Statistical Methods for Semiconductor Manufacturing

Gian Antonio Susto

PhD School on Information Engineering XXV Series, ICT Section Advisor: Prof. Alessandro Beghi

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Introduction •000	Virtual Metrology	VM with Time Series	VM: Publications	Predictive Maintenance	PdM: Applications	PdM: Publications	
Motivation							



- Semiconductor-based devices are pervasive (PCs, mobiles, cars, etc.)
- Semiconductor Manufacturing: one of the most technologically advanced with new products every months
- Constant search for improving process quality and control
- In the milestone paper [Edgar 2000] a huge margin of improvements for modeling and control in semiconductor manufacturing has been described
- 13 years have passed ...

T. Edgar, S. Butler, W. Campbell, C. Pfeiffer, C. Bode, S. Hwang, K. Balakrishnan, J. Hahn Automatic Control in Microelectronics Manufacturing: Practices, Challenges, and Possibilities *Automatica*, Vol. 36, Issue 11, Nov. 2000, Pag. 1567-1603

Introduction	Virtual Metrology	VM with Time Series	VM: Publications	Predictive Maintenance	PdM: Applications	PdM: Publications
Outline						

- Advanced Process Control (APC) systems have proliferated in the past years
- Two APC topics investigated
 - (a) Virtual Metrology (VM)
 - (b) Predictive Maintenance (PdM)
- Several challenging aspects tackled
- We will illustrate the following applications
 - (i) VM: Prediction of CVD thickness
 - (ii) VM: Multi-Step VM
 - (iii) VM with Time Series data
 - (iv) VM and Run-to-Run Control
 - (v) PdM for epitaxy
 - (vi) PdM for ion implantation

Introduction

tion Virtual Metrology

VM with Time Series

VM: Publication

Predictive Maintenanc

PdM: Applications

PdM: Publications

Summary of PhD activities



- Involvement in IMPROVE (Implementing Manufacturing science solutions to increase equiPment pROductiVity and fab pErformance): a 42 months, 37 million euro project
- Collaborations:
 - (a) Infineon Technologies AG, Austria (IFAT)
 - (b) STMicroelectronics
 - (c) University of Pavia
- Research periods abroad:
 - (a) IFAT in Villach, Austria
 - (b) National University of Ireland, Maynooth









Elements of Semiconductor Manufacturing



- The Wafer: main product of semiconductor industry
- Thin slice of silicon crystal used as substrate for microelectronic devices
- Production organized in Lots: groups of 25 wafers
- One process iteration, one wafer



- (a) Chemical Vapor Deposition (CVD)
- (b) Lithography
- (c) Etching

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(d) ..
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Introduction





- Several quantities (Y) on the wafer are costly to be measured, but they are necessary to monitor process quality
- Y only measured for few wafers in a lot
- VM system: model of a process for estimating Y based on the availability of tool and/or logistic data X
 - Regression Problem
 - ⇒ Black Box Modeling



- Besides accuracy a VM system must provide
 - (i) Fast Computation: new products every months, models needs to be recomputed frequently
 - (ii) Interpretability: to provide process insights and guidelines for control actions

VM: Challenge (1) - High Dimensionality

(1) High-Dimensionality: hundreds/thousands of input variables

Two approaches:

Virtual Metrology

- (i) Dimensionality Reduction (Correlation, PCA) two-step approach
- (ii) Variable Selection (Stepwise Selection, LARS, Regularization Methods) interpretable results



Regularization Methods Penalty on the complexity of the model:

$$\mathcal{L}(\theta) = \|\mathbf{Y} - \mathbf{X}\theta\|^2 + \lambda \mathcal{R}(\theta)$$

PdM: Applications

Different methods for different choice of R

(i) Ridge Regression $-R(\theta) = \sum_{j=1}^{p} \theta_j^2$ (ii) LASSO $-R(\theta) = \sum_{j=1}^{p} |\theta_j|$

iii) Elastic Net

$$R(\theta) = \alpha \sum_{j=1}^{p} \theta_j^2 + (1 - \alpha) \sum_{j=1}^{p} \theta_j^2$$

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 VM:
 Challenge (1) - High Dimensionality
 PdM: Publications
 PdM: Publications
 PdM: Publications



- RR suitable for highly correlated dataset
- LASSO provide sparse (more interpretable) models

