Data-Driven Multi-Element Arbitrary Polynomial Chaos for Uncertainty Quantification in Sensors

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A multi-element arbitrary polynomial chaos (ME-aPC) scheme is introduced for uncertainty quantification (UQ) in sensors. Similarly to the classical arbitrary polynomial chaos (aPC), the ME-aPC scheme is most usable in data-driven applications, in which the input uncertainty is represented numerically by raw data samples. In sensors, the input samples are usually obtained by real-time measurements. With the several examples considered in this paper, the proposed scheme is shown to have better numerical stability than the classical aPC, without compromising the accuracy of the solutions.

***Index Terms*—Uncertainty Quantification, Polynomial Chaos, Data-Driven, Multi-Element, Stochastic.**

I. Introduction

Studies of uncertainty quantification (UQ) play a key role in designing sensors that operate effectively in harsh and hostile environments. A common approach to performing such studies is to consider a stochastic model, in which inputs and outputs of a sensor are assumed as random variables. In this approach, the goal is to estimate the output probability density function (PDF) based on the input variability. For a moderate number of input variables, the generalized polynomial chaos (gPC) [1] is considered a fast and accurate method to perform this task. However, a key challenge in the classical gPC method is that input distributions are required to be fully known. In sensors, this might not be feasible as variation in inputs is usually represented in terms of limited data sets obtained from real-time measurements, and fitting the data with parametric distributions may introduce undesirable errors. In [2], Oladyshkin and Nowak addressed the aforementioned challenge by constructing a polynomial chaos (PC) scheme, based on the statistical moments rather than the probability distributions. This scheme can be referred to as arbitrary polynomial chaos (aPC). Yet, the aPC scheme may become unstable when high-degree polynomials are required to achieve accurate solutions [3]. The objective of the present paper is to show that by combining the aPC method with the multi-element (ME) technique [4], it is possible to reduce the degree of polynomials without compromising the accuracy of the outcomes. In particular, we apply and validate the proposed approach with model problems addressing several types of sensors.

II. Mathematical Framework for Data-Driven Applications

A. Non-intrusive polynomial chaos

We consider a probabilistic approach for uncertainty quantification, in which an uncertain input parameter x is related to an output metric y by a stochastic model $y = g(x)$. Both x and y are random variables with unknown probability density functions. x is represented in terms of M sample points (i.e, $x = \{x_1, x_2, \dots, x_M\}$) with a probability space $[a, b] \simeq [\min(x_i), \max(x_i)]_{1\le i\le M}$. y is a variable that we intend to approximate. In polynomial chaos approach, this is achieved by expressing the stochastic model $g(x)$ in terms of orthonormal polynomials $\Phi_i(x)$ through the expansion

$$y = g(x) = \sum_{i=0}^{N} c_i \Phi_i(x) \tag{1}$$

where N refers to the order of the expansion. Coefficients c_i are determined via $N + 1$ collocation points

$$\begin{bmatrix} \Phi_0(x_0) & \Phi_1(x_0) & \cdots & \Phi_N(x_0) \\ \Phi_0(x_1) & \Phi_1(x_1) & \cdots & \Phi_N(x_1) \\ \vdots & \vdots & \ddots & \vdots \\ \Phi_0(x_N) & \Phi_1(x_N) & \cdots & \Phi_N(x_N) \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_N \end{bmatrix} = \begin{bmatrix} y(x_0) \\ y(x_1) \\ \vdots \\ y(x_N) \end{bmatrix} \tag{2}$$

The expected value and the variance of y are given as

$$\mu_y = c_0, \quad \sigma_y^2 = \sum_{i=1}^{N} c_i^2 \tag{3}$$

B. Orthonormal Polynomials for an Arbitrary Distribution

The next step is to find the orthonormal polynomial basis $\{\Phi_1, ..., \Phi_N\}$. First we introduce orthogonal polynomials $P_k(x)$ which satisfy

$$P_k(x) = \sum_{i=0}^{k} p_{k,i} x^i, \quad k = 1, ..., N \tag{4}$$

where the subscript k refers to the order of the polynomial and $p_{k,i}$ are the polynomial coefficients. Note that the polynomials $P_k(x)$ may not be orthonormal. According to [2], the coefficients $p_{k,i}$ can be determined via the matrix

$$\begin{bmatrix} \mu_0 & \mu_1 & \cdots & \mu_k \\ \mu_1 & \mu_2 & \cdots & \mu_{k+1} \\ \vdots & \vdots & \ddots & \vdots \\ \mu_{k-1} & \mu_k & \cdots & \mu_{2k-1} \\ 0 & 0 & \cdots & 1 \end{bmatrix} \begin{bmatrix} p_{k,0} \\ p_{k,1} \\ \vdots \\ p_{k,k} \end{bmatrix} = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 0 \\ 1 \end{bmatrix} \tag{5}$$

where μ_i refers to the ith statistical moment. It satisfies the relation

$$\mu_i = \frac{1}{M}\sum_{j=1}^{M} x_j^i \tag{6}$$

Again, M refers to the size of the sample set, while x_j's are the sample points. Once the polynomials in (4) are determined, the orthonormal basis $\Phi_k(x)$ can then be obtained by the expression

$$\Phi_k(x) = \frac{P_k(x)}{||P_k||} \tag{7}$$

with

$$||P_k||^2 = \sum_{|\mathrm{s}|=2} \binom{2}{\mathrm{s}} \mathrm{p}_k^{\mathrm{s}} \mu_{r_k} \tag{8}$$

where

$$\mathrm{s} = \{s_0, s_1, \ldots, s_k\}, \quad \mathrm{p}_k^{\mathrm{s}} = \prod_{t=0}^{k} p_{t,k}^{s_t}, \quad \mu_{r_k} = \prod_{t=0}^{k} t s_t$$

The multi-index s refers to all combinations of s_i such that $s_0 + s_1 + \ldots + s_k = 2$. Equation (8) requires the availability of the first $2k+1$ moments.

