Improving adaptive generalized polynomial chaos method to solve nonlinear random differential equations by the random variable transformation technique

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Abstract

Generalized polynomial chaos (gPC) is a spectral technique in random space to represent random variables and stochastic processes in terms of orthogonal polynomials of the Askey scheme. One of its most fruitful applications consists of solving random differential equations. With gPC, stochastic solutions are expressed as orthogonal polynomials of the input random parameters. Different types of orthogonal polynomials can be chosen to achieve better convergence. This choice is dictated by the key correspondence between the weight function associated to orthogonal polynomials in the Askey scheme and the probability density functions of standard random variables. Otherwise, adaptive gPC constitutes a complementary spectral method to deal with arbitrary random variables in random differential equations. In its original formulation, adaptive gPC requires that both the unknowns and input random parameters enter polynomially in random differential equations. Regarding the inputs, if they appear as non-polynomial mappings of themselves, polynomial approximations are required and, as a consequence, loss of accuracy will be carried out in computations. In this paper an extended version of adaptive gPC is developed to circumvent these limitations of adaptive gPC by taking advantage of the random variable transformation method. A number of illustrative examples show the superiority of the extended adaptive gPC for solving nonlinear random differential equations. In addition, for the sake of completeness, in all examples randomness is tackled by nonlinear expressions.

Keywords: Nonlinear uncertainty, nonlinear random differential equations, adaptive generalized polynomial chaos, random variable transformation technique

1. Introduction

The consideration of uncertainty in modelling has experienced a significant increase over the last few years. Numerous researchers, with completely different backgrounds, are considering randomness in continuous models formulated by random differential equations (RDE's)

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to account for uncertainty quantification, and therefore providing more accurate and reliable mathematical models. The generalized polynomial chaos (gPC) method [1, 2], an extension of the classical PC method [3, 4], is one of the most adopted approaches to deal with uncertainty in RDE's. In its standard formulation, the application of gPC requires that every model input random parameter (coefficients, forcing terms, initial/boundary conditions) belongs to standard probabilistic distributions such as Gaussian, gamma, beta, exponential, etc., a hypothesis which often is not met in practice. With gPC, stochastic solutions are expressed as orthogonal polynomials of the input random parameters. Different types of orthogonal polynomials can be chosen to achieve better convergence. This choice is dictated by the key correspondence between the weight function associated to complete orthogonal polynomials in the Askey scheme and the probability density functions of standard random variables. However it is important to point out that, not all probability distributions yield a complete system of orthogonal polynomials. In [5], sufficient conditions are derived such that the polynomials are dense in the Hilbert space of square integrable functions. Also a counterexample is given, where the polynomials are not dense and thus some functions cannot be represented in a gPC expansion.

Recently, the authors, in collaboration with other colleagues, have developed a step-by-step computational technique to implement a version of gPC, termed adaptive gPC, for solving RDE's whose random inputs can have any probability distribution including the standard ones as well, [6]. It is important to clarify that the term *adaptive* is used to emphasize the weighting functions of the orthogonal polynomials are chosen to match the probability density of the individual random parameters. Adaptive gPC technique is aimed to provide researchers, who do not know the foundations of gPC, an easy guide to implement adaptive gPC in order to quantify uncertainty in models based on RDE's. In the context of standard gPC all model input parameters are assumed to be independent random variables (RV's), a hypothesis which is also kept in adaptive gPC method [1, 6]. In [6], a number of examples illustrates the competitiveness of adaptive gPC method to deal with linear and nonlinear RDE's, where random inputs have standard probability distributions, such as beta, uniform and Gaussian (see Examples 1–3 and 5), as well as, non-standard probability distributions generated by kernel distributions from sampled data (see Example 4). The examples include scalar and systems of RDE's (see Examples 1–4 and Example 5, respectively).

