Prediction of Multidimensional Spatial Variation Data via Bayesian Tensor Completion

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Abstract—This paper presents a multidimensional computational method to predict the spatial variation data inside and across multiple dies of a wafer. This technique is based on tensor computation. A tensor is a high-dimensional generalization of a matrix or a vector. By exploiting the hidden low-rank property of a high-dimensional data array, the large amount of unknown variation testing data may be predicted from a few random measurement samples. The tensor rank, which decides the complexity of a tensor representation, is decided by an available variational Bayesian approach. Our approach is validated by a practical chip testing data set, and it can be easily generalized to characterize the process variations of multiple wafers. Our approach is more efficient than the previous virtual probe techniques in terms of memory and computational cost when handling high-dimensional chip testing data.

Index Terms—Bayesian statistics, data analytics, process variation, tensor, tensor completion, variation modeling.

I. INTRODUCTION

Today’s nano-scale semiconductor manufacturing is subject to significant process variations (e.g., uncertain geometric and material parameters caused by imperfect lithography, chemical-mechanical polishing, and other steps) [1]. These process variations can propagate to circuit and system levels, and cause remarkable performance uncertainties and yield degradation. Therefore, extensive numerical modeling, simulation, and optimization techniques have been developed in the past decades to predict and control performance uncertainties of analog, digital, and mixed-signal design [2]–[13]. These numerical tools typically require a given detailed statistical model (e.g., a probability density function or a set of statistical moments) of the process variations. The statistical models of process variations are typically obtained by measuring and analyzing the performance data of a huge number of testing chips. The testing data can also be used for post-silicon yield analysis and performance tuning [14].

It is nontrivial to design and measure testing chips. First, one needs to carefully design and fabricate specialized circuits (e.g., ADC or ring oscillators) to measure or monitor the variation of certain parameters (e.g., Vth) [15]–[17]. For instance, a microprocessor may have hundreds of ring oscillators to monitor parametric variations, leading to large chip area overhead [18]. Second, one usually needs to measure many testing circuits on each die in order to extract statistical distributions or to characterize intradie/interdie spatial correlations. Testing these circuits can consume a large amount of time. Finally, hardware measurement may also permanently damage the chips due to mechanical stress [19].

Instead of measuring all circuits, virtual testing techniques aim to reduce the cost by measuring only a small number of samples. A representative example is the “Virtual Probe” technique [20], [21] and its variants [22], [23], which employ compressed sensing [24] to estimate all performance data from a few measurement samples. In order to estimate all data on a die with an n1 × n2 array of circuits, these techniques approximate the variation data by the linear combination of n1n2 basis functions [e.g., 2-D discrete cosine transformation (DCT) bases] of spatial axes x and y. When the approximation is very sparse (which is generally true in practice), the n1n2 coefficients can be estimated even if only N < n1n2 measurement samples are available. These techniques have proved to be more efficient than traditional approaches, such as Kriging prediction [25] and k-LSE estimation [26]. Compressed sensing is effective for processing 2-D data, but it has some shortcomings: 1) it is inefficient to exploit the structure of multidimensional data and 2) it involves large-scale optimization to compute all DCT coefficients. More detailed analysis will be given in Sections III-C and V.

This paper presents an alternative tensor approach to reduce the cost of modeling variations across multiple dies or wafers. Tensor computation [27] can reveal more information that cannot be captured by matrix- or vector-based computations (e.g., compressed sensing). By stacking all 2-D chip data as a multidimensional data array, we estimate them simultaneously with a small number of random samples. The full unknown multidimensional data set is characterized by several low-rank tensor factors, and the unknown tensor factors are adaptively computed by employing the recently developed variational Bayesian approach [28] with an automatic rank determination process. We demonstrate the effectiveness of our approach by a realistic data set with 717080 data samples describing the contact resitivity of 20 dies, which is beyond the computational capability of Virtual Probe [20]–[23].

