

Adaptive Polynomial-Chaos Algorithm with Dual-Criterion Sampling for Uncertainty-Quantification Problems

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This work addresses the development of reliable surrogates for electromagnetic problems with uncertainties, by introducing a new sampling approach for the computation of Polynomial-Chaos (PC) expansions via least squares. The proposed scheme adopts a sequential framework, enabling the development of an adaptive algorithm that promotes denser sample concentrations at areas with significant variance density of the quantity of interest. At the same time, a subset of samples is selected via a distance-based criterion, to ensure that the overall sample set preserves adequate space-filling properties. In this way, experimental designs balancing two different selection criteria are constructed, and their impact on the efficiency of PC computations is demonstrated herein via a number of tests.

Index Terms—Polynomials, sampling methods, stochastic systems, uncertainty.

I. INTRODUCTION

METHODOLOGIES BASED on the generalized Polynomial Chaos (PC) [1] have become indispensable tools for the analysis of electromagnetic problems with uncertainties [2,3]. Through the development of PC models for the Quantities of Interest (QoIs), uncertainty quantification and sensitivity studies are greatly facilitated. The standard non-intrusive computation of the PC expansion coefficients is typically achieved via the least-squares solution of an overdetermined system, which necessitates the sampling of the input-parameter space [4]. Naturally, the choice of these samples critically impacts the reliability of the PC formulae.

Aiming at improving the credibility of PC models, we develop an adaptive algorithm that incorporates a novel sampling approach. The construction of the surrogate starts with a typical low-order approximation and, as the order of the approximation increases, new basis functions and samples from the random space are progressively added. The latter are selected by constructively applying two different criteria: the first one prioritizes the sampling of regions with high variance density, similarly to other recent works [5], while the second one targets parts of the sample space that remain, till then, sparsely sampled. This balanced approach effectively addresses two distinct and equally important objectives, leading to PC computations with improved accuracy, as the results of this paper demonstrate.

II. POLYNOMIAL-CHAOS EXPANSIONS

For a scalar QoI y that depends on d independent random variables represented by the vector $\xi = [\xi_1 \dots \xi_d]^T$, the corresponding PC expansion has the form

$$y(\xi) = \sum_{\alpha \in \mathbb{N}_0^d} c_\alpha \Psi_\alpha(\xi), \quad (1)$$

where c_α are the expansion coefficients, $\Psi_\alpha(\xi)$ are the basis functions, and the multi-index $\alpha = (\alpha_1, \dots, \alpha_d)$ dictates the polynomial order with respect to each ξ_i . Specifically, each multivariate basis function is constructed as a product of univariate polynomials via $\Psi_\alpha(\xi) = \psi_{\alpha_1}(\xi_1) \times \dots \times \psi_{\alpha_d}(\xi_d)$. The

type of univariate polynomials depends on the corresponding input parameters (e.g. variables with uniform distributions necessitate Legendre polynomials). Typically, the truncation of the PC expansion (1) is necessary, by replacing $\mathbb{N}_0^d$ with a basis-index set $\mathcal{A} \subset \mathbb{N}_0^d$, leading to the approximation $\hat{y}(\xi)$ of the QoI. Here, the total-degree truncation scheme is applied: $\mathcal{A} = \{\alpha \in \mathbb{N}_0^d : \alpha_1 + \dots + \alpha_d \leq p_{\max}\}$, where $p_{\max}$ is the expansion's polynomial order, with the cardinality of $\mathcal{A}$ computed as $N = (d + p_{\max})! / (d! p_{\max}!)$.

For the calculation of the expansion coefficient c_α , a number of input samples are selected according to a specific technique, such as Latin-hypercube Sampling (LHS), and a corresponding number of equations with the following form are derived:

$$\sum_{\alpha \in \mathcal{A}} c_\alpha \Psi_\alpha(\xi^{(i)}) = y(\xi^{(i)}), \quad i = 1, \dots, C_s N. \quad (2)$$

C_s typically ranges from 2 to 5. Thus, the system of equations (2) is overdetermined and can be dealt with via least-squares. Once the PC model is available, metrics such as the mean and the variance of the QoI can be easily computed [1].

III. DUAL-CRITERION SAMPLING

The building of the PC surrogate starts with a low-order initial model (e.g. of 1st or 2nd degree), using samples selected via standard LHS. To extend the approximation to the immediately higher degree, the necessary additional samples are incrementally selected from a larger pool (formed beforehand also via LHS) and added to the active pool of samples. The new samples are selected one-by-one, alternating between two different criteria. According to the first one, we identify the sample from the larger pool where the highest variance density of the QoI is observed (as predicted by the current PC model). To apply the second criterion for the next sample, the minimum distance $d_{\min}$ between each sample from the larger pool and the samples of the active pool is evaluated, and the most suitable one is selected according to the maximum $d_{\min}$. Once a new sample is added to the active set, it is removed from the larger candidate pool and the PC model is updated accordingly. To prevent oversampling in specific regions of the random space, a rule regarding the minimum allowable distance

of a candidate sample from existing ones is also applied. Finally, a new basis function is added to the PC expansion every time C_s new samples are introduced to the active set. The procedure is terminated when the desired maximum polynomial order is achieved, or a predefined error criterion is satisfied.