Adaptive gPC belongs to the class of Galerkin-type methods. It consists of projecting weighted residuals onto a finite-dimensional subspace spanned by appropriate basis functions to obtain the constraints required to solve for the deterministic coefficients. This projection requires the construction of inner products defined by the expectations of input parameters. If $F(t, \mathbf{y}, \dot{\mathbf{y}}; \zeta_1, \ldots, \zeta_s) = \mathbf{0}$ denotes the RDE, with unknown stochastic process (SP) $\mathbf{y} = \mathbf{y}(t)$, and input random parameters $\zeta_1, \ldots, \zeta_s$, whose probability density functions (PDF's) are $f_{\zeta_1}(\zeta_1), \ldots, f_{\zeta_s}(\zeta_s)$, respectively, then, a basic tenet assumed in the development of the adaptive gPC presented in [6] is the polynomial dependence of the right-hand side of the RDE, F, upon the input random parameters $\zeta_1, \ldots, \zeta_s$ and the unknown process $\mathbf{y}(t)$. This permits to construct the required inner products directly in terms of the PDF's of input random parameters. As it was pointed out in [6] (see last paragraph in Section 3.1), the previous hypothesis limits the application of adaptive gPC since, if for example an input random parameter, say ζ, appears in the RDE by means of a non-polynomial transformation of itself, say $r(\zeta)$, then adaptive gPC will require the polynomial approximation of mapping r and, as a consequence, a loss of accuracy will be carried out in computations.

Throughout this paper the triplet $(\Omega, \mathcal{F}, \mathbb{P})$ will denote the common complete probability space where all real RV's are defined. In this contribution, we propose to overcome the above mentioned drawback by taking advantage of the random variable transformation (RVT) method

[7, 8]. RVT technique is a probabilistic method that permits determining the PDF $f_\xi(\xi)$ of an absolutely continuous real RV $\xi = r(\zeta)$ which results from mapping another absolutely continuous real RV $\zeta : \Omega \longmapsto \mathcal{D}_\zeta$, defined on the domain $\mathcal{D}_\zeta = \{\zeta \equiv \zeta(\omega) : \zeta_1 \leq \zeta(\omega) \leq \zeta_2,\ \omega \in \Omega\}$ and whose PDF $f_\zeta(\zeta)$ is given. Assuming that the domain of mapping r contains the entire range or codomain of RV and that $r : \mathcal{D}_\zeta \longmapsto \mathbb{R}$ is monotone and continuously differentiable, then

$$f_\xi(\xi) = f_\zeta(s(\xi)) \left| \frac{\mathrm{d}s(\xi)}{\mathrm{d}\xi} \right|, \qquad \mathcal{D}_\xi = \{\, \xi : \xi_1 \leq \xi \leq \xi_2 \}\,, \tag{1}$$

where $s(\xi) = \zeta$ is the inverse mapping of r on $\mathcal{D}_\zeta$, and $\left|\frac{\mathrm{d}s(\xi)}{\mathrm{d}\xi}\right|$ denotes the absolute value of the derivative of $s(\xi)$. If r is increasing (decreasing) on $\mathcal{D}_\zeta$, the domain $\mathcal{D}_\xi$ of $\xi = r(\zeta)$ is determined by $\mathcal{D}_\xi = \{\, \xi : \xi_1 = r(\zeta_1) \leq \xi \leq r(\zeta_2) = \xi_2\}$ ($\mathcal{D}_\xi = \{\, \xi : \xi_1 = r(\zeta_2) \leq \xi \leq r(\zeta_1) = \xi_2\}$), where for the sake of simplicity, as usual, the ω-notation has been omitted. In the case that mapping r is not monotone on its whole domain $\mathcal{D}_\zeta$, this can be split in several pieces where monotony is guaranteed. Indeed, if $r'(\zeta) \neq 0$ for all $\mathcal{D}_\zeta$ except at a finite number of points and for each $\xi \in \mathbb{R}$, there exist $m(\xi) \geq 1$ points: $\zeta_1(\xi), \zeta_2(\xi), \ldots, \zeta_{m(\xi)}(\xi) \in \mathcal{D}_\zeta$ such that

