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Recent Advancements of Uncertainty Quantification with Non-Gaussian Correlated Process Variations

(Invited Special Session Paper)

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***Abstract*—Uncertainty quantification techniques have been widely used to model devices, circuits, and systems with fabrication process variations. However, most existing techniques assume that all random parameters are mutually independent or Gaussian correlated, which is rarely true in practice. How to handle non-Gaussian correlated random parameters is a fundamental and long-standing challenge. In this paper, we review existing techniques and point out their limitations. Then, we summarize our recent work to address the theoretical and computational challenges caused by non-Gaussian correlations.**

I. Introduction

Variation-aware modeling, simulation, and optimization is a challenging task in nano-scale electronic and photonic circuit design. In commercial design automation tools, Monte Carlo is widely used due to its ease of implementation. However, Monte Carlo requires a huge number of simulation samples to achieve high accuracy. In the past decade, various stochastic spectral methods, such as stochastic collocation [1], stochastic Galerkin [2], and stochastic testing [3] have been applied or developed successfully in the design automation community, demonstrating orders-of-magnitude speedup over Monte Carlo in many design cases with a small or medium number of process variation parameters. Advanced numerical algorithms have also been developed for problems with many uncertain parameters [4] and with design hierarchy [5].

However, almost all existing stochastic spectral methods can only handle independent parameters. This is a very strong assumption. For instance, the device-level geometric and electrical parameters are often correlated due to the same fabrications step, and the parameters in system-level analysis depend on each other due to the coupling and feedback phenomena. Recent results [6] have shown that uncertainty correlation cannot be ignored in integrated photonics due to its high frequency and small wavelength.

This paper first reviews stochastic spectral methods and their variants to address non-Gaussian correlations. Then, we will summarize our recent uncertainty quantification techniques that can deal with non-Gaussian correlated uncertainties with significantly higher accuracy and computational efficiency.

II. Previous work

Without loss of generality, an uncertainty quantification tool uses $\boldsymbol{\xi} = [\xi_1, \ldots, \xi_d] \in \mathbb{R}^d$ to denote d random parameters with a joint distribution $\rho(\boldsymbol{\xi})$, and $y(\boldsymbol{\xi}) \in \mathbb{R}$ to denote the quantity of interest (eg., the frequency of a chip). When $y(\boldsymbol{\xi})$ is a smooth function of $\boldsymbol{\xi}$ and has a bounded variance, one may build a surrogate model

$$y(\boldsymbol{\xi}) \approx \sum_{|\boldsymbol{\alpha}|=0}^{p} c_{\boldsymbol{\alpha}} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}), \tag{1}$$

where $\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\}$ is a set of orthogonal and normalized polynomial basis function, and $c_{\boldsymbol{\alpha}}$ is its corresponding coefficient that can be computed via numerical techniques [1]–[3]. Assume that the total polynomial order $|\boldsymbol{\alpha}| = \alpha_1 + \ldots + \alpha_d$ is upper bounded by p. Then the total number of basis function is $N_p = \binom{p+d}{d}$. The basis functions can be defined adaptively based on the joint distribution $\rho(\boldsymbol{\xi})$.

Independent Cases. When the random parameters are Gaussian distributed, Hermite polynomials [7] can be used (possibly after a de-correlation process for Gaussian correlated uncertainties). When the parameters are non-Gaussian but independent, generalized polynomial chaos (gPC) [8] can be employed. The generalized polynomial chaos uses a three-term recurrence (TTR) relation [9] to generate some orthogonal basis functions $\{\psi_{k,\alpha_k}(\xi_k)\}$ for each random parameter ξ_k with a marginal density function $\rho_k(\xi_k)$, then tensorizes them as a multivariate basis function:

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \psi_{1,\alpha_1}(\xi_1)\psi_{2,\alpha_2}(\xi_2)\ldots\psi_{d,\alpha_d}(\xi_d). \tag{2}$$

Non-Gaussian Correlated Cases. It becomes a rather challenging task when the random parameters are non-Gaussian correlated, and limited work has been reported to address this challenge. In 2004, Soize [10] proposed to construct the basis function by modifying the generalized polynomial chaos:

$$\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}) = \frac{\psi_{1,\alpha_1}(\xi_1)\ldots\psi_{d,\alpha_d}(\xi_d)}{\rho(\boldsymbol{\xi})}\rho_1(\xi_1)\ldots\rho_d(\xi_d). \tag{3}$$

The resulting basis functions are orthogonal with respect to the joint density function $\rho(\boldsymbol{\xi})$, but they are not polynomials any more. This method has been employed by Weng [11] to quantify the impact of Gaussian-mixture process variations in silicon photonic devices. Although it turns out to be faster than Monte Carlo, the speedup is not as significant as expected because the basis functions are not smooth enough. Actually, the basis functions in (3) can be numerically unstable. In 2010,

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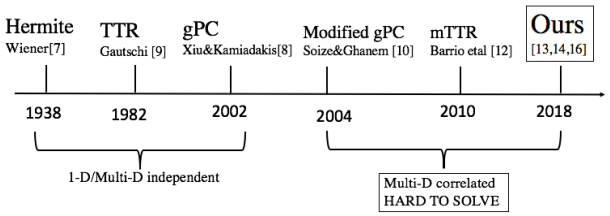

Fig. 1. Orthogonal basis functions for different kinds of uncertainties.

the three-term recurrence relation [9] was extended to multi-dimensional correlated cases (mTTR) [12], but the resulting polynomial basis functions are only weakly orthogonal.