Figure 1 illustrates the distribution of samples when the proposed approach is applied to the case of the simple test function $y(\xi_1, \xi_2) = \sin(\pi\xi_1)\sin(\pi\xi_2)$. Specifically, the left figure displays the function's variance density and the plot on the right presents the final sample distribution for a 10th-order approximation and $C_s = 3$ (the red samples are selected via the variance density criterion, the blue samples are chosen by maximizing the minimum distance from existing ones, the black samples correspond to the initial LHS set, and the gray circles denote unused samples from the larger pool). It becomes clear that integrating the combined criteria preserves space-filling properties and, at the same time, enhances the sampling concentration in the regions with significant variance density.

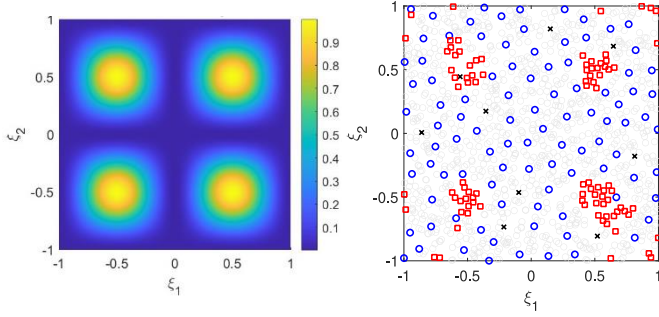


Fig. 1. Variance density of the test function (left) and distribution of samples via the new approach (right).

IV. EXPERIMENTAL VALIDATION

The performance of the proposed sampling strategy is first tested in the case of a nonlinear function, namely the Ishigami function,

$$y(\xi_1, \xi_2, \xi_3) = \sin \xi_1 + 7 \sin^2 \xi_2 + 0.1 \xi_3^4 \sin \xi_1 \quad (3)$$

with uniformly distributed variables ($\xi_i \in [-\pi, \pi]$, $i = 1, 2, 3$). The new technique is compared against the LHS, and the accuracy is assessed via the RMS cross-validation error:

$$e_{\text{RMC-CV}} = \sqrt{\frac{1}{M} \sum_{i=1}^M [y(\xi^{(i)}) - \tilde{y}(\xi^{(i)})]^2}, \quad (4)$$

with $M = 500$. The error lines for approximation orders up to 10 are plotted in Fig. 2, where the PC formulae computed with the new scheme displays higher efficiency, when compared to the expansions based on LHS. Specifically, except for the initial model with $p = 1$, the accomplished error reduction ranges from 15.3% to 52.4%, highlighting the potential of the proposed sampling algorithm.

For a second test case, we consider a partially filled rectangular waveguide with dimensions $w \times h \times (2d + l)$ [6]. A dielectric slab with dimensions $w \times h \times l$ is located in the middle of the configuration and its electromagnetic properties are characterized by the relative constants ϵ_r, μ_r . The nominal values of the uniformly-distributed problem geometric and electromagnetic parameters are $[w \ h \ l \ d \ \epsilon_r \ \mu_r]^T = [30 \text{ mm} \ 3 \text{ mm}$

$7 \text{ mm} \ 5 \text{ mm} \ 2 \text{ mm} \ 2.4]^T$, and a variation of $\pm 10\%$ around the mean values is considered. The QoI is the magnitude of the reflection coefficient of the TE₁₀ mode at 6 GHz, for which an analytical formula is derived in [6]. The absolute value of the % error in the variance of the reflection coefficient is depicted in Fig. 3, when polynomial models up to 5th order are computed. The reference value is obtained via a standard Monte-Carlo computation with 10^9 model evaluations. The results verify a clear advantage of the proposed sampling over LHS, as the relative variance error (averaged after 20 repetitions) is reduced by a factor ranging from 10% to 45.1%.

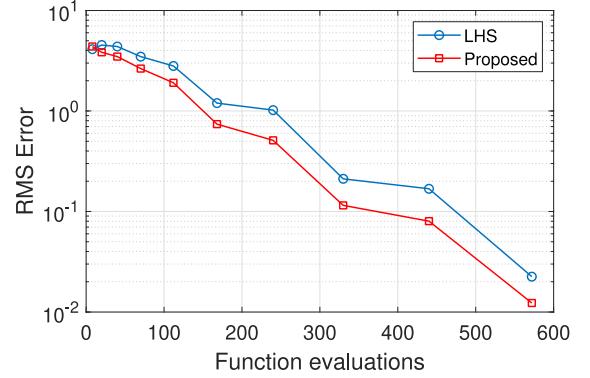


Fig. 2. RMS cross-validation error versus the number of function evaluations, in the case of the Ishigami function.

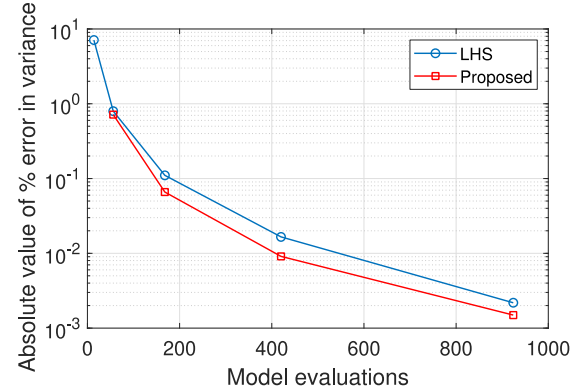


Fig. 3. Absolute value of the % error in the variance in the reflection coefficient at 6 GHz versus the number of model evaluations, in the case of the partially-filled waveguide problem.

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