$$r(\zeta_d(\xi)) = \xi, \quad r'(\zeta_d(\xi)) \neq 0, \qquad d = 1, 2, \ldots, m(\xi), \tag{2}$$

then

$$f_\xi(\xi) = \begin{cases} \displaystyle\sum_{d=1}^{m(\xi)} f_\zeta(\zeta_d(\xi)) \left| r'(\zeta_d(\xi)) \right|^{-1} & \text{if} \quad m(\xi) > 0, \\ 0 & \text{if} \quad m(\xi) = 0. \end{cases} \tag{3}$$

Throughout this paper, mappings playing the role of r in the above context will be assumed monotone for the sake of clarity in the presentation. We underline that in the context of solving random ordinary and partial differential and difference equations, RVT method has been successfully applied to compute both analytically and numerically, the first PDF associated to the solution SP (see for example, [9, 10, 11, 12, 13, 14, 15, 16, 17, 18]).

Finally, we recall a result that will be required later. If X is an absolutely continuous RV defined on the domain $\mathcal{D}(X)$ and with PDF $f_X(x)$, and from it one constructs a new RV $Y = \mathfrak{M}(X)$, where $\mathfrak{M}$ is a continuous mapping, then the expectation of Y can be obtained as follows

$$\mathbb{E}[Y] = \int_{\mathcal{D}(X)} \mathfrak{M}(x) f_X(x)\, \mathrm{d}x\,. \tag{4}$$

This paper is organized as follows. In Section 2, an extended version of adaptive gPC method which is able to solve RDE's when its input random parameters appear by non-polynomial transformations of themselves is presented. In Section 3, several examples illustrating the improvement of the extended version of adaptive gPC against standard gPC method are presented. Conclusions are drawn in Section 4.

2. Development

In this section, we will develop an extended version of adaptive gPC based on [6]. For the sake of clarity in the presentation, we will keep the same notation used in [6].

Let us consider the initial value problem (IVP)

$$\begin{cases} F(t, \mathbf{y}, \dot{\mathbf{y}}) &= \mathbf{0}, \\ \mathbf{y}(t_0) &= \widehat{\mathbf{y}}_0, \end{cases} \qquad F : \mathbb{R}^{2q+1} \longrightarrow \mathbb{R}^q, \tag{5}$$

where t is the independent variable, and let

$$\mathbf{y} = \mathbf{y}(t) = (y^1(t), y^2(t), \ldots, y^q(t))^\top, \qquad \widehat{\mathbf{y}}_0 = (y^1(t_0), y^2(t_0), \ldots, y^q(t_0))^\top, \tag{6}$$

be the vector of unknown functions and the initial condition, respectively. As usual, $\mathbf{0} = (0, 0, \ldots, 0)^\top$ stands for the zero vector of dimension q, being $\top$ the transpose operator for vectors and matrices. We will assume that $\boldsymbol{\zeta} = (\zeta_1, \ldots, \zeta_s)$ are the model input random parameters in the IVP defined by (5)–(6). These are assumed to be mutually independent RV's with univariate PDF $f_{\zeta_l}(\zeta_l)$, $1 \leq l \leq s$. The value s is usually referred to as the order of the chaos. For the sake of clarity in the presentation and, without loss of generality, hereinafter we will assume that $\zeta_1, \ldots, \zeta_h$, $1 \leq h \leq s$, appear both in the RDE as in the initial condition in (5), by means of non-polynomial transformations, say $\xi_i = r_i(\zeta_i)$, $1 \leq i \leq h$, of themselves. As it was pointed out, in the following the mappings r_i, $1 \leq i \leq h$, will be assumed monotone; otherwise formula (3) would be applied. To fix ideas, this means that terms of the form $\ln(\zeta_1), \exp(\zeta_2), \ldots, \arctan(\zeta_h)$, for example, could appear in the IVP (5), whereas the rest of input random parameters are $\zeta_{h+1}, \ldots, \zeta_s$. The unknowns $y^1(t), y^2(t), \ldots, y^q(t)$ are assumed to appear polynomially in the RDE (5).

