Applications of Sparse Modelling and Principle Component Analysis for the Virtual Metrology of Comprehensive Multi-dimensional Quality

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Abstract: This paper discussed the virtual metrology (VM) modelling of multi-class quality to describe the relationship between the variables of a production machine's condition and the estimated/forecasted product quality soon after finishing the machine processing. Applications of PCA and LASSO technique of the Sparse modelling were introduced to define the multi-dimensional quality. Because the high accuracy and quick computations are required for the VM modelling, in this study, the PCA-LASSO combination was applied before building the VM models based on the kernel SVM (kSVM), particularly the linear kernel for real-time use. As the result of evaluation of a CVD (Chemical vapor deposition) process in an actual semiconductor factory, LASSO and linear-SVM could reduce the scale of the machine variable's set and calculation time by almost 57% and 95% without deterioration of accuracy even without PCA. In addition, as the PCA-LASSO, the multi-dimensional quality was rotated to the orthogonality space by PCA to summarize the extracted variables responding to the primary independent hyperspace. As the result of the PCA-LASSO combination, the scale of machine variables extracted was improved by 83%, besides the accuracy of the linear-SVM is 98%. It is also effective as the pre-process of Partial Least Square (PLS).

1 INTRODUCTION

Semiconductor manufacturing is characterized by a sequence of sophisticated manufacturing processes, often exceeding several hundred production steps. The process basically consists of main 10 or less types of processes repeated, for example, washing, deposition of materials on a semiconductor wafer, a photo-lithography, an etching, a polishing, an annealing, an intermediate test, and so on (Y.Naka, K.Sugawa, and C. McGreavy, 2012).

Here the intermediate test is a quality check process which occupies 30% of the whole of the production process. Though the intermediate test aims the fast detection of the quality defects to prevent to pile more cost and time before the final test, the time and the cost for the intermediate test is also serious in 100%-inspections . Virtual metrology (VM) has become widely studied all over the world to reduce both the defects and the cost of the test (or the test itself) as the research area of "advanced process control" since 2005 as in AEC/APC (Advanced equipment control/Advanced process control) symposium around the world.

2 QUALITY DISCRIMINATION MODELLING FOR VIRTUAL METROLOGY

This study has advanced in 3 phases. As the first, Arima (2011) applies kSVM for multi-class VM modelling mainly for high accuracy. Second is the application of the LASSO (Least Absolute Shrinkage and Selection Operator) for automatic variable extractions and fast computation of kSVM (Arima, Ishizaki, and Bu, 2015). The third phase is for all of those; automated variable extraction, the high accurate quality detection, and the fast computation. This paper mainly describe the third phase in Section 3 after explaining the results and

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issues of the first and the second phases in this section.

2.1 Problem Descriptions

The target process in this study is a plasma-CVD (Chemical vapor deposition) process. CVD is one type of thin-film formation processes and uses the vapor process of a target material such that the snow falls into the ground. The thickness of the film is measured by nine points on a wafer after the CVD process as the quality test for the CVD process (Fig.2-1). Note that there are some types of layout of the nine points. The measured data is composed into 2 factors (dimensions), “Design conformity (Dc)” and “Uniformity (Uf)” for every wafer. Table. 2-1 shows one example of nine classes (3x3).

Not only Dc but also Uf is very important because the larger wafer size leads the more defects besides the higher throughput [wafers/unit time]. For example, 30mm-size wafer is used in the target factory, and the thickness sometimes much varies on a wafer. The thickness influences the final quality of the product such as the electrical resistance and the current value.

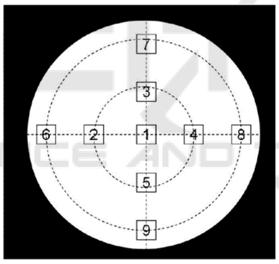


Figure 2-1: Film thickness measured by nine points.

Table 2-1: Multi-dimensional quality class definition (nine classes for 2-dimension).