Fig. 1 has summarized some representative techniques for handling various uncertainties. Recently, we have developed some new techniques to handle non-Gaussian correlations with significantly higher accuracy and numerical efficiency.

III. Summary of Recent Advancements

A. New Basis Functions

The first question one needs to answer is: how can we choose a "good" set of orthogonal basis functions? It is known that we can approximate a smooth function by a set of d-dimensional monomials $\mathbf{b}(\boldsymbol{\xi})$. Therefore, we can orthogonalize $\mathbf{b}(\boldsymbol{\xi})$ to get a set of orthogonal multivariate polynomial basis functions. A Cholesky decomposition approach was presented in [13]. The key is to construct a matrix $\mathbf{L}$ satisfying

$$\mathbf{LML}^T = \mathbf{I}, \tag{4}$$

where $\mathbf{M} = \mathbb{E}[\mathbf{b}(\boldsymbol{\xi})\mathbf{b}(\boldsymbol{\xi})^T]$ and $\mathbf{I}$ is the identity matrix. Here, $\mathbb{E}$ is the expectation operator. Consequently, $\mathbf{L}^{-1}\mathbf{b}(\boldsymbol{\xi})$ is the desired orthogonal basis functions. This idea was also implemented by a functional Gram-Schmidt method in [14]. The basis functions in [13], [14] have the similar nice property as the generalized polynomial chaos does: they are smooth, orthogonal, and converge fast for smooth $y(\boldsymbol{\xi})$. Furthermore, they allow one to obtain the expectation and variance of $y(\boldsymbol{\xi})$ in a closed form.

B. A New Stochastic Collocation Method

The second question is: how can we calculate the coefficients $\{c_{\boldsymbol{\alpha}}\}$. Because the basis functions are orthogonal and normalized, it is a natural idea to extend the classical stochastic collocation [1] to non-Gaussian correlated cases. The key challenge is to choose a set of quadrature samples and weights $\{\boldsymbol{\xi}_k, w_k\}$ to perform a numerical projection:

$$c_{\boldsymbol{\alpha}} = \mathbb{E}[y(\boldsymbol{\xi})\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})] \approx \sum_{k=1}^{M} y(\boldsymbol{\xi}_k)\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_k)w_k. \tag{5}$$

It is preferred to make the total number of quadrature points, M, as small as possible. While efficient techniques exist for independent cases [15], choosing numerical quadrature samples for non-Gaussian correlated cases is a hard problem.

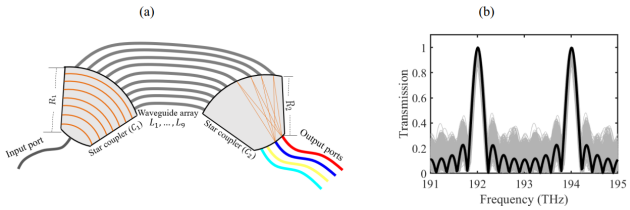

Fig. 2. (a) Schematic of AWG with 9 waveguide arrays; (b) The nominal transmission rate from input to output Port 1. The black curve shows the result without any uncertainties, and the grey lines show the effects caused by the fabrication uncertainties of radius R_1, R_2 and waveguide lengths $L_1, \ldots, L_9$.

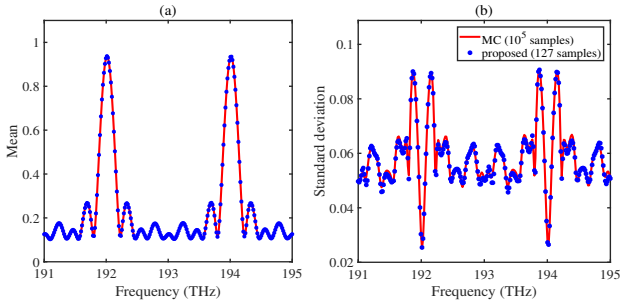

Fig. 3. Simulation results for AWG [16]. (a) mean value of the transmission rate; (b) standard deviation of the transmission rate obtained by our proposed method and Monte Carlo (MC).

