Data-Driven Polynomial Chaos Basis Estimation

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ABSTRACT: A non-intrusive uncertainty quantification scheme based on Polynomial Chaos (PC) basis constructed from available data is introduced. The method uses properly parametrized basis functions in order to let them adapt to the given input-output data instead of predefining them based on the probability density function of the uncertain input variable. Model parameter estimation is effectively dealt with through a Separable Non-linear Least Squares (SNLS) procedure that allows the simultaneous estimation of both the PC basis and the corresponding coefficients of projection. Method's effectiveness is demonstrated through its application to the uncertainty propagation modelling in two examples: a nonlinear differential equation with uncertain initial conditions and a nonlinear single degree-of-freedom system with an uncertain parameter. Comparisons with classical PC expansion modelling based on the Wiener-Askey scheme are used to illustrate the method's performance and potential advantages.

Polynomial Chaos (PC) expansion has been demonstrated to effectively model uncertainty propagation in a number of engineering problems. The main advantage of the PC representation is its low computational cost, compared to that of traditional approaches such as the classical Monte-Carlo, and its ease of use for model-based analysis, e.g. for the purposes of statistical characterization of the output, reliability and global sensitivity analysis.

Nevertheless, PC expansion for uncertainty quantification in real applications remains challenging mainly due to problems arising from the statistical characterization of the input variables, as well as the process of determining a sparse PC basis, in the sense of including only a small number of basis functions which may still provide high approximation accuracy. With regard to the first problem, although Xiu and Karniadakis (2002) have extended the initially proposed PC of Gaussian processes on Hermite polynomials proposed by Wiener, to a number of common continuous and discrete Probability Density Functions (PDFs) through the Wiener-Askey scheme, estimating the statistical distribution of input variables may be a nontrivial task since bounded, multi-modal, or discontinuous PDFs may be found to best fit given measured data (Oladyshkin and Nowak (2012)). In such cases, fitting the given data to a common PDF may significantly reduce the accuracy of the expansion, while on the other hand transformations to standard PDFs normally lead to slower convergence rates.

The crucial problem of selecting specific PC subspaces is also an open problem that has been treated in a number of recent studies (for example see Blatman and Sudret (2011)), with a common approach being the forward selection procedure which builds up the PC model by adding bases till no further improvement is achieved, according to a predetermined criterion. In most cases however, such approaches require the estimation of a large number of candidate models.

Moreover, potential limitations of the Wiener-Askey expansion scheme arise in situations where discontinuities or complex relationships characterize the dependency of the output variable on the random input data (Le Maître et al. (2004)).

The aim of the present study is to circumvent the aforementioned difficulties associated with PC basis construction. Toward this end, the PC is not based on basis functions of a fixed form, but instead we use orthogonal B-splines functions with a-priori unknown properties that may be adapted to the specific random input variable characteristics. This is accomplished through appropriate basis function parametrization which allows for direct estimation of the splines knots, and a Separable Nonlinear Least Squares (SNLS) type procedure (Golub and Pereyra (2003)) that achieves simultaneous estimation of the basis functions and the coefficients of projection through a reduced dimensionality, constrained non-quadratic optimization problem. The method's effectiveness is examined via a Monte Carlo study and comparisons with the classical PC method based on the Wiener-Askey scheme are made.

1. POLYNOMIAL CHAOS EXPANSION

PCE based on the Wiener-Askey scheme concerns the expansion of a random output variable on polynomial chaos basis functions which are orthonormal to the probability space of the system's random inputs. More specifically, let us consider a system $\mathscr{S}$ which has M random input parameters represented by independent random variables $\{\Xi_1,\ldots,\Xi_M\}$, gathered in a random vector Ξ of prescribed joint PDF $p_\Xi(\xi)$ (Blatman and Sudret (2011)).

The system output, denoted by $Y = \mathscr{S}(\Xi)$ will also be random. Provided that Y has finite variance, it can be expressed as follows:

$$Y = \mathscr{S}(\Xi) = \sum_{j\in\mathbb{N}} c_j \phi_{d(j)}(\Xi) \tag{1}$$

where c_j are unknown deterministic coefficients of projection, d is the multivariate index of the PC basis, and $\phi_{d(j)}(\Xi)$ are the PC functions orthonormal to $p_\Xi(\xi)$. These basis functions $\phi_{d(j)}(\Xi)$ may be constructed through tensor products of the corresponding univariate functions associated through the corresponding probability distributions (Xiu and Karniadakis (2002)).