II. BASICS OF TENSOR

We first describe a few key definitions related to tensor, which are necessary to understand this paper. We refer the readers to [27] for a detailed introduction of tensor and [29] for tensor computation in electronic design automation.

Definition 1: A tensor is a high-dimensional generalization of a matrix. A matrix X ∈ Rn1×n2 is a second-order tensor, and its element indexed by (i1,i2) can be denoted as x(i1,i2). For a general dth-order tensor X ∈ Rd1×· · ·×d d , its element indexed by (i1, · · · , id) can be denoted as x(id)···(id).

Fig. 1 shows a matrix and a third-order tensor, respectively. In this paper, we denote scalars by lowercase letters (e.g., x), vectors (tensors of order one) by boldface lowercase letters (e.g., x), matrices (tensors of order two) by boldface capital letters (e.g., X), and higher-order
The inner product is defined as

\[ \langle \mathbf{X}, \mathbf{Y} \rangle = \sum_{i_1 \ldots i_d} x_{i_1 \ldots i_d} y_{i_1 \ldots i_d}. \]  

**Definition 2:** Given any two tensors \( \mathbf{X} \) and \( \mathbf{Y} \) of the same size, their inner product is defined as

\[ \langle \mathbf{X}, \mathbf{Y} \rangle = \sum_{i_1 \ldots i_d} x_{i_1 \ldots i_d} y_{i_1 \ldots i_d}. \]  

**Definition 3:** Given \( n \) tensors \( \{ \mathbf{X}^{(m)} \} \) of the same size, their generalized inner product is defined as

\[ \langle \mathbf{X}^{(1)}, \ldots, \mathbf{X}^{(n)} \rangle = \prod_{i_1 \ldots i_d} x_{i_1 \ldots i_d}^{(m)}. \]  

Since tensors are a generalization of matrices and vectors, the above definitions of (generalized) inner product apply to matrices and vectors as well.

**Definition 4:** The Frobenius norm of a tensor \( \mathbf{X} \) is further defined as

\[ \| \mathbf{X} \|_F = \sqrt{\langle \mathbf{X}, \mathbf{X} \rangle}. \]  

**Definition 5:** A tensor \( \mathbf{X} \in \mathbb{R}^{n_1 \times \ldots \times n_d} \) is rank-1 if it can be written as the outer product of \( d \) vectors

\[ \mathbf{X} = \mathbf{u}_1 \circ \ldots \circ \mathbf{u}_d \iff x_{i_1 \ldots i_d} = \mathbf{u}_1(i_1) \cdots \mathbf{u}_d(i_d) \]  

where \( \mathbf{u}_k(i_k) \) denotes the \( i_k \)th element of vector \( \mathbf{u}_k \in \mathbb{R}^{n_k} \).

### III. TENSOR-BASED CHIP TESTING

Different from the previous virtual probe techniques [20]–[23] that employ compressive sensing, this section formulates the virtual testing as a tensor completion problem.

**A. Problem Formulation**

We consider the variations of \( n_3 \) dies on a wafer, and assume that each die has \( n_1 \times n_2 \) circuits (e.g., ring oscillators) which can capture spatial correlations. Instead of measuring all \( n_1 n_2 n_3 \) testing circuits, we aim to estimate their performance by measuring only \( N \) circuits, with \( N \ll n_1 n_2 n_3 \). In order to achieve this goal, we first stack all dies as a 3-D data array. As shown in Fig. 2, the whole data set of die \( i_1 \) is a matrix \( \mathbf{X}_1 \). We can see \( \mathbf{X}_1 \) as \( i_1 \)th slice of a tensor \( \mathbf{X} \in \mathbb{R}^{n_1 \times n_2 \times n_3} \). Now the virtual testing problem can be formulated as tensor completion. Assume that \( N \) measurement results \( x_{i_1 i_2 i_3} \) are given, \( (i_1, i_2, i_3) \in \Omega \), and \( \Omega \) denotes the indices of measured samples. Then, we have the following problem:

Given \( x_{i_1 i_2 i_3} \) for \( (i_1, i_2, i_3) \in \Omega \), find \( \mathbf{X} \).