Recently, an efficient optimization-based quadrature technique was proposed in [14], [16]. If $y(\boldsymbol{\xi})\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})$ can be approximated by basis functions bounded by order $2p$, we instead seek for $\{\boldsymbol{\xi}_k\}_{k=1}^M$ and $\{w_k\}_{k=1}^M$ by minimizing the integration error of all basis functions up to oder $2p$:

$$\min_{\boldsymbol{\xi}_k, w_k} \sum_{|\boldsymbol{\alpha}|=0}^{2p} \left(\sum_{k=1}^{M} \Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi}_k)w_k - \mathbb{E}[\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})] \right)^2. \tag{6}$$

With a good initial guess and an iterative clustering technique in [16], high-quality quadrature samples and wights can be computed, and M can be automatically determined.

The above technique has been tested by some synthetic and practical benchmarks in [16], demonstrating $700\times$ to $6000\times$ speedup than Monte Carlo. The speedup factor is much higher than that in [11]. For the arrayed waveguide grating (AWG) [17] shown in Fig. 2, the predicted uncertain transmission rates via a 2nd-order stochastic model is almost the same with that from Monte Carlo using 10^5 simulation samples, as shown in Fig. 3.

C. Theoretical Results

Error Bound. It is shown in [16] that the approximation error in (1) is upper bounded as

$$\|y(\boldsymbol{\xi}) - \tilde{y}(\boldsymbol{\xi})\|_2 \leq C_1\delta + C_2\epsilon, \tag{7}$$

under some weak assumptions. Here δ is the distance from $y(\boldsymbol{\xi})$ to the p-th order polynomial subspace, ϵ is ℓ_1 norm of the objective function in (6) at the computed quadrature samples and weights, $C_1, C_2 \geq 0$ are some constants. This theoretical

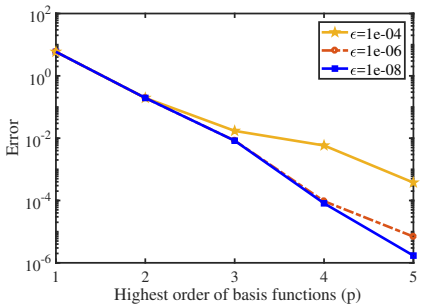

Fig. 4. Convergence rate for the synthetic example [16]. Here ϵ is the numerical error of optimization defined in (6). This figure demonstrates the error estimated in (1): the stochastic collocation algorithm shows a nearly exponential convergence rate as p increases and before ϵ dominates the error.

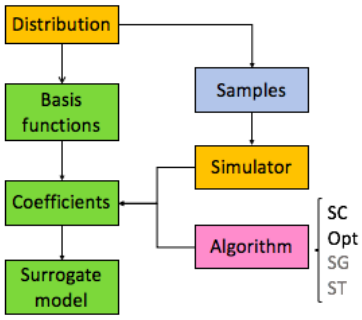

Fig. 5. Flow chart for building surrogate models with non-Gaussian correlated uncertainties. The parameter distribution and simulator are specified by users.

result implies that a nearly exponential convergence rate can be obtained if $y(\boldsymbol{\xi})$ is smooth enough and when ϵ does not dominate the error. This has been observed on a synthetic example in [16], as shown in Fig. 4.

Number of Quadrature Samples. The lower and upper bounds for the number of quadrature points was also estimated in [16]. Assume that M pairs of quadrature samples and weights are obtained from (6) to ensure an $2p$-th-order integration accuracy, then there exists at least one $M \in [N_p, N_{2p}]$.

D. Adaptive Compressive Sensing for High-dimensional Case

Our techniques in [14], [16] work very well for low-dimensional problems, but they become less efficient as the number of random parameters increases. In order to address the scalability issue, a high-dimensional solver was further proposed in [13], [18] by employing the following techniques:

- A tensor-train technique to build high-dimensional basis functions for Gaussian-mixture uncertainties;
- An ℓ_0 minimization solver to compute the sparsest coefficients in the surrogate model;
- An adaptive sampling technique based on a rank-revealing QR initialization, and D-optimal, R-optimal, and E-optimal criterion to reduce the number of simulation samples.

E. A Toolbox for Non-Gaussian Correlated Parameters

Recently we released a Matlab toolbox for stochastic collocation with non-Gaussian correlated uncertainties. The code is posted online [1]. The main blocks are illustrated in Fig. 5. Given the joint distribution $\rho(\boldsymbol{\xi})$, the basis functions $\{\Psi_{\boldsymbol{\alpha}}(\boldsymbol{\xi})\}$ are first built based on Section III-A. Then the coefficients are computed via the stochastic collocation (SC) approach in Section III-B or the optimization (Opt) approach in Section III-D.

Other techniques such as stochastic Galerkin (SG) and stochastic testing (ST) can also be developed for non-Gaussian correlated cases. The toolbox will be updated in the future.

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