For every RV ξ_i, $1 \leq i \leq h$, which results from the non-polynomial transformation of input random parameter ζ_i by the mapping r_i, let us define the following inner product

$$\langle g_1(\xi_i), g_2(\xi_i)\rangle_{\xi_i} = \int_{\mathrm{supp}(\xi_i)} g_1(\xi_i) g_2(\xi_i) f_{\zeta_i}(s_i(\xi_i)) \left|\frac{\mathrm{d}s_i(\xi_i)}{\mathrm{d}\xi_i}\right| \mathrm{d}\xi_i, \quad 1 \leq i \leq h, \tag{7}$$

being, g_1, g_2 deterministic functions such that the above integrals exist; s_i, the inverse mapping of r_i; and $\mathrm{supp}(\xi_i)$ the domain or support of RV ξ_i, $1 \leq i \leq h$. For each one of the rest of the input random parameters ζ_j, $h+1 \leq j \leq s$, we define the following inner product

$$\left\langle g_1(\zeta_j), g_2(\zeta_j)\right\rangle_{\zeta_j} = \int_{\mathrm{supp}(\zeta_j)} g_1(\zeta_j) g_2(\zeta_j) f_{\zeta_j}(\zeta_j)\, \mathrm{d}\zeta_j, \quad h+1 \leq j \leq s. \tag{8}$$

Now, for each type of input random parameter, either $\{\xi_i : 1 \leq i \leq h\}$ or $\{\zeta_j : h+1 \leq j \leq s\}$, we will construct an orthogonal polynomial basis using the Gram-Schmidt method from the canonical basis truncated at a common degree p:

$$\begin{array}{rcll} C^p_{\xi_i} & = & \{1, \xi_i, (\xi_i)^2, \ldots, (\xi_i)^p\}, & 1 \leq i \leq h, \\ C^p_{\zeta_j} & = & \{1, \zeta_j, (\zeta_j)^2, \ldots, (\zeta_j)^p\}, & h+1 \leq j \leq s, \end{array} \tag{9}$$

respectively. In this manner, two sets of orthogonal polynomials are constructed, say

$$\begin{array}{rcll} \Xi^p_{\xi_i} & = & \{\phi^i_0(\xi_i), \phi^i_1(\xi_i), \ldots, \phi^i_p(\xi_i)\}, & 1 \leq i \leq h, \\ \Xi^p_{\zeta_j} & = & \{\phi^j_0(\zeta_j), \phi^j_1(\zeta_j), \ldots, \phi^j_p(\zeta_j)\}, & h+1 \leq j \leq s, \end{array} \tag{10}$$

where, without loss of generality, we will assume that $\phi^i_0(\xi_i) = 1$, $1 \leq i \leq h$, and, $\phi^j_0(\zeta_j) = 1$, $h+1 \leq j \leq s$. The degree of polynomials $\{\phi^i_0(\xi_i), \phi^j_0(\zeta_j)\}$; $\{\phi^i_1(\xi_i), \phi^j_1(\zeta_j)\}$; $\ldots$; $\{\phi^i_p(\xi_i), \phi^j_p(\zeta_j)\}$ is $0, 1, \ldots, p$, respectively. If the first-order polynomials $\phi^i_1(\xi_i)$ and $\phi^j_1(\zeta_j)$ have the following representation

$$\phi^i_1(\xi_i) = a_i + b_i \xi_i, \quad \phi^j_1(\zeta_j) = c_j + d_j \zeta_j, \quad b_i, d_j \neq 0, \tag{11}$$

where the coefficients a_i, b_i, c_j and d_j are determined by Gram-Schmidt orthogonalization process, then, notice that both type of input random parameters, ξ_i and ζ_j, have the following simplest representations in terms of the bases $\Xi^p_{\xi_i}$ and $\Xi^p_{\zeta_j}$, respectively

$$\begin{aligned} \xi_i &= -\frac{a_i}{b_i}\phi^i_0(\xi_i) + \frac{1}{b_i}\phi^i_1(\xi_i) \quad , \quad 1 \le i \le h, \\ \zeta_j &= -\frac{c_j}{d_j}\phi^j_0(\zeta_j) + \frac{1}{d_j}\phi^j_1(\zeta_j) \quad , \quad h+1 \le j \le s. \end{aligned} \tag{12}$$

