

Statistical Methods for Semiconductor Manufacturing

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- 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
- \blacksquare 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

- 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

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Summary of PhD activities T objectives of T is a constraint a constraint a constraint and specific all types of specific all types of

- **Involvement in** *IMPROVE* **(***Implementing* Manufacturing science solutions to increase equiPment pROductiVity and fab pErformance): a 42 months, 37 million euro project **10 Solutions Providers:** PDF Solutions,
- **Proballaborations:** \blacksquare Condition direction.
- (a) Infineon Technologies AG, Austria (IFAT)
- (b) STMicroelectronics $\binom{n}{k}$, C. Angle Denoten British
- (c) University of Pavia UNIPO, CNR-IEI ITALIA, FH-WIENER, FH-WIENER, FH-WIENER, FH-WIENER, FH-WIENER, FH-WIENER, FH-WIENER, FH-WIENER,
- **Research periods abroad:**
	- (a) IFAT in Villach, Austria
- The main idea, building the consortium with many different semiconductor manufacturers, was to (b) National University of Ireland, Maynooth

Elements of Semiconductor Manufacturing

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- **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

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One process iteration, one wafer

Hundreds of processes:

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

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- 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

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

- Two approaches:
	- (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:

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

Different methods for different choice of R

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

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

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VM: Challenge (2) - Data Fragmentation

- **(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*

VM: Prediction of CVD thickness

■ Collaboration with Infineon Technologies AG, Austria

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■ Chemical Vapor Deposition (CVD): chemically growing a layer upon the wafer

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Prediction of the thickness of the deposited layer from tool variables (temperatures, pressures, flows, etc.)

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(i) High data fragmentation:

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- 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)**

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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: Challenge (3) - Run-to-Run and VM 1/2

-
- penalization $\frac{6}{4}$ $\frac{4}{-3}$ $\frac{2}{-1}$ 0 1 2 $\frac{3}{4}$

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VM: 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)

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Modeling

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

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$$
S = \{x_i \in \mathbb{R}^{1 \times p}, y_i \in \mathbb{R}\}_{i=1}^n \Rightarrow Y = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix} X = \begin{bmatrix} x_1^1 & \cdots & x_1^p \\ \vdots & & \vdots \\ x_n^1 & \cdots & x_n^p \end{bmatrix}
$$

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

Input Space Representation

- Data not always organized in $n \times p$ matrix (x^j not always scalar)
- Representation with little information loss not always trivial

i.e. text data mining

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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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Introduction: Problem Statement

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	- (i) *p* time series input
	- (ii) Irregularly sampled measures

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Introduction: Problem Statement

- Typical settings for modeling of industrial processes:
	- (i) *p* time series input
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	- (iii) Sampling can vary observation-wise

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

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Introduction: Problem Statement

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TSL: Mathematical Formulation

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n observations, *p* time series: *i*-th observation \mathcal{X}_i

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

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

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 $x_i^{(j)}(t)$ samples

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

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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

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

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Regressor matrix

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

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

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

*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 $\mathcal N$ segments $[\tau_1 \ldots \tau_N]$
- \blacksquare Regressor matrix

 $\Phi = [\Phi_1 \dots \Phi_i \dots \Phi_n]$

populated with

$$
\Phi_j[i, k] = \text{Avg}[z_{i,s}^{(j)} : t_{i,s}^{(j)} \in \tau_k].
$$

Drawbacks:

- (i) 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*)

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

Model structure:

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

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

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SAFE: Regularization

Objective Function:

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

where

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

$$
\mathcal{R}(\beta) = \sum_{j=1}^{p} \left\langle \beta^{(j)}, \beta^{(j)} \right\rangle_{L^2}
$$
 Ridge Regression

Looking for

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

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

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$$
\mathcal{R}(\beta) = \sum_{j=1}^{p} \left\langle \beta^{(j)}, \beta^{(j)} \right\rangle_{L^2}
$$
 Ridge Regression

Looking for

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

 \blacksquare The previous cannot be handled directly:

- (*i*) we just have samples of $x_i^{(j)}(t) \Rightarrow$ **approximate** $x_i^{(j)}(t)$
- (ii) $\beta^{(j)}(t)$ have infinite degrees of freedom \Rightarrow **parametrize** $\beta^{(j)}(t)$

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SAFE: Time Series Approximation

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

$$
\hat{\mathcal{L}} = \hat{\mathcal{F}} + \lambda \mathcal{R}
$$
\n
$$
\hat{\mathcal{F}} = \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \int_{-\infty}^{\infty} \beta^{(j)}(t) \hat{x}_i^{(j)}(t) dt - y_i \right)^2
$$