		Uniformity			
		a	b	c	abc
Design conformity	A	46	18	6	70
	B	14	2	8	24
	C	2	0	4	6
	ABC	62	20	18	100

For VM, quality was categorized by multi classes of 2 factors (dimensions), “Uniformity” and “Design conformity” as shown in Table.2-1. Table 2-1 shows the case of nine classes as the result of 3-class definition for each factor. The measures and thresholds depend on the definition of the class. For example of Table. 2-1, Dc was defined by the sum total of square error between designed and actual film thickness, and the boundaries of classes ‘A' and ‘B' or ‘B' and ‘C' were set as 3-quantiles between the minimum and maximum values. Surface uniformity (Uf) was defined by the standard deviation of the film thickness, and the boundaries of classes ‘a' and ‘b' or ‘b' and ‘c' were set similarly as 3-quantiles. This is only one example as the first phase definition. The i-th wafer belongs to one of those 3x3=9 classes, and maintains the multi-dimensional quality class expression as YC (i). Number in Table.2-1 is the probability of the sample data. Note that a different engineering action should be done for the different colour in it.

On the other hand, conditions of a production machine, used to explain the product quality, are monitored on 18 sensors (EQC) settled in four types of subunits of a machine (Fig.2-2). Soon after the process end, 5 basic statistics are calculated, and 90 variables can be used for VM. Note that the original wave data of each EQC cannot be opened for any publications, and the statistics are used in this paper.

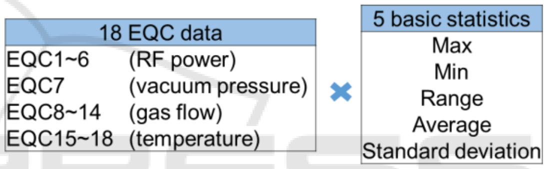


Figure 2-2: Machine variable set for experiment.

The challenge of VM here is to estimate/predict the class of each product quality only by using the machine data and the VM model that has been learned by the set of machine data and the class data of each product quality in a learning data set. Table.2-2 shows the combinations of machine variables to evaluate the VM accuracy. Note that only the average and the standard deviation (SD) for each EQC are used for the first phase. The choice of the statistics is also based on engineering knowledge.

Table 2-2: 13 combinations of machine variables for the performance evaluations ((x): # of variables).

parameter set No.	Avarage	SD	parameter set No.	Avarage	SD
1	EQC1-18(18)	EQC1-18(18)	8	EQC8-14(7)	EQC8-14(7)
2	EQC1-18(18)	-	9	EQC8-14(7)	-
3	-	EQC1-18(18)	10	-	EQC8-14(7)
4	EQC1-6(6)	EQC1-6(6)	11	EQC5-18(7)	EQC5-18(7)
5	EQC1-6(6)	-	12	EQC5-18(7)	-
6	-	EQC1-6(6)	13	-	EQC5-18(7)
7	EQC7(1)	EQC7(1)			

2.2 The First Phase – SVM Applications

As the first, S. Arima (2011) has examined VM of an actual plasma-CVD process. Before applying the kSVM, 2σ/3σ methods and the combination of the Hotelling-T^2 and Q-statistics are evaluated for easier 2-class discrimination problem. The former is a basic statistical process control (SPC), and the latter is a representative of the multivariate statistical process control (MSPC). The accuracy of the latter stays low (67%) though a false error (False Positive of confusion matrix) is much improved than the former case. The reason why the low accuracy is that the data is not ideally distributed along the normal distribution, for example, subunit4: temperatures.

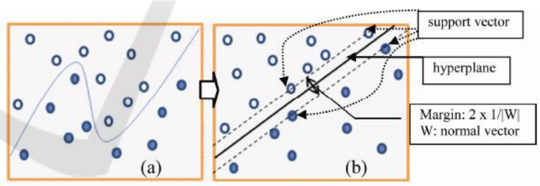
Support Vector Machines (SVM) was originally introduced to address the Vapnik's (1995) structural risk minimization principle and is now famous for high accuracy in application fields (e.g. Lee,et.al., 2015). The basic idea of SVM is to map the data into a higher dimensional space called feature space and to find the optimal hyperplane in the feature space that maximizes the margin between classes as shown in Fig.2-3. A kernel function, such as the Polynomial, the Gaussian (hereafter RBF: Radial basis function), the Linear, or the Sigmoid kernel are used to map the original data to feature space. the simplest SVM deals with a two-class classification problem—in which the data is separated by a hyperplane defined by a number of support vectors. Support vectors are a subset of the training data used to define the boundary between the two classes.