VM: Challenge (2) - Data Fragmentation

VM with Time Series

- (2) Data Fragmentation: thousands of products run, different tool settings (recipes), equipment composed of 2/3 chambers
- No single modeling for each logistic path, not enough data. Two approaches:
 - (i) smart data clustering (PCA, information-theory elements)
 - (ii) multi-task modeling

Virtual Metrology



VM: Prediction of CVD thickness

- Collaboration with Infineon Technologies AG, Austria
- Chemical Vapor Deposition (CVD): chemically growing a layer upon the wafer
- Prediction of the thickness of the deposited layer from tool variables (temperatures, pressures, flows, etc.)
- (i) High data fragmentation:

Virtual Metrology

- 10 products run, different recipes
- tool with 3 chambers (A, B, C) and 2 sub-chambers (1, 2)
- (ii) High number of variables (\approx 450)
 - Modeling with Neural Networks and Least Angle Regression (LARS)



VM: Multi-Step Modeling

VM with Time Series

Virtual Metrology

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- Collaboration with University of Pavia and Infineon Technologies AG, Austria
- Quality features of a certain wafer depend on the whole processing
- Multi-level: Generalized Additive Model (sum η logistic effects)

$$f(X) = \sum_{k=1}^{\eta} f_k(X_k)$$



VM: Publications Virtual Metrology VM with Time Series VM: Publications Predictive Maintenance PdM: Applications PdM: Publications VM: Publica





 State of the art: Reliance Index (RI) based penalization



VM: Publications Predictive Maintenance PdM: Applications Predictive Maintenance ON PdM: Challenge (3) - Run-to-Run and VM 2/2



- Information Theory elements
- Penalization on VM measures based on
 - (i) statistical distance
 - (ii) iterations from last physical measure

VM: Challenge (4) - Time Series Learning (TSL)

VM with Time Series

Modeling

Training dataset (n observations): p regressors x^j and a scalar target value y

$$S = \left\{ x_i \in \mathbb{R}^{1 \times p}, \ y_i \in \mathbb{R} \right\}_{i=1}^n \quad \Rightarrow \quad Y = \left[\begin{array}{cc} y_1 \\ \vdots \\ y_n \end{array} \right] \ X = \left[\begin{array}{cc} x_1^1 & \dots & x_1^p \\ \vdots & & \vdots \\ x_n^1 & \dots & x_n^p \end{array} \right]$$

Goal: create a predictive model *f* to provide predictions for $\tilde{x} \notin S$

Input Space Representation

- Data not always organized in n × p matrix (xⁱ not always scalar)
- Representation with little information loss not always trivial

i.e. text data mining





Introduction: Problem Statement

- Typical settings for modeling of industrial processes:
 - (i) *p* time series input



Goal

Build a regressor matrix and aggregate the input information in summary features with small loss of information

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TSL: Mathematical Formulation

VM with Time Series

n observations, *p* time series: *i*-th observation X_i

$$\mathcal{X}_i = [x_i^{(1)}(t) \ \dots \ x_i^{(j)}(t) \ \dots \ x_i^{(p)}(t)], \ t \in [0, 1], \forall j$$

A scalar output *y*: training dataset $S = \{X_i, y_i\}_{i=1}^n$ for learning *f*



• $x_i^{(j)}(t)$ samples

 $\left\{t_{i,s}^{(j)}, \ z_{i,s}^{(j)}\right\}_{s=1}^{\mathcal{N}_{i,j}}$

PdM: Applications

Difform length and sampling timestamps

$$\mathcal{N}_{i,j} \neq \mathcal{N}_{i,m}, \ \mathcal{N}_{i,j} \neq \mathcal{N}_{k,j}$$
$$t_{i,s}^{(j)} \neq t_{i,s}^{(m)}, t_{i,s}^{(j)} \neq t_{k,s}^{(j)}$$

Noisy observations

$$z_{i,s}^{(j)} = x_i^{(j)}(t_{i,s}^{(j)}) + v_{i,s}^{(j)} \quad v_{i,s}^{(j)} \sim N(0,
ho_j^2)$$

 Introduction
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 VM: Publications
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 PdM: Public