C. Multi-Element Decomposition

Some model problems involve the evaluation of high-degree polynomials in order to achieve the required accuracies. This can be challenging as the matrix in (5) might become ill-conditioned in such cases [3]. Alternatively, the multi-element approach [4] can be used to reach the attempted accuracies still by using relatively low-degree polynomials. In this approach, the random space is decomposed into d non-overlapping intervals. Then the non-intrusive polynomial chaos (see Section II-A) is applied locally on each element. Consequently, the global mean μ_y and variance σ_y^2 are computed as

$$\mu_y = \sum_{l=1}^{d} \mu_{y,l} h_l, \quad \sigma_y^2 = \sum_{l=1}^{d} [\sigma_{y,l}^2 + (\mu_{y,l} - \mu_y)^2] h_l \tag{9}$$

where $\mu_{y,l}$ and $\sigma_{y,l}$ are the local mean and variance on element l, respectively. $h_l = M_l/M$, with M_l being the number of samples in element l.

D. Error Estimation

The output measures defined in (3) and (9) vary with different realizations of the same sample size. Let Z_{Approx} refer to an output measure obtained from distribution sampling. For error evaluation, we take n realizations of $Z_{\text{Approx}}(n)$, and compute its mean $\mu_{Z_{\text{Approx}}}$ and standard deviation $\sigma_{Z_{\text{Approx}}}$. Typically, $Z_{\text{Approx}}(n)$ is considered to follow a normal distribution. Based on that and on the 3-sigma rule, the maximum relative error can be approximated as

$$\varepsilon \simeq \frac{\max\{||(\mu_{Z_{\text{Approx}}} \pm 3\sigma_{Z_{\text{Approx}}}) - \mathrm{Z}_{\text{Exact}}||\}}{||\mathrm{Z}_{\text{Exact}}||} \tag{10}$$

with $\mathrm{Z}_{\text{Exact}}$ computed by the exact distribution.

III. Numerical Examples

A. Capacitive Moisture Sensor

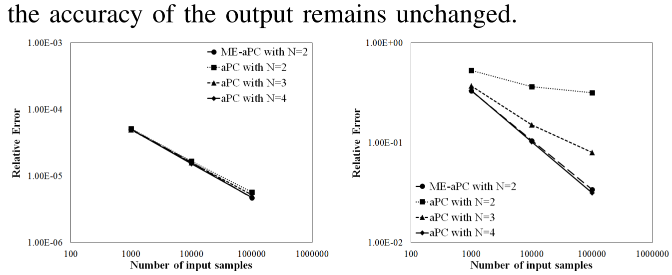
A basic capacitive moisture sensor consists of dielectric substrate with thickness d and permittivity ϵ, inserted between two conducting plates each of area A. The capacitance of the sensor is given by relation $C = \epsilon A/d$, where ϵ satisfies

$$\epsilon = \left(1 + \frac{1.5826}{10^6 T}\left(P_{ma} + \frac{0.36 P_{ws}}{T}\right) RH\right)\epsilon_0 \tag{11}$$

with ϵ_0 being the permittivity of free-space, T is the absolute temperature, and RH is the relative humidity. P_{ma} and P_{ws} refer to the pressure of moist air and saturated water vapor, respectively. They are given by the expressions

$$P_{ma} = 133.322 e^{20.386 - 5132/T}$$
$$P_{ws} = 133.322 \times 10^{0.66077 + 7.5(T - 237.15)/T}$$

The goal here is to estimate the sensor capacitance C given that the operating temperature T is under uncertainty. T is considered to follow normal distribution with expected value $\mu_T = 300$ K and standard deviation $\sigma_T = 0.2\mu_T$ K. The other inputs are given as: $d = 1$ mm, $A = 100$ mm^2, and $RH = 0.4$. Figure 1 shows the maximum relative error of the expected value and the standard deviation of the sensor capacitance vs. number of T samples, obtained with aPC and ME-aPC schemes. In ME-aPC the input domain is decomposed into 8 elements. For the expected values, it is clear that the results obtained with aPC and ME-aPC are in good agreement, even when the order of the polynomial chaos expansion is the same for both schemes (i.e. $N = 2$). However, for the standard deviation, the results show that the same rate of convergence obtained by aPC at $N = 4$ is attained by ME-aPC with $N = 2$. In other words, by using the ME-aPC approach the degree of the polynomials is reduced by 2, while the accuracy of the output remains unchanged.



(a) Expected value (b) Standard deviation

Fig. 1: Convergence rate of expected value and standard deviation of C vs. number of T samples, with $\mu_T = 300$ K and $\sigma_T = 0.2\mu_T$ K.

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