The kernel-SVM (kSVM) is compared with the linear discriminant analysis for the binary classifications problem as the first. The kSVM performs better than the linear discriminant analysis for the 2-class model, though each of those achieves more than 80% of accuracy. Next is the multi-class discriminant in Table.2-1. The linear and the nonlinear discriminant analyses are compared with the kSVM (Fig. 2-4). Here, SVMs were originally designed for binary classifications. However, many real-world problems have more than two classes. Most researchers view multi-class SVMs as an extension of the binary SVM classification problem as summarized by Wong and Hsu (2006). Two approaches, one-against-all and one-against-one methods, are commonly used. The one-against-all method separates each class from all others and constructs a combined classifier. The one-against-one method separates all classes pairwise and constructs a combined classifier using voting shemes In this study, the former approach is used.

Independent from the combination of machine variables, the kernel-SVM achieves the best in the three methods. Beside that, the accuracy of the standard linear and non-linear discriminations (5-dimension) are less than 60% and 20%, respectively. 100% accuracy is achieved when the variables of all machine sub-units are used for the RBF-SVM learning (x=1, 2, or 3).

However, it also shows that when there are not enough variables in the data set for leaning step, the accuracy in the test step stays lower level. Since the semiconductor manufacturing is going to be a high-mix and low-volume production system in these years, and the number of samples can be used in the learning step (is limited to several tens in some cases. Therefore, we applied LOOCV (leave-one-out cross-validation) to the problem. LOOCV involves using one sample as the validation data in the test step and the remaining samples as the training data in the learning step. This is repeated on all samples one by one to cut the original samples on a validation data and the training data. We confirmed the high accuracy of SVM using LOOCV to respond to such a case of small data set. The 9-class discrimination can be solved by using several tens samples in this study. However, note that the accuracy of kSVM model depends on the variables considered, the number of classes, and the data size.

$$\Phi : x_i \in X^p \rightarrow z_i = F(x_i) \in Z^q (p < q), \quad \langle z_i, z_j \rangle = K(x_i, x_j)$$



Note: *Solid line*: the optimal separating hyperplane $<w, z> + b = 0$; *Dashed line*: $<w, z> + b = 1, -1$.

Figure 2-3: Kernel SVM: (a) non-linear discrimination needed and (b) mapping from original space to feature space by a kernel function.

As the summary of the first phase, SVM was applied to construct an accurate VM model that provided multi-class quality prediction of the product. The VM model predicted with 100% accuracy the quality of the product after a CVD process. The accuracy depends on the set of input variables, and the best here is a case variables of all subunits are included.

We got the following issues for the practical use in the mass production as the result of the SVM applications of the first phase:

1) Machine variables are selected manually based on

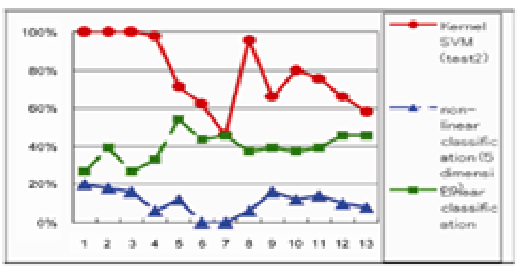


Figure 2-4: Case#2 -VM accuracy -nine classes. (x={1,2,…13}: # EQC variables set in Table 2-2).

the engineering knowledge, and the best combination of the variables are empirically detected. The issue is to automatically extract the variables from the wider scope.
2) SVM using the RBF kernel could achieve the highest accuracy for the VM model as the result of comparison of the Polynomial kernel or the Sigmoid kernel. However, for the large model it is difficult to build the VM model based on RBF-SVM in a realistic time period. For example, 10 hours for learning when RBF is used for the final test process of an actual factory. The issue is to utilize a different kernel function of high speed without unallowable deterioration of the accuracy.

2.3 LASSO Applications

Second phase is for automatic variable extractions and fast computation of SVM learning, and so LASSO technique is applied and evaluated.

2.3.1 Problem Definition

In the first phase, much adaptive accuracy of RBF-SVM could be evaluated by numerical experiments of discrimination of multi-class quality by using actual fab data. However, 13 different variable sets are comparably evaluated to get the best accuracy in that case. The number of the variables (M=90) are larger than the number of samples (e.g. n=50), and thus some of those are selected based on engineering knowledge (Table.2-2). Here, the sparse modelling is a rapidly progressing in recent. It is one important research area of the compressed sensing, and it has very wide application fields such as a medical data processing (rapid image sensing of MRI or CT), the earth science (data-driven modelling and forecasting), and so on. Note that the deep learning method also can extract meaningful variables but it requires a big data to analyze, and so it cannot be used in this case. This paper focuses on the automatic variable extraction which can be used even when M >n.