As already mentioned, the main drawback of the classic PC expansion, especially for real-data applications, is the statistical characterization of the input variables and the selection problem related with the choice of an appropriate functional subspace. Even if this is only a small price to pay for rendering the estimation of an uncertainty propagation model into a deterministic estimation problem, this selection is of crucial importance for accurate modelling. Indeed, despite the fact that theoretically any "extended" (of high dimensionality) PC subspace may achieve good tracking of the parameter evolution, this is not true when we have to select only a small number of functions due to reasons of statistical efficiency and model parsimony (economy of representation).

On the contrary, the use of PC basis adapted on the selected input variables data is proposed in this study. Toward this end, the basis functions are determined by an a-priori unknown vector of parameters δ which has also to be estimated along with the coefficients of projection θ. In this way, the basis may be automatically adapted on the data in order to achieve higher accuracy in the case the uncertainty propagation is highly nonlinear, leading to an output which does not follow the distribution of the input. In the sequel, a data-driven PC basis estimation framework based on B-spline functions is described. Based on the attractive properties of the B-splines functions, both smooth or abrupt uncertainty propagation relationships may be efficiently expanded on the constructed basis.

1.1. Adaptable B-spline functions

The values of the input variable Ξ are considered to be samples drawn from a PDF which may be approximated by a continuous piecewise polynomial function of order k (de Boor, 2001, Chs. 7-8). Then, according to the theorem of Curry and Schoenberg (de Boor, 2001, pp. 97-98), a basis of splines (B-splines) may be constructed for the corresponding piecewise polynomial space. By considering, for the purposes of simplicity, a bounded PDF and the univariate case, the B-splines are fully defined by an appropriate nondecreasing sequence of points (*knots*) $\tau = [\tau_1,\ldots,\tau_{p+k}] \in [\alpha,\beta] \subset \Re$ (where p is the basis dimensionality). The aforementioned theorem leaves open the selection of the first k and last k knots. However, imposing no continuity conditions at the endpoints, $\tau_1 = \ldots = \tau_k = \alpha$ and $\tau_{p+1} = \ldots = \tau_{p+k} = \beta$ may be selected. This choice is also consistent with the fact that the constructed basis provides a valid representation only for the interval $[\tau_k, \tau_{p+1}]$, that is $[\alpha, \beta]$.

Thus, in terms of the above quantities the B-splines of order k may be described by the functional subspace parameter vector $\delta \triangleq [\tau_{k+1}, \ldots, \tau_p]^T$ of dimension $\dim(\delta) = p - k$ consisting of the non-decreasing sequence of the free internal knots. The variable $Y = \mathscr{S}(\Xi)$ is then expressed as:

$$Y = \sum_{j=1}^{p} c_j \cdot \phi_j^k(\Xi, \delta) \tag{2}$$

where $\phi_j^k(\Xi, \delta)$ denotes the sequence of B-splines of order k. There are several ways to define the B-spline functions $\phi_j^k(\xi, \delta)$ for a given realization ξ. A convenient one is by the means of the Cox-de Boor recursion formula for the normalized B-splines (de Boor, 2001, p. 90):

$$\phi_j^1(\xi, \delta) = \begin{cases} 1 & \text{if } \tau_j \leq \xi < \tau_{j+1} \\ 0 & \text{otherwise} \end{cases} \tag{3a}$$

$$\begin{aligned} \phi_j^i(\xi, \delta) = w_{j,i}(\xi) \cdot \phi_j^{i-1}(\xi, \delta) + \\ + (1 - w_{j,i}(\xi)) \cdot \phi_{j+1}^{i-1}(\xi, \delta), \text{ for } 1 < i \leq k \end{aligned} \tag{3b}$$

where

$$w_{j,i}(\xi) = \begin{cases} \frac{\xi - \tau_j}{\tau_{j+i-1} - \tau_j} & \text{if } \tau_j < \tau_{j+i-1}, \\ 0 & \text{otherwise.} \end{cases} \tag{3c}$$