■ Radial Basis function Kernel

$$
\mathcal{K}(t_1, t_2) \quad := \quad e^{-\frac{(t_1 - t_2)^2}{2\omega^2}} \\
\qquad = \quad \sqrt{2\pi}\omega G(t_1, \omega^2; t_2)
$$

it follows that

$$
\hat{x}_i^{(j)}(t) = \sqrt{2\pi}\omega_{(j)}\sum_{s=1}^{N_{i,j}}c_{i,s}^{(j)}G(t_{i,s}^{(j)},\omega_{(j)}^2;t)
$$

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

SAFE: Shape Function Parametrization

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

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$$
\beta^{(j)}(t) = \sum_{k=1}^{\gamma} \alpha_k^{(j)} G(\mu(k), \sigma^2; t)
$$

$$
\mu(k) = \frac{k-1}{\gamma - 1}
$$

The loss function then becomes

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

Theorem

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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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SAFE: Shape Function Parametrization

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

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

$$
\hat{\mathcal{F}} = \sum_{i=1}^{n} \left(\sum_{j=1}^{p} \sum_{k=1}^{\gamma} \alpha_k^{(j)} \overline{\delta}_i^{(j)}(k) - y_i \right)^2 = ||\Phi\theta - Y||^2
$$

\n
$$
\Phi = \begin{bmatrix} \overline{\delta}_1^{(1)}(1) & \cdots & \overline{\delta}_1^{(1)}(\gamma) & \overline{\delta}_1^{(2)}(1) & \cdots & \overline{\delta}_1^{(p)}(\gamma) \\ \vdots & \vdots & \ddots & \vdots \\ \overline{\delta}_n^{(1)}(1) & \cdots & \overline{\delta}_n^{(2)}(\gamma) & \overline{\delta}_n^{(2)}(1) & \cdots & \overline{\delta}_n^{(p)}(\gamma) \end{bmatrix}^2 \quad \theta = [\alpha_1^{(1)} \alpha_2^{(1)} \cdots \alpha_k^{(j)} \cdots \alpha_\gamma^{(p)}]'
$$

■ 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

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Experiment 1: Sinusoid Dataset

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

$$
x(t) = \sin(t\omega + \delta)
$$

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$$
\omega \sim \mathcal{U}(0.01, 10)
$$

\n
$$
\delta \sim \mathcal{U}(0, 2\pi)
$$

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

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

Statistical Moments based approach cannot filter important portions of the signal

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

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VM: Publications 1/2

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G.A. Susto, A. Beghi, C. De Luca

A Virtual Metrology System for Predicting CVD Thickness with Equipment Variables and Qualitative **Clustering**

16th IEEE Conference on Emerging Technologies and Factory Automation, Toulouse (France), September 5-9th, 2011

G.A. Susto, A. Beghi

Least Angle Regression for Semiconductor Manufacturing Modeling *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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An Information Theory-based Approach to Data Clustering for Virtual Metrology and Soft Sensors *3rd International Conference on Circuits, Systems, Control, Signals*, Barcelona (Spain), October 17-19th, 2012, pp. 198-203

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A Virtual Metrology System Based on Least Angle Regression and Statistical Clustering *Applied Stochastic Models in Business and Industry*, On-line access stage, 2012

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G.A. Susto, A. Schirru, S. Pampuri, G. De Nicolao, A. Beghi An Information-Theory and Virtual Metrology-based approach to Run-to-Run Semiconductor Manufacturing Control *8th IEEE International Conference on Automation Science and Engineering*, Seoul (South Korea), August 20-24th, 2012, pp. 91-96 Best Student Paper Finalist awarded by IEEE Robotics and Automation Society S. Pampuri, A. Schirru, G.A. Susto, G. De Nicolao, A. Beghi, C. De Luca Multistep Virtual Metrology Approaches for Semiconductor Manufacturing Processes *8th IEEE International Conference on Automation Science and Engineering*, Seoul (South Korea), August 20-24th, 2012, pp. 358-363

A. Schirru, G.A. Susto, S. Pampuri, S. McLoone Learning from Time Series: Supervised Aggregative Feature Extraction *51st IEEE Conference on Decision and Control*, Maui (US), December 10-14th, 2012, pp. 5254-5259

A. Schirru, G.A. Susto, S. Pampuri, S. McLoone Supervised Aggregated Feature Extraction for Functional Regression in Time Series Space *IEEE Transactions on Neural Networks and Learning Systems*, Under Review

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PdM Intro: Maintenance Policies

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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

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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

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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

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

- (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.

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

- 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.

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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

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Thank you for your attention !

Statistical Methods for Semiconductor Manufacturing

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