2.3.2 Methods - Lasso

Basic Least-square method is used to estimate coefficients **C**$\in \mathbb{R}^M$ to minimize the estimation error (Eq.2) in the linear regression (Eq.1) from the data set $\{ (\boldsymbol{x_i}, y_i) \in \mathbb{R}^M \times \mathbb{R};\ i = 1,2,\cdots n \}$. Here, if some variables in $\boldsymbol{x}$ may not contribute to estimate Y, some of values in “C” should be zero to reduce the variance of the estimation result. That responds to “parse” case. LASSO proposed by Tibshirani (1996) is the estimation method of the sparse coefficient vector to reduce the variance of the estimation result (Eq.3).

$$Y = C^T X, Y = (y_1, y_2, \cdots y_n)^T, X = \begin{pmatrix} {x_1}^T \\ {x_2}^T \\ \vdots \\ {x_n}^T \end{pmatrix} \quad (1)$$

$$Er = \sum_{i=1}^{n} (y_i - {x_i}^T c)^2 = \|y - Xc\|_2^2 \quad (2)$$

$$\min_c \|y - Xc\|_2^2 \quad s.t. \|c\|_1 \le \lambda \ \ (\lambda > 0) \quad (3)$$

2.3.3 Numerical Results

In case of the class definition of Fig.2-1, we empirically selected variables of 2 kinds of statistics as the result (Table.2-2). Here, we try to “automatically extract the variables by applying the sparse modelling, and evaluate those accuracy as well. The significant variables for the design conformity (V(D)) and for the uniformity” (V(U)) are extracted (Table.2-4). The-10-hold cross validation is used for LASSO, and the set of variables are selected when the lambda is minimum as shown in Figures 2-5 and 2-6.

VM model of kSVM is built by using conjoint form of variables (e.g. V(D)∪V(U)) as the first case. Its accuracy of each kernel is evaluated for 2-demensional quality classification by using the LOOCV. A linear kernel is the best for the Lasso-kSVM as shown in Table 2-5.

2.3.4 Issues for the next

We got the following issues for the practical use in the mass production as the result of the SVM applications of the second phase. Automated procedure of VM modelling should be proposed.
1) LASSO regression model can achieve the compression of the variables and computational time

much, however, we have to consider about the multi-objective model. The multi-dimensional classes of product quality may not be in the relationship of linearly independent each other because it has been defined by the engineering knowledge. In that case, the join set of variables can be redundant. The exclusion is still 7 variables as common of Dc and Uf (Table 2-4).

2) It is required to compare with other multi-objectives models such as PLS (Partial Least Squares) often used in chemo-metrics research area.

Table 2-4: Variable extractions by Lasso -(Design conformity(D) / Uniformity (U) /Both (B)).

Variables extracted		Sensor No. 1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
statistics	Min	U			U			U			U			U	U				
	Max	U						D				U	D	U	U	B	U	B	
	Range				U			D					U					U	U
	Average		B						U	U	B		B		U	D	U	U	U
	Std. dev.				U				U	B		U	B	U		U			

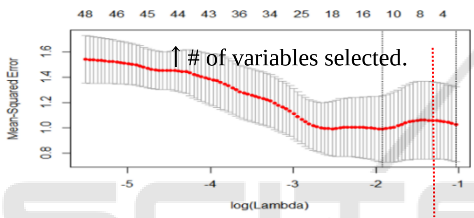


Figure 2-5: Cross validation for Lasso parameter (λ - [min, lse] = [0.1462973, 0.3540583]) for i) D.

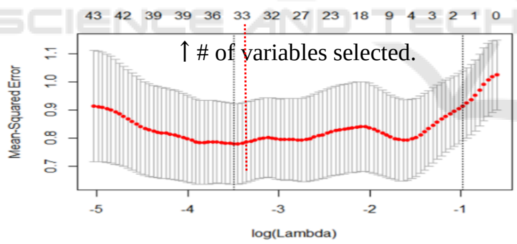


Figure 2-6: Cross validation for Lasso parameter (λ - [min, lse] = [0.03037, 0.37440]) for ii) U.