This formulation can be easily extended to handle multiple wafers: one can add another index \( i_k \) to indicate a specific wafer, and the whole data set \( \mathbf{X} \) is a fourth-order tensor.

**B. Low-Rank Tensor Completion**

The problem in (4) has an infinite number of solutions, since we do not have any information about the un-given samples. Therefore, some constraints should be added. For instance, a \( \ell_1 \) regularization is used in Virtual Probe [20], [21] because heuristic experience shows that a 2-D DCT transform of the data on each die has very sparse coefficients.

In this paper, we estimate the unknown variation data based on a different heuristic: we find that \( \mathbf{X} \) in the chip testing problem usually has a low-rank property in the high-dimensional space. Intuitively, this is because two reasons. First, there exist strong spatial correlations. Second, the fabrication data samples depend on the same fabrication process, and some fabrication process have much stronger influence in causing process variations. Similar to matrices, a low-rank tensor can be written as the sum of some rank-1 tensors

\[ \mathbf{X} = \sum_{j=1}^{r} \mathbf{u}^j_1 \circ \cdots \circ \mathbf{u}^j_d. \]  

This factorization is called the CANDECOMP/PARAFAC (CP) factorization, which is one of several popular factorization formats [27]. Having a few samples of \( \mathbf{X} \), we attempt to compute the factors in (5) and to determine the rank \( r \). Many tensor completion methods were introduced, but most approaches tend to have an inaccurate tensor rank and latent factors estimation, and eventually lead to the problem of over-fitting or weak predictive performance. In this paper, we choose to employ the variational Bayesian CP factorization model [28] to solve our problem. We will introduce the key ideas of variational Bayesian CP factorization in Section IV.

**C. Comparison With Virtual Probe**

The tensor completion approach can be considered as a more flexible generalization of the virtual probe [22]. In order to demonstrate this, we consider the problem of approximating a \( d \)-variable function \( f(t_1, \ldots, t_d) \), where \( t_i \in [0, T_i] \) is a continuous variable for \( i = 1, 2, \ldots, d \).

We discretize \([0, T_i]\) into \( n_i - 1 \) segments of length \( \Delta_i = T_i/(n_i - 1) \), then the \((t_1, t_2, \ldots, t_d)\)th element of \( \mathbf{X} \) can be regarded as the discretized value of \( f(t_1, \ldots, t_d) \)

\[ x_{i_1 \ldots i_d} = f(t_1 = (i_1 - 1)\Delta_1, \ldots, t_d = (i_d - 1)\Delta_d). \]  

This formulation can be easily extended to handle multiple wafers: one can add another index \( i_k \) to indicate a specific wafer, and the whole data set \( \mathbf{X} \) is a fourth-order tensor.
The virtual probe technique [20] is equivalent to approximating $f(t_1,\ldots,t_d)$ by some given and fixed basis functions
\[ f(t_1,\ldots,t_d) = \sum_{i_1=1}^{n_1} \cdots \sum_{i_d=1}^{n_d} c_{i_1\ldots i_d} u_{i_1}^{(1)}(t_1) u_{i_2}^{(2)}(t_2) \cdots u_{i_d}^{(d)}(t_d). \]
Here, $[u_{i_1}^{(1)}(t_k)]$ are some predefined basis functions, and $[c_{i_1\ldots i_d}]$ are the unknown weights. In [20], the basis functions are specifically chosen as some Fourier basis functions. This choice of basis functions normally leads to a sparse representation; however, it is not guaranteed optimal. For instance, the Fourier basis function is not a good choice to approximate a nonsmooth function $f(t_1,\ldots,t_d)$.

IV. BAYESIAN CP FACTORIZATION

We employ the variational Bayesian approach [28] to solve our problem, due to its automatic rank determination and low computational cost. The key ideas are summarized below.