B-splines are characterized by a number of properties which make them particularly attractive for data-driven PC expansion applications. A significant property of B-splines is their local support, that is $\phi_j^k[\xi, \delta] \neq 0$ only for $\xi \in [\tau_j, \tau_{j+k})$. Due to this local support, the resulting basis may consist of splines with various characteristics and therefore may be capable of tracking parameters with mixed type of evolution, that is alternating patterns of smooth and abrupt changes of the PDF. Moreover, B-splines are locally linearly independent, that is they provide a basis for the piecewise polynomial space even for an interval $[\alpha, \beta] \subseteq [\tau_1, \tau_{p+k}]$. Finally, by selecting the proper B-splines order k, various degrees of smoothness may be achieved. For example, for $k = 1$ the basis consists of piecewise constant functions, for $k = 2$ linear B-splines, for $k = 3$ quadratic, for $k = 4$ cubic, and so on. Yet, smoothness may also be controlled by the proximity of knots (de Boor, 2001, Ch. 9). A thorough analysis of B-splines and their properties may be found in de Boor (2001).

Constraints on δ. The internal knots $\tau_{k+1}, \ldots, \tau_p$ form a nondecreasing sequence of real numbers defined in the open set (α, β). Thus, they have to satisfy proper constraints related with their bounds and their order relation.

Simple constraints may be defined for the case of internal knots with multiplicity one. This is not restrictive in view of the fact that a B-spline with an internal knot of multiplicity $m > 1$ may be approximated by replacing this knot by m simple knots nearby (de Boor, 2001, p. 106).

Thus, an appropriate order relation constraint, suitable for numerical purposes (as it prevents the knots from coalescing when their distance becomes practically equal to zero) is:

$$\tau_j - \tau_{j-1} > \varepsilon, \quad j = k+1, \ldots, p+1, \tag{4}$$

where $0 < \varepsilon \ll (\beta - \alpha)$ is a selected, sufficiently small separation parameter.

Therefore, the following $p-k+1$ inequality constraints are imposed on the parameter vector δ:

$$\left.\begin{aligned} \tau_{k+1} - \tau_k = \tau_{k+1} - \alpha &\geq \varepsilon \\ \tau_{k+2} - \tau_{k+1} &\geq \varepsilon \\ &\vdots \\ \tau_p - \tau_{p-1} &\geq \varepsilon \\ \tau_{p+1} - \tau_p = \beta - \tau_p &\geq \varepsilon \end{aligned}\right\} \Longrightarrow$$

$$\begin{bmatrix} -1 & 0 & \ldots & 0 & 0 \\ 1 & -1 & \ldots & 0 & 0 \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & \ldots & 1 & -1 \\ 0 & 0 & \ldots & 0 & 1 \end{bmatrix} \cdot \underbrace{\begin{bmatrix} \tau_{k+1} \\ \tau_{k+2} \\ \vdots \\ \tau_{p-1} \\ \tau_p \end{bmatrix}}_{\delta} - \begin{bmatrix} -\alpha - \varepsilon \\ -\varepsilon \\ \vdots \\ -\varepsilon \\ \beta - \varepsilon \end{bmatrix} \leq 0 \tag{5}$$

which are also depicted schematically in Fig. 1.

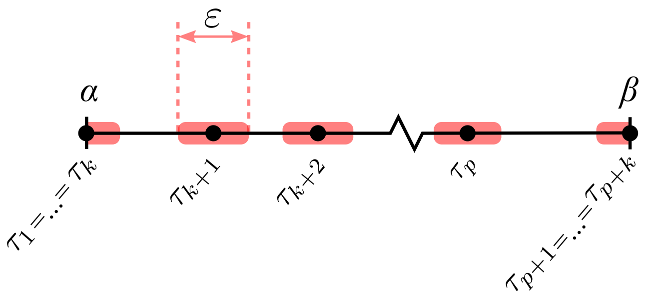

Figure 1: Constraints imposed on δ. The distance between two internal knots has to be larger than ε. The first and last internal knots have also to be ε away from the endpoints α and β, respectively.