Table 2-5: VM accuracy – Lasso-kSVM.

Quality class of VM	variables set [# of variables]	Kernel RBF	Kernel Linear
Design conformity (A,B,C)	V(D) [11]	92	88
Uniformity (a,b,c)	V(U) [35]	84	100
2D quality (A,B,C) X (a,b,c)	V(D) U V(U) [39]	90	100
			accuracy [%]

3 PCA AND LASSO APPLICATIONS

3.1 Problem Definition

In this section, we will discuss an automated VM procedure using PCA-LASSO and the kernel SVM to solve the issues mentioned in section 2.3.4. PLS is able to analyze the case the sample size is less than the number of the variables.

3.2 Method - PCA and PLS

3.2.1 Basics of PCA and PLS

Principal component analysis (PCA) is a mathematical procedure that transforms a number of possibly correlated variables into a smaller number of uncorrelated variables called principal components. PCA rotates the axes of the original variable coordinate system to new orthogonal axes, called principal axes, such that the new axes coincide with directions of maximum variation of the original observations (Fig.3-1(graph)).The regression is the modelling of relational expression between the objective variable(s) *Y* and the explanatory variables *X*. Coefficients are estimated under the conditions of lowest estimation errors by the Least-square or another method. There are some regression models using PCA (Fig.3-1). PCR is a representative in which PCA is applied only to *X*. On the other hand, both *X* and *Y* are rotated by PCA before regression in PLS.

3.2.2 PCA Application for Quality Definitions

The PCA is applied for a multi-dimensional quality definition. As the first case, PCA is used to 2-demensional quality data (Design conformity (Dc) and Uniformity (Uf)) to rotate to the orthogonality space. After the PCA, the class is defined under the threshold of 3-quantiles for each dimension. In the second PCA application, we newly define the multi-dimension of the quality as shown in Table.3-2 as the result of PCA using original thickness values of 9 points. The primary principle component (PC1) shows the level of thickness and it responds to the "Design conformity" (Dc'). The second and the third principle component (PC2, PC3) show the deflection of the thickness and respond to "Uniformity" (Uf ’). The threshold of quality class can be defined by:

i) Probability (e.g. normal distribution case)

ii) Quantiles (e.g. uniform distribution case, etc.)
Based on the distribution of the principal component scores (Fig. 3-3), only PC1's score is statistically adapt to the normal distribution as the result of One-sample Kolmogorov-Smirnov test (D = 0.55944, p-value = 2.998e-15, alternative hypothesis: two-sided). Here, i) is selected for defining classes of Dc' and ii) is used for defining classes of Uf '. The threshold here is defined as shown in Table 3-5 for i). On the other hand, the 3-quantiles is used for ii).

b) Multiple Linear Regression (MLR)

$$y_i = \beta_0 + \beta_1 x_{i1} + \ldots + \beta_p x_{ip} + \varepsilon_i$$

c) PCR(Principle Component Regression)

$$\begin{cases} Y_i = \beta_0 + \beta_1 Z_{i1} + \ldots + \beta_r Z_{ir} + \varepsilon_i \\ Z_{ir} = a_{r1}x_{i1} + a_{r2}x_{i2} + \ldots + a_{rm}x_{im} \end{cases}$$

e) PLS(Partial Least Squares) regression

$$\begin{cases} X = \bar{X} + \sum_{a=1}^{r} t_a p_a + E,\ y = \bar{y} + \sum_{a=1}^{r} t_a q_a + f, \qquad \beta = W(P^T W)^{-1} q \\ W = (w_1, w_2, \cdots), \quad P^T = (p_1, p_2, \cdots)^T \qquad q = (q_1, q_2, \cdots)^T, \\ w_i = \frac{X^T t_i}{\|X^T t_i\|}, \quad t_i = \sum_{k=1}^{m} x_{ik} w_k = x_{i1}w_1 + x_{i2}w_2 + \cdots + x_{im}w_m \\ p_i = \frac{X^T t_i}{t_i^T t_i}, q_i = \frac{y^T t_i}{t_i^T t_i} \end{cases}$$