Let $\mathbf{X} = \mathbf{X} + \varepsilon$ be a noisy tensor, and the true latent tensor $\mathbf{X}$ is generated by a CP model
\[ \mathbf{X} = \sum_{j=1}^{r} u_j^{(1)} \circ \cdots \circ u_j^{(d)} = \sum_{j=1}^{r} \mathbf{U}_j^{(1)} \cdots \mathbf{U}_j^{(d)}. \]

The noise term $\varepsilon$ is an independent identically distributed Gaussian distribution, $\varepsilon \sim \prod_{i \in \Omega} \mathcal{N}(0, \tau^{-1})$. Here, we have used $u_j^{(i)}$ to denote the factor vector of dimensionality $k$ in the $j$th outer product; we use the matrix $\mathbf{U}_j = [u_j^{(1)},\ldots,u_j^{(d)}] \in \mathbb{R}^{n \times r}$ to denote all factor vectors associated with the $k$th dimension.

A. Probabilistic Model

Suppose $\Omega$ denotes the indices of some observed entries in $\mathbf{Y}$, the observed tensor $\mathbf{Y}_\Omega$ is defined as
\[ \mathbf{Y}_\Omega = \left\{ \begin{array}{ll} y_{i_1\ldots i_d} & \text{if } (i_1,\ldots,i_d) \in \Omega \\ 0 & \text{otherwise.} \end{array} \right. \]

We further denote $u_{i,j} = (u_{i,j}^{(1)},\ldots,u_{i,j}^{(d)})^T \in \mathbb{R}^{r \times 1}$, i.e., the transpose of the $j$th row of matrix $\mathbf{U}_j$. Combining the noise distribution and the CP model, we get the observation model that is factorized over the observed tensor entries
\[ p(\mathbf{Y}_\Omega | [\mathbf{U}_j]_{k=1}^{d}, \tau) = \prod_{(i_1,\ldots,i_d) \in \Omega} \mathcal{N}(y_{i_1\ldots i_d} | [u_{i,j}]_{j=1}^{d}, \tau^{-1}). \]

The selection of a latent tensor rank, $r$, has been a challenging task. Previous probabilistic models rely on a predetermined tuning parameter chosen either by cross-validations or maximum likelihood. However, the Bayesian CP factorization method [28] is able to automatically determine the tensor rank as part of the Bayesian inference process. This approach uses a set of hyper-parameters ($\lambda = [\lambda_1, \lambda_2, \ldots, \lambda_r]$) to control the rank. Each $\lambda_j$ controls the magnitude of the $j$th column of each $\mathbf{U}_j$. Further, a sparsity-inducing prior distribution is placed over all the latent factors, given by
\[ p(\mathbf{U}_j | \lambda) = \prod_{i,j=1}^{n} \mathcal{N}(u_{i,j} | \mathbf{0}, \Lambda^{-1}), \forall k \in [1,d] \]
where $\Lambda = \text{diag}(\lambda)$ is the precision matrix. Note that the larger $\lambda_j$, the smaller elements in the $j$th column of $\mathbf{U}_j$. The hyper-priors over $\lambda$ and $\tau$ are Gamma distributions, factorized over each dimensionality of the latent tensor $\mathbf{X}$, given by
\[ p(\lambda) = \prod_{j=1}^{r} \text{Ga}(\lambda_j | a_0, b_0) \]
\[ p(\tau) = \text{Ga}(\tau | a_0, b_0) \]
where $a_0, b_0$ (scalars) and $c_0, d_0$ (vectors) are selected heuristically.