 TSL:
 Classical Approaches - Statistical Moments



Regressor matrix

$$\Phi = [\Phi_1 \ \dots \ \Phi_j \ \dots \ \Phi_p]$$

where $\Phi_j \in \mathbb{R}^{n \times k_{max}}$ is

$$\Phi_{j}[i, k] = m^{(k)} \left(\left\{ z_{i,s}^{(j)} \right\}_{s=1}^{\mathcal{N}_{i,j}} \right)$$

 k_{\max} highest considered moment order, $m^{(k)}(\cdot)$ is the *k*-th sample moment

Drawbacks:

- (i) Loss of dependency between information and time
- (ii) Independent data points: little statistical meaning for autocorrelated time series



TSL: Classical Approaches - Systematic Sampling



- Interval [0, 1] divided into *N* segments [τ₁ ... τ_N]
- Regressor matrix

 $\Phi = [\Phi_1 \ \dots \ \Phi_j \ \dots \Phi_p]$

populated with

$$\Phi_j[i,k] = \operatorname{Avg}[\boldsymbol{Z}_{i,s}^{(j)} : t_{i,s}^{(j)} \in \tau_k].$$

Drawbacks:

- Number of segments to be selected as trade-off: temporal resolution vs robustness to noise
- (ii) Different features computed with different numbers of values: data reliability issues (*PCA a possible solution*)

SAFE: Supervised Aggregative Feature Extraction

SAFE: A methodology to include temporal information in the regression matrix Φ.
 Assumption: the input x_i^(j) influences y through a weighted integration



 $f(\mathcal{X}_i) := \sum_{i=1}^p \left\langle x_i^{(j)}(t), \beta^{(j)}(t) \right\rangle_{L^2}$

 $\langle f,g\rangle_{L^2}=\int_{-\infty}^{\infty}f(t)g(t)dt$

SAFE: Regularization

Objective Function:

$$\mathcal{L}(\beta) = \mathcal{F}(\beta) + \lambda \mathcal{R}(\beta)$$

where

$$\mathcal{F}(\beta) = \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \int_{-\infty}^{\infty} \beta^{(j)}(t) x_{i}^{(j)}(t) dt - y_{i} \right)^{2}$$
$$\mathcal{R}(\beta) = \sum_{j=1}^{p} \left\langle \beta^{(j)}, \beta^{(j)} \right\rangle_{L^{2}} \quad \text{Ridge Regression}$$

Looking for

$$\beta^* = \arg \min_{\beta} \mathcal{F}(\beta) + \lambda \mathcal{R}(\beta)$$

- The previous cannot be handled directly:
 - (i) we just have samples of $x_i^{(j)}(t)$
 - (ii) $\beta^{(j)}(t)$ have infinite degrees of freedom

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- The previous cannot be handled directly:
 - (i) we just have samples of $x_i^{(j)}(t) \Rightarrow \text{approximate } x_i^{(j)}(t)$ (ii) $\beta^{(j)}(t)$ have infinite degrees of freedom \Rightarrow parametrize $\beta^{(j)}(t)$

SAFE: Time Series Approximation

VM with Time Series

 \blacksquare We consider an approximation of the fitness function $\mathcal L$

$$\hat{\mathcal{L}} = \hat{\mathcal{F}} + \lambda \mathcal{R}$$

 $\hat{\mathcal{F}} = \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \int_{-\infty}^{\infty} \beta^{(j)}(t) \hat{x}_{i}^{(j)}(t) dt - y_{i} \right)^{2}$

Radial Basis function Kernel

Virtual Metrology

$$\begin{aligned} \mathcal{K}(t_1, t_2) &:= e^{-\frac{(t_1 - t_2)^2}{2\omega^2}} \\ &= \sqrt{2\pi}\omega G(t_1, \omega^2; t_2) \end{aligned}$$

it follows that

$$\hat{x}_{i}^{(j)}(t) = \sqrt{2\pi}\omega_{(j)}\sum_{s=1}^{\mathcal{N}_{i,s}} \boldsymbol{c}_{i,s}^{(j)} \boldsymbol{G}(t_{i,s}^{(j)}, \omega_{(j)}^{2}; t)$$

Approximation of x_i^(j)(t) obtained as a weighted sum of Gaussian densities

SAFE: Shape Function Parametrization

VM with Time Series

Parametrization of $\beta^{(j)}$ as linear combination of γ Gaussian densities

$$\begin{aligned} \beta^{(j)}(t) &= \sum_{k=1}^{\gamma} \alpha_k^{(j)} G(\mu(k), \sigma^2; t) \\ \mu(k) &= \frac{k-1}{\gamma-1} \end{aligned}$$