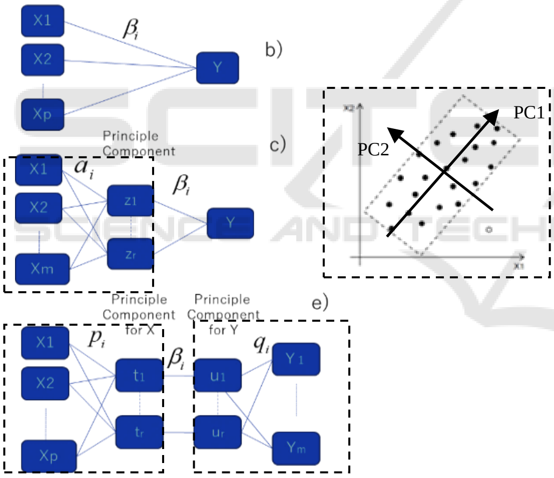


Figure 3-1: Multivariate regression models.

Table 3-1: PCA result - factor loading (PC1, 2, 3).

	Original variables of quality measured								
	QC1	QC2	QC3	QC4	QC5	QC6	QC7	QC8	QC9
PC1	0.292	0.350	0.350	0.335	0.352	0.350	0.303	0.288	0.370
PC2	0.177	0.189	0.263	0.454	0.076	0.010	(0.333)	(0.076)	(0.731)
PC3	(0.660)	0.087	0.126	0.390	0.155	(0.030)	(0.396)	(0.260)	0.373

Table 3-2: PCA result - factor loading (PC1, 2, 3).

	original variables of quality								
	QC1	QC2	QC3	QC4	QC5	QC6	QC7	QC8	QC9
PC1	0.292	0.350	0.350	0.335	0.352	0.350	0.303	0.288	0.370
PC2	0.177	0.189	0.263	0.454	0.076	0.010	(0.333)	(0.076)	(0.731)
PC3	(0.660)	0.087	0.126	0.390	0.155	(0.030)	(0.396)	(0.260)	0.373

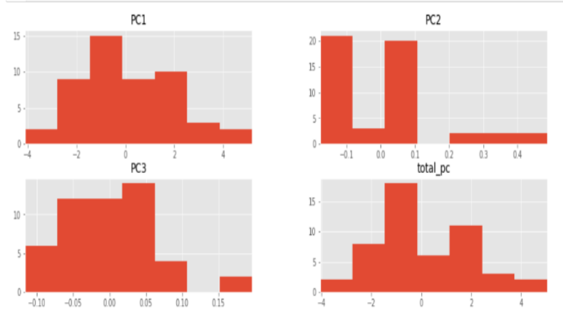


Figure 3-3: PCA result -principal component scores.

Table 3-5: The threshold for i (yi: the score, μ: average, σ:standard deviation).

a	μ - σ ≦yi≦ μ + σ
b	μ -2σ≦yi< μ - σ, μ + σ <yi≦ μ +2σ
c	yi< μ -2σ, μ +2σ<yi

3.3 Numerical Results

3.3.1 Automated VM Procedure

The procedure of PCA-LASSO and kSVM
STEP-1: PCA to define the multi-dimensional quality. Select a few principal components by the cumulative contribution ratio becomes over 80*% or so. (*depend on the target accuracy)
STEP-2: LASSO to extract the significant machine variables
STEP-3: Select the principal component to use in the following step. Check the LASSO result (e.g. PC2 is excepted because of no variables selected.)
STEP-4: Select the threshold type for each PCs. Check the distributions of principal component scores for selected PCs (e.g. PC1 and PC3 is set to the probability-type and to the quantiles)
STEP-5: Define the class for all samples (e.g. product wafer here)
STEP-6: SVM learning and class discriminations.

3.3.2 PCA-LASSO (1) and Kernel SVM

As the first case, PCA is used to 2-demensional quality data (Dc2 and Uf2) to rotate to the orthogonality space. The threshold of quality class can be defined by the 3-quantiles for each dimension. Combination of LASSO and linear-SVM appear the best accuracy again (100%) even if PCA is used. In the same case, the accuracies of RBF-SVM and Polynomial-SVM result 82% and 92%, respectively. In case of PCA-LASSO (1), PC2 is excepted because no machine variables are selected in the LASSO regression, and only the primary principle component (PC1) represents both the "Design conformity" and "Uniformity" (PC1: Dc2 & Uf2). Note that PLS regression cannot work well in this case. Error is detected in calculation.