1.2. PCE model parameter estimation

The proposed data-driven PCE model estimation problem involves the estimation of the parameter vector δ consisting of the B-splines internal knots and the coefficients of projection vector c from the available N-samples long set of data $\xi = [\xi_1, \ldots, \xi_N]^T$ and $y = [y_1, \ldots, y_N]^T$. Using the B-spline functions of Eq. (3) (for given k and p), the PCE model may be re-written in the following nonlinear regression form:

$$\begin{aligned} y_n &= \sum_{j=1}^{p} c_j \cdot \phi_j^k(\xi_n, \delta) + e_n(\delta, c) \Rightarrow \\ \Rightarrow y_n &= \underbrace{\begin{bmatrix} \phi_1^k(\xi_n, \delta) \\ \phi_2^k(\xi_n, \delta) \\ \vdots \\ \phi_p^k(\xi_n, \delta) \end{bmatrix}^T}_{\phi(\xi_n, \delta)_{(p\times 1)}} \cdot \underbrace{\begin{bmatrix} c_1 \\ c_2 \\ \vdots \\ c_p \end{bmatrix}}_{c_{(p\times 1)}} + e_n(\delta, c) \end{aligned} \tag{6}$$

or equivalently by using the stacked signal and innovations sequence vectors $y = \left[y_1, \ldots y_N\right]^T$ and $e(\delta, c) = \left[e_1(\delta, c), \ldots, e_N(\delta, c)\right]^T$:

$$y = \Phi(\xi, \delta) \cdot c + e(\delta, c) \tag{7}$$

where $\Phi(\xi, \delta) = \left[\phi_1^k(\xi_1, \delta), \ldots, \phi_p^k(\xi_N, \delta)\right]^T$.

The estimation of the model parameter vectors δ and c may be based on the minimization of the Prediction Error (PE) criterion $V(\delta, c) = \|e(\delta, c)\|^2$ consisting of the sum of squares of the model's errors, subject to the constraints discussed in the previous section which guarantee the linear independence of the basis functions, that is:

$$\begin{aligned} &[\hat{\delta}^T, \hat{c}^T]^T = \arg\min_{\delta, c} V(\delta, c) = \arg\min_{\delta, c} \|e(\delta, c)\|^2 \\ &\text{subject to} \quad H(\delta) \leq 0 \end{aligned} \tag{8}$$

In this relation, arg min stand for "argument minimizing", $\|\cdot\|$ indicates Euclidean norm, and $e(\delta, c)$ the model error being provided by the model expression of Eq. (6). A hat designates estimator/estimate of the indicated quantity.

The nonlinear dependence of the basis functions $\phi_j^k(\xi, \delta)$ on the parameter vector δ renders the PE-based estimation problem a nonlinear optimization problem with linear inequality constraints. This problem may be solved through common iterative constrained nonlinear optimization methods with respect to the $\dim(c) + \dim(\delta) = p + p - k$ parameters and by utilizing the gradient of the objective function $V(\delta, c)$.

However, by taking into consideration the fact that the parameters c and δ form two completely disjoint sets more efficient estimation methods may be derived. Such problems are referred to as Separable Nonlinear Least Squares (SNLS) problems and an efficient method for their solution is the Variable Projection (VP) method introduced in early seventies by Golub and Pereyra (1973), which is based on the fact that c appears linearly in the model function $\Phi(\xi, \delta) \cdot c$. Thus, if we assume known nonlinear parameters δ, the $\hat{c}$ estimate may be readily obtained through the ordinary least squares equation:

$$\begin{aligned} &\hat{c} = \left(\Phi^T(\xi, \delta) \cdot \Phi(\xi, \delta)\right)^{-1} \Phi^T(\xi, \delta) \cdot y \Rightarrow \\ &\Rightarrow \hat{c} = \Phi^{\dagger}(\xi, \delta) \cdot y \end{aligned} \tag{9}$$

with † denoting pseudo-inverse. Hence, the model errors may be obtained as

$$\begin{aligned} &e(\delta, c) = y - \Phi(\xi, \delta) \cdot c \Rightarrow \\ &\Rightarrow e_{\text{VP}}(\delta) = y - \Phi(\xi, \delta) \cdot \Phi^{\dagger}(\xi, \delta) \cdot y \Rightarrow \\ &\Rightarrow e_{\text{VP}}(\delta) = \left(I - \Phi(\xi, \delta) \cdot \Phi^{\dagger}(\xi, \delta)\right) \cdot y \end{aligned} \tag{10}$$

and as a consequence the optimization problem of Eq. (8) takes the *variable projection* functional form:

$$\hat{\delta} = \arg\min_{\delta} \| \left(I - \Phi(\xi,\delta)\cdot\Phi^{\dagger}(\xi,\delta)\right)\cdot y\|^2 \quad \text{subject to} \quad H(\delta) \leq 0 \tag{11}$$

with $H(\delta)$ denoting the linear constraint functional. In this way, the nonlinear parameters δ may be estimated through Eq. (11) by the means of constrained nonlinear optimization techniques with only $p-k$ unknown parameters, while c may be subsequently estimated through linear least square optimization (Eq. (9)). The method is referred to as VP method as the matrix $\left(I - \Phi(\xi,\delta)\cdot\Phi^{\dagger}(\xi,\delta)\right)$ is the projector on the orthogonal complement of the column space of $\Phi(\xi,\delta)$ (Golub and Pereyra (2003)).

The minimization of the VP functional entails a number of advantages compared to the original minimization problem. The most important is the dimensionality reduction of the nonlinear optimization problem – while this reduction does not imply changes to the stationary points (minima and maxima) of the original problem. This holds under the rather mild condition of constant (not necessarily maximum) rank of the regression matrix $\Phi(\xi,\delta)$ over the whole parameter search space of δ. However, in our case the constraints described in the previous section define an appropriate parameter space in which the constant full rank of $\Phi(\xi,\delta)$ is guaranteed.

Nonetheless, the cost for reducing the dimension of the nonlinear optimization problem is the increased complexity of the VP objective function $V_{\mathrm{VP}}(\delta)$ gradient computation. Golub and Pereyra in their aforementioned study derived the necessary relationships for the differentiation of a pseudoinverse matrix and concluded to the required gradient with respect to the nonlinear parameter vector. Approximate solutions which aim at computational time reduction have also been proposed in the literature. A comparison and asymptotic analysis study for the three most frequently used algorithms may be found in Ruhe and Wedin (1980). In the present study we follow the Golub and Pereyra exact approach.

2. NUMERICAL CASE STUDY

2.1. *Test case I*

For this first example we consider the following differential equation governing the movement of a particle being under the influence of a potential field and a friction force (Le Maître et al. (2004)):

$$\frac{d^2X}{dt^2} + 2\frac{dX}{dt} = -\frac{35}{2}X^3 + \frac{15}{2}X \tag{12a}$$

with uncertain initial initial position

$$X(t=0,\xi) = 0.05 + 0.2\xi, \quad \xi \sim \mathscr{U}(-1,1) \tag{12b}$$

and vanishing velocity

$$\left.\frac{dX}{dt}\right|_{t=0} = 0 \tag{12c}$$

The analytical prediction of the steady state position of the particle is given by

$$\begin{cases} X(t\to\infty,\xi) = -\sqrt{15/35}, & \xi < -0.25, \\ X(t\to\infty,\xi) = \sqrt{15/35}, & \xi > -0.25, \end{cases} \tag{13}$$

This uncertainty propagation problem was solved in Le Maître et al. (2004) through the Galerkin approach and the proposed therein Wiener-Haar expansion model. Nonetheless, in the present study the non-intrusive regression problem of the initial conditions uncertainty propagation to the steady state solution (for $t = 10$ s) is considered, that is $Y = X(t = 10s,\xi)$. For this reason Eq. (12) is simulated for $N = 100$ times, with the corresponding samples of the uncertain parameter ξ being drawn from the standard uniform distribution through the Latin Hypercube Sampling (LHS) method (Helton and Davis (2003)). A Runge-Kutta scheme is utilized for performing time integration with a time step $\Delta t = 0.001$ s. The output $y_n (n = 1,\ldots,100)$ versus the corresponding input variables ξ_n are shown in Fig. 2.