The loss function then becomes

Virtual Metrology

$$\hat{\mathcal{F}} = \sum_{i=1}^{N} \left[\sqrt{2\pi} \sum_{j=1}^{p} \omega_{(j)} \sum_{k=1}^{\gamma} \alpha_{k}^{(j)} \sum_{s=1}^{N_{i,j}} c_{i,s}^{(j)} \int_{-\infty}^{\infty} \left(G(\mu(k), \sigma^{2}; t) G(t_{i,s}^{(j)}, \omega_{(j)}^{2}; t) \right) dt - y_{i} \right]^{2}$$

0.5

Theorem

Let $a, b, x \in \mathbb{R}^{p}$ and $A, B \in \mathbb{R}^{p \times p}$, it holds that

$$\int_{-\infty}^{\infty} G(a, A; x) G(b, B; x) dx = G(a, A + B; b)$$

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PdM: Applications

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0.6

0.8

PdM: Publications

SAFE: Shape Function Parametrization

$$\hat{\mathcal{F}} = \sum_{i=1}^{n} \left(\sqrt{2\pi} \sum_{j=1}^{p} \omega_{(j)} \sum_{k=1}^{\gamma} \alpha_{k}^{(j)} \sum_{s=1}^{N_{i,j}} c_{i,s}^{(j)} G(\mu(k), \sigma^{2} + \omega_{(j)}^{2}; t_{i,s}^{(j)}) - y_{i} \right)^{2}$$

Defining

$$\delta_{i,s}^{(j)}(k) = \sqrt{2\pi} c_{i,s}^{(j)} \omega_j G(\mu(k), \sigma^2 + \omega_{(j)}^2; t_{i,s}^{(j)}), \qquad \overline{\delta}_i^{(j)}(k) = \sum_{s=1}^{N_{i,j}} \delta_{i,s}^{(j)}(k),$$

we obtain the compact formulation

$$\hat{\mathcal{F}} = \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \sum_{k=1}^{\gamma} \alpha_{k}^{(j)} \overline{\delta}_{i}^{(j)}(k) - y_{i} \right)^{2} = ||\Phi\theta - Y||^{2}$$
$$\Phi = \begin{bmatrix} \overline{\delta}_{1}^{(1)}(1) & \dots & \overline{\delta}_{1}^{(1)}(\gamma) & \overline{\delta}_{1}^{(2)}(1) & \dots & \overline{\delta}_{1}^{(p)}(\gamma) \\ \vdots & \vdots & \vdots & \vdots \\ \overline{\delta}_{n}^{(1)}(1) & \dots & \overline{\delta}_{n}^{(1)}(\gamma) & \overline{\delta}_{n}^{(2)}(1) & \dots & \overline{\delta}_{n}^{(p)}(\gamma) \end{bmatrix} \quad \theta = [\alpha_{1}^{(1)} \alpha_{2}^{(1)} \cdots \alpha_{k}^{(j)} \cdots \alpha_{\gamma}^{(p)}]'$$



Testing against classical feature extraction approaches

- (i) Statistical Moments
- (ii) Systematic Sampling
- (iii) PCA on Systematic Sampling
- Results based on Ridge Regression
- n = 500:
 70% training
 30% validation
- p = 1 with [35, 45] samples for observation

Noise:

 $v_{i,s}^{(j)} \sim N(0, 0.1)$

Comparison in terms of RMSE

Experiment 1: Sinusoid Dataset

VM with Time Series

- Only an unknown part of the input signal affects the output
- Input:

Virtual Metrology

$$egin{array}{rcl} \mathbf{x}(t) &=& \sin(t\omega+\delta) \ \omega &\sim& \mathcal{U}(0.01,10) \ \delta &\sim& \mathcal{U}(0,2\pi) \end{array}$$



$$y = \int_{0.3}^{0.7} x(t) dt$$

= $\frac{\cos(0.3\omega + \delta) - \cos(0.7\omega + \delta)}{\omega}$

 Statistical Moments based approach cannot filter important portions of the signal



PdM: Applications

PdM: Publications





 SAFE outperforms statistical moments even when the target is a global feature of the signal