3.3.3 PCA-LASSO (2) and Kernel SVM

Here we use the result of PCA using original thickness values of 9 points (PC1: Revised design conformity (Dc'), PC3: Revised uniformity (Uf ')). 2nd-principal component PC2 is excepted because no machine variables are selected by LASSO.

Three principal components were obtained by PCA, and 12 variables for PC1 and 4 variables for PC3 were chosen. Variable sets for PC1 and PC3 are expressed as V(Dc')and V(Uf '). Since each principal component is orthogonal, the variables chosen for each principal component tend to be uncorrelated, that is, they are exclusive. Thus, variables included in the union can explain the original objective variables without waste. The variable set used for the SVM learning is defined as the union of the variables extracted by LASSO: $V(Dc') \cup V(Uf')$

Linear-SVM appears again the best accuracy for all (98%) in addition to the shortest computational time. RBF-SVM is lower accuracy (82%) though it can keep its accuracy based on best parameters for the gamma function. In addition, the computational time is the largest for all. The accuracy of the Polynomial-SVM stays about 90%.

Note that the result of the variable extraction of this PCA-LASSO is helpful pre-process for PLS regression though the PLS regression cannot be solved when the original input data without the representative object variables and extracted explanatory variables. This is one type of cases that PLS regression does not go well because the data set includes an explanatory (independent) variable irrelevant to an objective (dependent) variable. Even though in such a case, PLS regression can succeed by the pre-process of variable extraction of the PCA-LASSO regression. The best number of objective variables, that is principal components here, is the same as the number of selected objective variables in PCA. "3" is the best of the lowest RMSE (root-mean-square error) as shown in Fig. 3-4.

3.3.4 PCA-LASSO (3) and Kernel SVM

We can use the result of PCA to define comprehensive index by using the contribution rate (thus Eigen values), Eigen vectors, and so on. However the result of LASSO for the comprehensive index is not so effective here.

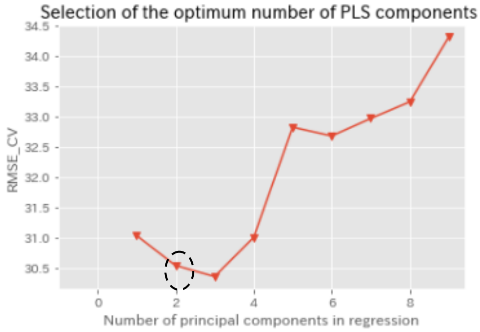


Figure 3-4: Selection of # of objective variables (principal components here) for PLS.

3.4 Summary of Variable Extractions

PCA is combined to LASSO regressions instead of PCR (Fig.3-1) or PLS (Fig.3-1, or as a pre-process of PLS) to extract the optimal and smallest set of variables for comprehensive VM modelling of multi-dimensional quality. As the result of comparison of PCA-LASSO (1) and (2), the compaction rate is improved by about 66.7% and 83.3% besides the exclusion rate' improvement (Table 3-7). In case of PCA-LASSO (1), PC2 is excepted because no machine variables are selected in LASSO regression, and only the primary principle component (PC1) represents both the design conformity and uniformity (Dc2 & Uf 2:PC1). That is caused the original definition of the 2 factors of thickness is not linearly independent. In such a case, compression rate is lower than the other case. The exclusion rate becomes much lower in the proposed PCA-LASSO cases (Tables 3-6, 3-8, 3-9, 3-10). See appendix-A for the coefficients of the variables.

3.5 Conclusions of the Third Phase

In this section, automated VM procedure using PCA-LASSO and kernel SVM is proposed and evaluated. PCA is combined to LASSO regressions instead of using PCR or PLS to extract the reasonable and smallest set of variables for comprehensive VM modelling of multi-dimensional quality. In addition, the liner-kernel SVM using the variables selected LASSO regressions achieves the highest accuracy. LASSO and linear-kernel SVM can compress the scale and computational time much in the model learning without deterioration of the accuracy.

Table 3-6: The number of machine variables extracted.

	# of variables (total) V(D+U)=V(D)∪V(U)	# of depricated variables V(D*U)=V(D)∩V(U)
Original	90	-
LASSO (Dc, Uf)	39	7
PCA-LASSO(1) (pc1: Dc2 & Uf2)	30	0
PCA-LASSO(2) (pc1: Dc', pc3:Uf')	15	1

Table 3-7: Compaction rate and Exclusion rate.