The criterion of the normalized sum of squared errors:

$$NSE = \frac{\sum_{n=1}^{N} e_n^2}{\sum_{n=1}^{N} y_n^2}\ (\%) \tag{14}$$

is utilized for evaluating the performance of the different expansion schemes. The calculated NSE values of the data-driven expansion based on adaptable B-spline basis of various orders $k = 1,\ldots,4$ is

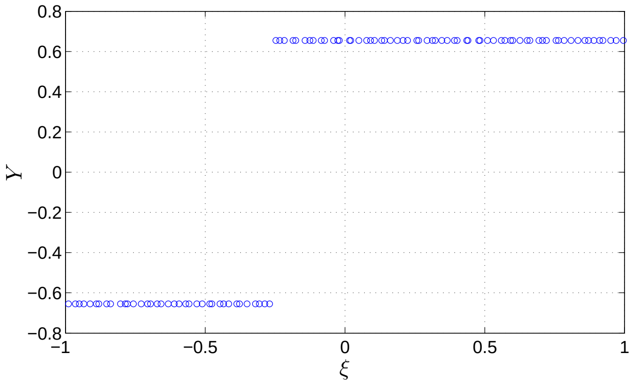

Figure 2: Steady-state position of the moving particle $Y = X(t = 10s, \xi)$ versus the corresponding input variable ξ for the 100 simulations conducted.

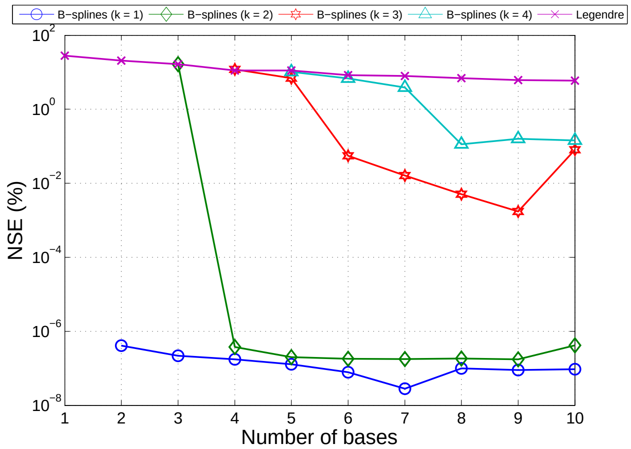

Figure 3: Test case I: NSE criterion values for the expansion models based on classical PC (Legendre polynomials) and the introduced data-driven method (B-splines of order $k = 1, \ldots, 4$).

shown in Fig. 3 along with those obtained by the classical PC expansion based on Legendre polynomials. For all cases, the maximum number of bases has been limited to 10. It is noted that a constraint parameter ε equal to 0.02 is selected for the data-driven approach while the SNLS optimization is initialized by values estimated through a gradient-free Particle Swarm Optimization (PSO) algorithm (Engelbrecht (2006)) . This extra step is taken in order to reduce the possibility of wrong convergence of the optimization procedure to local minima due to arbitrary initialization.

The results of Fig. 3 reveal superior performance of the proposed method since the discontinuity of the input-output relationship is correctly captured, as expected, by the B-splines with $k = 1$ and only two bases, that is a single internal knot estimated to be at $\xi = -0.2678$. On the other hand, a large number of Legendre polynomials are necessary to achieve similar accuracy.

2.2. *Test case II*

In this second example the test case of a hysteretic dissipative SDOF system is examined. The SDOF system is actually a mass-damper systems with an additional element producing a nonlinear restoring force $F(t)$ described by the Bouc-Wen model (Fig. 4):

$$m\frac{dX^2}{dt} + c\frac{dX}{dt} + F(t) = U(t) \tag{15a}$$

$$F(t) = \lambda k_\ell X(t) + (1-\lambda)k_\ell Z(t) \tag{15b}$$

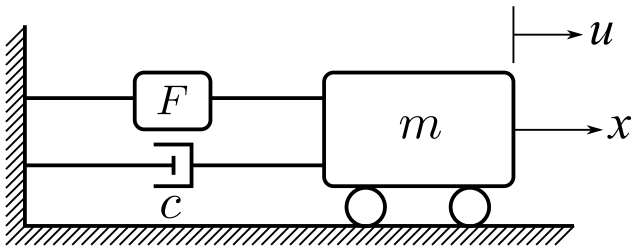

Figure 4: Single degree of freedom system with hysteretic restoring force.

with

$$\dot{Z}(t) = A\dot{X}(t) + \beta\left|\frac{dX}{dt}\right||Z(t)|^{n-1}Z(t) - \gamma\frac{dX}{dt}|Z(t)|^n \tag{15c}$$

λ designating the post- to pre-yield stiffness k_ℓ ratio, and A, $\beta > 0$, γ and n the dimensionless quantities controlling the shape of the hysteresis loop (Ismail et al. (2009)).