Together, the overall probabilistic model can be expressed as the following joint distribution:
\[ p(\mathbf{Y}_\Omega, \mathbf{U}_1,\ldots,\mathbf{U}_d | \lambda, \tau) = p(\mathbf{Y}_\Omega | [\mathbf{U}_j]_{k=1}^{d}, \tau) \prod_{j=1}^{d} p(\mathbf{U}_j | \lambda)p(\lambda)p(\tau). \]
where the normal distribution function $\tau$ and noise precision are predicted data can be measured as $|\mathcal{Y} - \tilde{\mathcal{Y}}|_F / \|\mathcal{Y}\|_F$. As shown in Fig. 4, our approach can predict the spatial variation data with a very small sampling ratio: the relative error decreases to around 0.2% as the sampling ratio is greater than 10%; the relative errors are below 1% for all ten experiments. As shown in [15], the chip variation data typically has some certain patterns in the spatial domain. However, these patterns are not easy to capture, since they depend on very small variations across a die or a wafer. Our approach is capable of predicting the spatial patterns of the multiple-die data set simultaneously. We show the results of tensor completion by using a 15% sampling ratio and by fixing the maximum rank as 15. The top part of Fig. 5 shows the exact variation patterns of two chips obtained by measuring all testing circuits. The bottom of Fig. 5 shows the predicted variation pattern by our approach with a 15% sampling rate.

### CPU TIME FOR VIRTUAL PROBE AND OUR METHOD WITH 15% SAMPLES

| Methods                      | Slice-By-Slice | 3-D Array |
|------------------------------|----------------|-----------|
| Virtual Probe                | 62,947 s (17.5 h) | Out of Memory |
| Proposed Method              | 325 s (5.5 min) | 67 s      |

### B. Comparison With Virtual Probe

We further compare our approach with the virtual probe on this realistic data set. Our data set has $144 \times 256 \times 20$ entries. Suppose we observe 15% of the data, the Virtual Probe approach then has to solve a linear equation with 110,592 rows and 737,280 columns. Computing such a large-scale matrix and importing it into the physical memory is far beyond the capability of our desktop computer. In contrast, the Bayesian tensor completion takes only 1 min to predict such a large-scale 3-D data array with an accuracy of 0.2%, as shown in Table I. Since the Virtual Probe technique is unable to directly process the high-volume 3-D data, we perform another round of comparison by predicting the 3-D data array slice-by-slice. Specifically, we use Virtual Probe and tensor completion to predict the 20 individual slices of $144 \times 256$ matrices based on 15% given samples. The Virtual Probe approach can work in this case, and it generates one model for each individual slice. However, Virtual Probe is extremely time-consuming: it takes 17.5 h to predict all slices as shown in Table I. In contrast, our Bayesian tensor completion finishes...
the prediction in only 5.5 min and with the similar level of accuracy. This is because that Virtual Problem has to solve a large-scale under-determined equation, whereas tensor completion only needs to compute a small number of unknown low-rank factors.

Remarks: Our proposed approach employs the variational Bayesian method [28] to estimate the tensor rank probabilistically. Once the algorithm converges, we can compute the expected value of each \( \lambda_j \); a large \( \lambda_j \) indicates very small \( \Psi_k \) for all \( k = 1, \ldots, d \), thus the \( j \)th outer product in (8) will vanish, and a tensor rank deficiency is detected. We should choose a maximum rank that is greater than the true rank; otherwise, some tensor factors cannot be captured. However, if the selected maximum rank is too large, extensive data will be required to infer the latent variables, causing higher computational cost. Table II has shown the predicted ranks with respect to different maximum ranks when the sampling ratio is fixed as 15%. The predicted rank remains below 20 with the relative errors around 0.2%; the relative error decreases as the predicted rank increases to capture some small variations. However, a large maximum rank may cause over-fitting, and may overestimate the true rank.

VI. CONCLUSION

This paper has presented a tensor framework to predict the spatial variation data of semiconductor fabrications. Our key idea is to estimate the data of multiple dies simultaneously by performing tensor completion in a higher-dimensional data space. The approach has been implemented with a recently developed variational Bayesian approach which automatically determines the tensor rank in a probabilistic way. The numerical experiments on a contact plug resistivity variation data set has shown excellent performance. High accuracy (e.g., a 0.2% relative error) has been achieved with a small (e.g., 10%) sampling ratio. The proposed approach has also correctly predicted the spatial patterns of multiple dies simultaneously. Our proposed approach has easily handled a huge 3-D data set in 1 min, whereas the Virtual Probe technique failed to work due to its huge cost of physical memory and computational resources.

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