At this point, we want to represent the solution SP $\mathbf{y}(t)$ and the initial condition $\widehat{\mathbf{y}}_0$ in terms of a basis, say $\Xi = \{\Phi_k\}$, constructed from the previous bases $\Xi^p_{\xi_i}$, $1 \le i \le h$, and, $\Xi^p_{\zeta_j}$, $h+1 \le j \le s$. The elements of this basis Ξ represent multidimensional expansion polynomials which depend on RV's ξ_i, $1 \le i \le h$, and ζ_j, $h+1 \le j \le s$. They are constructed by the tensor product

$$\Phi_k(\boldsymbol{\nu}) = \phi^1_{p_1}(\xi_1) \times \cdots \times \phi^h_{p_h}(\xi_h) \times \phi^{h+1}_{p_{h+1}}(\zeta_{h+1}) \times \cdots \times \phi^s_{p_s}(\zeta_s), \tag{13}$$

where $\boldsymbol{\nu} = (\xi_1, \ldots, \xi_h, \zeta_{h+1}, \ldots, \zeta_s)$ and the multi-index $\mathbf{p} = (p_1, \ldots, p_h, p_{h+1}, \ldots, p_s)$ can be reformulated by means of a single index k using the graded lexicographic order, i.e., $\mathbf{p} > \mathbf{q}$ if and only if $|\mathbf{p}| \ge |\mathbf{q}|$ and the first nonzero entry in the difference $\mathbf{p} - \mathbf{q}$ is positive, being $|\mathbf{p}| = p_1 + \cdots + p_h + p_{h+1} + \cdots + p_s$ [2, p.66]. This permits the following representations of the solution SP, its derivative and the initial condition

$$\mathbf{y}(t) = \sum_{k=0}^{P} \mathbf{y}_k(t)\Phi_k(\boldsymbol{\nu}), \quad \dot{\mathbf{y}}(t) = \sum_{k=0}^{P} \dot{\mathbf{y}}_k(t)\Phi_k(\boldsymbol{\nu}), \quad \widehat{\mathbf{y}}_0 = \sum_{k=0}^{P} \mathbf{y}_{0,k}(t_0)\Phi_k(\boldsymbol{\nu}). \tag{14}$$

In practice, the order of truncation P in the above sums remains completely determined once the common degree p of the sets $C^p_{\xi_i}$ and $C^p_{\zeta_j}$ introduced in (9) and, an specific degree of the multidimensional polynomials (13) to be contained in the expansions (14), have been fixed.

On account of the previous development, substituting (14) in (5), one gets the following representation of the IVP

$$F\left(t, \sum_{k=0}^{P} \mathbf{y}_k(t)\Phi_k(\boldsymbol{\nu}), \sum_{k=0}^{P} \dot{\mathbf{y}}_k(t)\Phi_k(\boldsymbol{\nu})\right) = \mathbf{0}, \tag{15}$$

$$\widehat{\mathbf{y}}_0 = \sum_{k=0}^{P} \mathbf{y}_{0,k}(t_0)\Phi_k(\boldsymbol{\nu}), \tag{16}$$

which involves both, transformed model input random parameter $\xi_1, \ldots, \xi_h$ and the rest of inputs $\zeta_{h+1}, \ldots, \zeta_s$, since $\boldsymbol{\nu} = (\xi_1, \ldots, \xi_h, \zeta_{h+1}, \ldots, \zeta_s)$.