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Predictive Mainte

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PdM: Applications Pd 000 00

PdM: Publications

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VM: Publications 1/2



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IEEE Multi-Conference on Systems and Control, Dubrovnik (Croatia), October 3-5th, 2012, pp. 658-663 Best Student Paper Winner awarded by IEEE Control Systems Society



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PdM Intro: Maintenance Policies



1) Run-to-Failure Maintenance - R2F

When repairs or restore actions are performed only after the occurrence of a failure

"If it's not broken don't fix it"

Common Policy in the fabs

PdM Intro: Maintenance Policies



2) Preventive Maintenance

Maintenances carried out on a planned schedule with the aim of anticipating the process failures

Failures are usually warded off but unnecessary maintenances are performed Introduction Virtual Metrology VM with Time Series VM: Publications Predictive Maintenance PdM: Applications PdM: Publications occessor

PdM Intro: Maintenance Policies



3) Predictive Maintenance - PdM

Maintenance actions are taken after the verification of conditions indicating the degradation of the process/equipment. A *PdM* system predicts when such actions have to be taken

Proposed Policy

Predictive Maintenance (PdM): Techniques

- While all VM problems are regression ones, for PdM, depending on the problem, several techniques may be suitable
 - [Wu 2007]: regression methods (Neural Networks, Elastic Nets)
 - [Baly 2012]: classification methods (Support Vector Machines)
 - [Pampuri 2011]: survival models
 - **[Butler 2010]**: *filtering and prediction* (Particle Filters)

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A Neural Network Integrated Decision Support System for Condition-Based Optimal Predictive Maintenance Policy IEEE Transactions on Systems, Man and Cybernetics, (37), pp. 226-236, 2007

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Proportional Hazard Model with L1 Penalization Applied to Predictive Maintenance in Semiconductor Manufacturing IEEE Conference on Automation Science and Engineering, Trieste, 24-27 Aug, 2011



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Particle Filters for Remaining Useful Life Estimation of Abatement Equipment Used in Semiconductor Manufacturing IEEE Conference on Fault-Tolerant Systems, Nice, 6-8 Oct, 2010



- (1) Problem Definition not standard approaches, solutions tailored for each problem
- (2) Small Amount of Observations maintenances are usually not many for statistical modeling
- (3) PdM Evaluation non-trivial evaluation of the impact of a PdM module and its advantages w.r.t. R2F and PvM approaches



Performances must be evaluated in terms of

- Type I error not prevented maintenances (N_{UB})
- Type II error process iterations (N_{BL}) that may have been performed if the maintenance interventions suggested by the PdM would not have been performed

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PdM: Filtering and Prediction for Epitaxy 1/2

 Temperature difference measured by pyrometers is a key value in Epitaxy control

Virtual Metrology

- With Filtering and Prediction techniques (Kalman Predictor, Particle Filter) an estimation of temperature difference can be provided
- The PdM module provide a confidence level of control action need at next process step





PdM: Applications

Wafer temperature (solid, blue) and prediction (dash, black).

- The end-user is provided with:
 - (i) an estimation of next values of temperature difference with confidence levels;
 - (ii) an estimation of runs to be processed before a maintenance action is needed.

PdM: Publications





- The previous work has been developed with Infineon Technologies AG, Austria sited in Villach and with the collaboration of University of Pavia
- The PdM module, ROOME (pRedictive tOOI for Monitoring Epitaxy) has been implemented in C# in a GUI that it is currently used in production.



PdM: Regression for Ion-Implantation

- Collaboration with STMicroelectronics Italia and University of Pavia
- Breakings of Tungsten Filament is the biggest problem for maintenance engineers
- We propose a PdM module to predict filament breakings based on tool variables
- Module based on Elastic Nets to deal with high dimensionality



Introducti	on Virtual Metrology	VM with Time Series	VM: Publications	Predictive Maintenance	PdM: Applications	PdM: Publications •O
Pdl	M: Publica	ations				
	G.A. Susto, A. Sch A Predictive Mainte 23rd IEEE/SEMI A (US), May 15-17th, Best Student Pape	irru, S. Pampuri, A. I nance System base dvanced Semicondu 2012 r Winner awarded by	Beghi ed on Regulariz <i>ictor Manufactu</i> y the Semicond	ation Methods for lor ring Conference, pp. uctor Equipment and	n-Implantation 175-180, Sarato I Materials Interr	ga Springs national
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Thank you for your attention !

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