[%]	Compaction rate =(90-V(D+U))/90	Exclusion rate ={V(D+U)-V(D*U)}/V(D+U)
Original	0.00%	-
LASSO (Dc, Uf)	56.67%	82.05%
PCA-LASSO(1) (pc1: Dc2 & Uf2)	66.67%	100.00%
PCA-LASSO(2) (pc1: Dc', pc3:Uf')	83.33%	93.33%

Table 3-8: Machine variables extracted by LASSO. (※D: Design conformity, U: Uniformity, B:both).

Variables extracted		Sensor No.																	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
statistics	Min	U			U			U			U			U	U				
	Max	U						D				U	D	U	U	B	U	B	
	Range				U			D					U					U	U
	Average		B						U	U	B		B		U	D	U	U	U
	Std. dev.				U				U	B		U	B	U		U			

Table 3-9: Variables extraction of PCA-LASSO (1). (※PC1: Design conformity & Uniformity).

Variables extracted		Sensor No.																	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
statistics	Min	PC1											PC1		PC1	PC1			
	Max	PC1					PC1	PC1		PC1		PC1		PC1	PC1		PC1	PC1	
	Range			PC1			PC1						PC1			PC1			
	Average	PC1	PC1		PC1						PC1				PC1			PC1	
	Std. dev.				PC1	PC1	PC1			PC1			PC1	PC1	PC1				

Table 3-10: Variables extraction of PCA-LASSO (2). (PC1: Design conformity, PC3: Uniformity, B:both).

Variables extracted		Sensor No.																	
		1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
statistics	Min								PC1	PC3									PC1
	Max							PC1	PC1			PC1		PC1					
	Range				PC1														
	Average							PC3										PC1	B
	Std. dev.			PC3					PC1						PC1				PC1

4 CONCLUSIONS

This study discussed the modelling of virtual metrology in 3 phases. The first is the application of SVM for multi-class virtual metrology mainly for high accuracy. The second phase is LASSO application for automatic variable extractions and fast computation of Linear-SVM learning. Finally the third phase is for all; automated extractions of the best set of machine variables, the high accurate quality discriminations for the multi-dimensional classes, and the fast computation for a practical use.

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REFERENCES

Y.Naka, K.Sugawa, C. McGreavy., 2012. *Introduction to VLSI Process Engineering*, Springer.

APC Conference (USA) (Oct. 22nd, 2018 access) http://www.cvent.com/events/apc-conference-xxx-2018/event-summary-a8d0f8ae27e84ecf97862bdc1b4c7b01.aspx.

EUROPEAN ADVANCED PROCESS CONTROL AND MANUFACTURING CONFERENCE (Oct. 22nd, 2018 access): https://www.apcm-europe.eu/home/.

AEC/APC symposium Asia (Oct. 22nd, 2018 access): https://www.semiconportal.com/AECAPC/index_e.html.

Literatures in "*Metrology*" and "*Advanced process control*" sessions of *IEEE Transaction on Semiconductor Manufacturing* (since 2011).

S. Arima, 2011. Virtual Metrology-based Engineering Chain Management by Multi-classification of Quality using Support Vector Machine for Semiconductor Manufacturing, *Int. J. Industrial and Systems Engineering* No.8 Vol.1, Inderscience pub., pp.1-18 .

S. Arima., et.al., 2015. Applications of machine learning and data mining methods for advanced equipment control and process control, *Proceedings of AEC/APC symposium Asia 2015*, DA-O-34 (pp.1-6).

Vapnik, V.N. ,1995. *The Nature of Statistical Learning Theory*, New York: Springer-Verlag.

Wong, W. and Hsu, S. ,2006. Application of SVM and ANN for image retrieval, *European Journal of Operations Research*, Vol. 173, pp.938–950.

T. Lee, C. O. Kim., 2015. Statistical Comparison of Fault Detection Models for Semiconductor Manufacturing Processes, *IEEE Trans. on Semi. Manufacturing*, 28(1), pp.80-91, IEEE.

R.Tibshirani.,1996. Regression shrinkage and selection via the lasso, *J. R. Statist. Soc. B*, 58(1), pp.267-288.

R. A. Johnson, D. W. Wichern., 2007. *Applied Multivariate Statistical Analysis*, Prentice Hall.