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Bayesian inference for mining semiconductor manufacturing big data for yield enhancement and smart production to empower industry 4.0

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ABSTRACT

Big data analytics have been employed to extract useful information and derive effective manufacturing intelligence for yield management in semiconductor manufacturing that is one of the most complex manufacturing processes due to tightly constrained production processes, reentrant process flows, sophisticated equipment, volatile demands, and complicated product mix. Indeed, the increasing adoption of multimode sensors, intelligent equipment, and robotics have enabled the Internet of Things (IOT) and big data analytics for semiconductor manufacturing. Although the processing tool, chamber set, and recipe are selected according to product design and previous experiences, domain knowledge has become less efficient for defect diagnosis and fault detection. To fill the gaps, this study aims to develop a framework based on Bayesian inference and Gibbs sampling to investigate the intricate semiconductor manufacturing data for fault detection to empower intelligent manufacturing. In addition, Cohen's kappa coefficient was used to eliminate the influence of extraneous variables. The proposed approach was validated through an empirical study and simulation. The results have shown the practical viability of the proposed approach.

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1. Introduction

Semiconductor fabrication facilities (fabs) are the most capital-intensive and fully automated manufacturing systems, in which similar equipment and processes are employed to produce integrated circuits via lengthy complicated processes with tightly constrained production processes, reentrant process flows, sophisticated equipment, and waiting time limits to fulfill the volatile demands of high product mix. The yield learning curve of semiconductor manufacturing [1–3] has demonstrated that data analytics, cumulative engineering training, and domain knowledge have significantly enhanced yield, and thus integrated yield enhancement methods [4] and [5] are widely employed. However, high dimensionality and multi-collinearity [6] among the operation variables cause difficulty in embracing the independent condition for statistical testing and conventional analysis. Furthermore, the increasing adoption of multimode sensors, intelligent equipment, and robotics have enabled the Internet of Things (IOT) and advanced analytics of automatically collected big data for predicting process behavior and identifying defective tools, chambers, and products to improve

the yield and productivity [7–9] for smart production of semiconductor manufacturing. On the other hand, numerous fundamental demands for computational issues such as variable selection and data preparation are excessively dependent on domain knowledge. Therefore, substantial differences exist between research results and actual processes, and thus researchers have combined technological and psychological factors to improve the interaction between systems and behavior [10–12].

Indeed, building an accurate function of process data in industrial settings is difficult since the process variables are highly correlated [13] and [14], in which high collinearity occurs in high-dimensional modeling because of an increased probability of dependency among the parameters. Furthermore, generating a training set that can circumvent this phenomenon is difficult, since the variables cannot be dropped without understanding the interactions among parameters [15]. On the other hand, process engineers are interested in identifying a few essential variables to effectively identify root causes. Alternatively, a novel approach to hedge and compensate the critical dimension variation of the developed-and-etched circuit patterns via a short-loop processes is evolved for yield enhancement [16]. Also, advanced process control (APC) with dynamically adjusted proportional-integral run-to-run controller is developed to compensate overlay errors [5]. Since hundreds of factors must be considered simultaneously to accurately characterize the yield performance, a retrospective design of experiment (DOE) data mining that matches potential designs with a

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huge amount of data automatically collected to enable effective and efficient data analytics [17].

To fill the gaps for dealing with multi-collinearity and empirical variable selection behavior, this study aims to develop a framework based on Bayesian inference and Gibbs sampling for analyzing semiconductor manufacturing big data with high volume of variables, where Cohen's kappa coefficient was used to eliminate the influence of extraneous variables. Indeed, the proposed Gibbs sampling methodology has been used for deep learning [17], high-dimensional linear regression [18], and prior knowledge learning [19]. To estimate the validity of the proposed approach, simulation and an empirical study were conducted with data collected in a world leading semiconductor manufacturing company.

The remainder of the paper is organized as follows: Section 2 introduces the fundamental material for application to semiconductor manufacturing. Section 3 presents a research framework with detailed procedures. Section 4 details the validation of the framework with simulation and subsequently empirical study in Section 5. Section 6 concludes with a discussion of results and further research directions.

