1$ , the predicted value for Y is  $C_2$  which translates to a 0.228 probability that this value will be within specification limits of [LSL, USL]. Therefore, a decision may be made to scrap/hold this product in wafer fabrication and not allow it to continue on to probe. The actual value for this particular observation was 7 units below the lower specification limit.

Based upon this graph, there appears to be a linear relationship between Y and x. However, there is a fair amount of noise in the data that can not be modeled adequately with the regressor variable alone. This prediction equation is explaining 49% of the variation in Y while 51% of the variation is unexplained. This may lead to unreliable predictions. The procedure can be evaluated by selecting  $p \leq c$ , where  $p = \Pr\{LSL < Y < USL\}$  and, for example,  $c=0.50$  and holding any product for further investigation that meets this criteria. The following table provides an example for evaluating the procedure with historical data:

|                | Test Scraps | Test Accepts |
|----------------|-------------|--------------|
| Product Y Good | <b>3</b>    | 116          |
| Product Y Bad  | 2           | <b>10</b>    |

The areas that are bolded are the combinations for making an error. Specifically, there were 3 instances where this test would have scrapped product with acceptable Y values; 2 instances where this test would have scrapped product with unacceptable Y values; 116 instances where this test would have accepted product with acceptable Y values; and 10 instances where this test would have accepted product with bad Y values. Once again, it should be noted that all of these 131 observations would have passed for x based upon its “in-line” specification limits.

## CONCLUSIONS

In this paper, it has been shown how to replace in-line specification limits with an alternative approach that relies on the relationship between the in-line value and a final product parameter.

This was accomplished with a combination of linear regression and the Gibbs sampler. The  $100(1-\alpha)\%$  credible bands for the probability that a device is within specification limits clearly provides some insight to the engineer regarding the fit of the model to the data.

This technique can be effective under the right conditions. This data set possessed a considerable amount of noise in the response. There are large dispersions in the Y values for the same values of x. This may be indicative of a measurement capability problem. This is also reflected by large credible intervals and a prediction equation which predicts nonsense values of Y for values of x that are close to its lower “in-line” specification limit.

However, this analysis did lead to an alternative approach to releasing product and setting appropriate specification values that are based upon process knowledge. The Gibbs sampler was easily supported by the SAS system and proved to be a valuable addition to the engineer’s arsenal of process analysis tools.

This application was straightforward because it only involved one in-line parameter and one functional test parameter. There are several ways that this problem can be expanded or further studied:

- ◆ observe appropriate range of in-line parameters using design of experiments;
- ◆ account for measurement error in x and y;
- ◆ model in-line parameters as random variables;
- ◆ adjust model for missing factors or terms;
- ◆ watch out for correlation not causation;
- ◆ consider a multivariate approach using multiple functional test parameters;
- ◆ add cost / risk criteria to model to determine when to scrap and when to move product.

## ACKNOWLEDGMENTS

The author would like to acknowledge Dr. Balgobin Nandram who is an associate professor of statistics at Worcester Polytechnic Institute for his ideas for using the Gibbs sampler. Mark Kelley, who is a Yield Enhancement Engineer at Unitrode

Corporation, also deserves mention for bringing this problem to my attention.

## REFERENCES

1. Casella, George and George, Edward I. (1992), "Explaining the Gibbs Sampler." *The American Statistician*, 16, 167-174.
2. Meyers, Raymond (1990), *Classical and Modern Regression With Applications, second edition*, Boston, Massachusetts: PWS-KENT.
3. Tanner (1993), *Tools for Statistical Inference*, New York: Springer-Verlag.

SAS, SAS/ETS, SAS/IML, SAS/QC, SAS/STAT are registered trademarks or trademarks of SAS Institute Inc. in the USA and other countries. ® indicates USA registration.

Brenda S. Cantell, Unitrode Corporation 7  
Continental Blvd, Merrimack, NH 03054, (603)429-  
8948, cantell@uicc.com.