The nonlinear SDOF system is considered to be subject to a static random force equal to 100 N, while it is characterized by uncertainty of the parameter $\lambda \equiv \xi \sim \mathscr{U}(0,1)$. The properties of the system are summarized in Table 1.

Again the regression problem of the uncertainty propagation to the steady-state displacement (for $t = 20$ s) of the SDOF hysteretic system is considered, that is $Y = X(t = 20s, \xi)$. The system is simulated $N = 100$ times, with the equations of motion describing the system being integrated through

Table 1: Properties of the SDOF system with hysteretic restoring force.

mass	$m = 1$ kg
damping coefficient	$c = 1$ N/ (m/s)
linear stiffness coefficient	$k_\ell = 100$ N/m
post- to preyield stiffness ratio	$\lambda \sim \mathscr{U}(0,1)$
hysteretic loop shape parameters	$A = 1, n = 3$
	$\beta = 1, \gamma = 1$

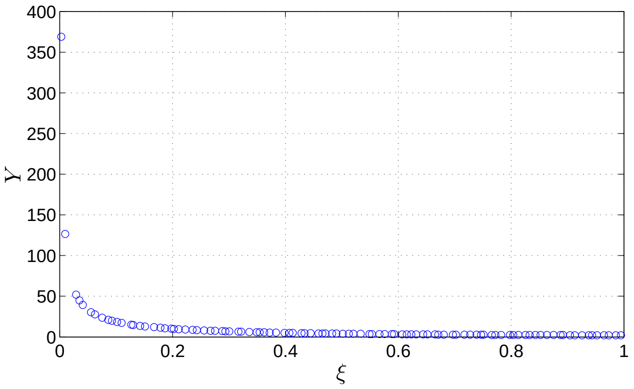

Figure 5: Steady-state displacement of the hysteretic SDOF system $Y = X(t = 20s, \xi)$ versus the corresponding input variable ξ for the 100 simulations conducted.

a Runge-Kutta scheme with a time step $\Delta t = 0.01$ s. The values of the output variable versus those of the uncertain input variable are shown in Fig. 5.

The normalized sum of squared errors criterion achieved by the classical PCE based on Legendre polynomials for various degrees $p = 1, \ldots, 10$ is contrasted to those of a data-driven expansion based on B-splines of various orders $k = 1, \ldots, 4$ in Fig. 6. As clearly shown the data-driven expansion outperforms the classical PC model for B-splines order of $k = 3$ and $k = 4$, yet with a much larger convergence rate.

3. CONCLUSIONS

A data-driven uncertainty quantification scheme has been introduced. The method is based on proper basis function parametrizations and an SNLS type procedure which allows the efficient solution of the parameter estimation problem. The method's effectiveness has been assessed through two uncertainty propagation representation test case studies. Comparisons with classical PCE based on the Wiener-Askey scheme, demonstrated

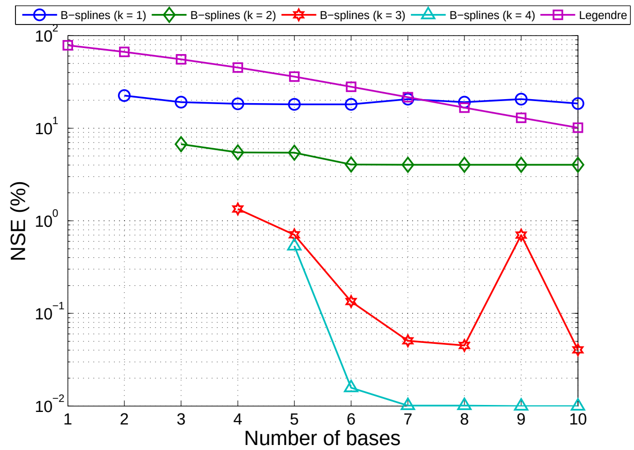

Figure 6: Test case II: NSE criterion values for the expansion models based on classical PC (Legendre polynomials) and the introduced data-driven method (B-splines of order $k = 1, \ldots, 4$).

the method's advanced capabilities and superior performance characteristics. Future work will include the comparison of the method with other data driven methods such as the arbitrary PC (aPC) introduced in Oladyshkin and Nowak (2012), and the extension of the method for the intrusive PC approach.

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