2. Fundamental

The notation and terminologies used in this paper are as follows:

- i Index of process steps
- j Index of manufacturing tools
- l Index of observations
- k Number of process steps
- s_i Number of manufacturing tools in the i th step
- m_{s_i} Number of manufacturing chambers for each tool in the i th step
- M Number of process variables
- N Number of observations
- X_{il} Nominal factor set of step-tool-chamber information (process variable)
- $\mathbf{XN} \times M$ matrix of process information
- $\mathbf{YN} \times 1$ matrix of yield percentage
- $\mathbf{Y}^c N \times 1$ matrix of yield category
- $\hat{\mathbf{Y}}^c N \times 1$ matrix of predicted yield category
- p Prior probability for the $i_{s_i-m_{s_i}}$ th binary variable
- \mathbb{I} Indicator function

Wafer fabrication is complex and lengthy that consists of segments of process steps including oxidation/deposition/metallization, lithography, etching, ion implantation, photo-resist strip, cleaning, inspection, and measurement. Fig. 1 illustrates a segment/short-loop of process steps, and at each step, the wafer is fabricated by a specific tool. A number of alternative tools and chambers may be qualified for performing the same process in a step. However, only one of the many tool-chamber features is applied to a wafer. In particular, since hundreds of factors must be considered simultaneously to accurately characterize the yield performance, a retrospective design of experiment (DOE) data mining that matches potential designs with a huge amount of data automatically collected to enable effective and efficient data analytics [20].

Suppose that k process steps exist for completing a product. s_i denotes the number of manufacturing tools in the i th step, where $i = 1, \dots, k$. Similarly, m_{s_i} represents the number of manufacturing chambers for the j th corresponding tool in the i th step, when $1 \leq j \leq s_i$. Hence, the total set of process variables is estimated using

$$M = \sum_{i=1}^k \sum_{j=1}^{s_i} m_{s_i} = \sum_{i=1}^k s_i * m_{s_i}.$$

To achieve shorter production cycle time, faster process development, higher yield efficiency, and lower contamination risk,

cluster tools that consist of specific processing, cleaning, or cooling chambers, with loading and unloading chambers are increasingly employed in semiconductor manufacturing. Without loss of generality, the tool compounds and process chambers are noted with singular nominal factors as the following explanation.

2.1. Approximate inference for distribution of nominal data

A categorical distribution, i.e., a multinomial distribution, is a generalization of the Bernoulli distribution for a categorical random variable with more than two possible outcomes [21]. In the present study, categorical distribution was used to construct the nonparametric Bayesian model for multivariate nominal data.

Bayesian models can represent dependency among variables, in which current knowledge about model parameters is expressed by prior distribution, denoted as $p(\theta)$, and will be updated with new evidence θ' with the likelihood $p(\theta'|\theta)$ to derive the posterior distribution. If posterior and prior probability distributions are from the same family of distributions, they are then called conjugate distributions, and the prior is called a conjugate prior. In particular, Dirichlet distribution is a conjugate prior for the categorical distribution of multinomial data.

However, quantifying the idea of a Bayesian model is difficult for multinomial data because of the complexity in estimating the parameters of the Dirichlet distribution. Nevertheless, one approach to facilitate this difficulty is to sample values from the distribution before computing the sample statistics.

Sampling from an arbitrary distribution can be extremely complicated. However, the Markov chain Monte Carlo (MCMC) method has facilitated Bayesian statistics [22] that can be applied widely. A Markov chain is a sequence of events with a distribution that depends only on the outcome of the previous event. One basis of Markov chain theory posits that, if the probabilities associated with different events are constructed in the correct manner and the chain has a sufficient length, then the event distribution can be made equal to any arbitrary distribution, including a posterior distribution.

Gibbs sampling is an MCMC technique that is suitable for this task. The concept of Gibbs sampling involves generating posterior samples by eliminating each variable for sampling from its conditional distribution, with the remaining variables fixed to their current values.

The Gibbs sampling-based searching algorithm [23] was originally proposed by George and McCulloch [24]. Garcia-Donato and Martinez-Beneito [25] showed that this simple sampling strategy combined with estimates based on the frequency of visits (the one implemented in the present study) provides extremely reliable results.

The Gibbs sampler is used to estimate the posterior distribution and assess the model parameters [26] and [27]. However, the sampler is particularly favorable for sampling from imbalanced class distribution [28]. Gibbs sampling was preferred since it functions efficiently in the presence of multi-collinearity and high dimensionality.

2.2. Cohen's kappa coefficient

Cohen's kappa is a statistical method that measures the levels of agreement between two raters, each of which is classified into several exclusive categories.

A brief overview of nonparametric techniques shows that kappa is most typically applied to predictive models devised using unbalanced data [29]. This study employed the kappa coefficient for data clearance and variable association.

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