In order to solve this IVP, the coefficients $\mathbf{y}_k(t)$, $0 \le k \le P$, must be determined. For that, we define the following inner product, that represents an ensemble average of RV's $g_1(\boldsymbol{\nu})$ and $g_2(\boldsymbol{\nu})$,

$$\langle g_1(\boldsymbol{\nu}), g_2(\boldsymbol{\nu})\rangle_{\boldsymbol{\nu}} = \int_{\mathrm{supp}(\boldsymbol{\nu})} g_1(\boldsymbol{\nu}) g_2(\boldsymbol{\nu}) f_{\boldsymbol{\nu}}(\boldsymbol{\nu})\, \mathrm{d}\boldsymbol{\nu}, \tag{17}$$

where

$$f_{\boldsymbol{\nu}}(\boldsymbol{\nu}) = \left(\prod_{i=1}^{h} f_{\zeta_i}(s_i(\xi_i)) \left|\frac{\mathrm{d}s_i(\xi_i)}{\mathrm{d}\xi_i}\right|\right)\left(\prod_{j=h+1}^{s} f_{\zeta_j}(\zeta_j)\right), \qquad \boldsymbol{\nu} = (\xi_1, \ldots, \xi_h, \zeta_{h+1}, \ldots, \zeta_s)\,. \tag{18}$$

Notice that by [19, Th.3, p.92], mutually independence of RV's ζ_l, $1 \le l \le s$, entails mutually independence of RV's $\xi_i = r_i(\zeta_i)$, $1 \le i \le h$, and, ζ_j, $h+1 \le j \le s$, and hence the above factorization of the weighting function $f_{\boldsymbol{\nu}}(\boldsymbol{\nu})$ through the PDF's of each ζ_l, $f_{\zeta_l}(\zeta_l)$, $1 \le l \le s$, is legitimated.

Coefficients $\mathbf{y}_k(t)$, $0 \le k \le P$ are determined by setting a deterministic IVP based on a system of $P+1$ differential equations whose unknowns are just $\mathbf{y}_k(t)$. This system, usually referred to as auxiliary system, is built by multiplying each equation of random differential system (15) by elements of the orthonormal basis $\Xi = \{\Phi_k\}$ defined by (13) and then, taking the ensemble average $\langle\ \rangle_{\boldsymbol{\nu}}$ defined by (17)–(18). This permits simplifying the deterministic system of differential equations taking advantage of orthogonality. In order to establish the initial condition associated to this system, we first multiply (16) by $\{\Phi_k\}$ and then, the ensemble average $\langle\ \rangle_{\boldsymbol{\nu}}$ is taken again. This yields the computation of coefficients $\mathbf{y}_{0,k}(t_0)$ as follows

$$\mathbf{y}_{0,k}(t_0) = \langle \widehat{\mathbf{y}}_0, \Phi_k(\boldsymbol{\nu}) \rangle_{\boldsymbol{\nu}}, \quad 0 \le k \le P. \tag{19}$$

In practice, numerical integration schemes are required to solve the auxiliary system together with the initial conditions (19), i.e., to compute $\mathbf{y}_k(t)$, $0 \le k \le P$. From them, approximations for the mean, $\mathbb{E}[\mathbf{y}(t)]$, and the variance-covariance matrix, $\Sigma_{\mathbf{y}(t)}$, can be obtained on account of the following relationships:

$$\mathbb{E}[\mathbf{y}(t)] = \langle \mathbf{y}(t) \rangle_{\boldsymbol{\nu}} = \mathbf{y}_0(t), \qquad \Sigma_{\mathbf{y}(t)} = \sum_{k=1}^{P} \mathbf{y}_k(t)(\mathbf{y}_k(t))^\top \left\langle (\Phi_k(\boldsymbol{\nu}))^2 \right\rangle_{\boldsymbol{\nu}}. \tag{20}$$

The diagonal elements of $\Sigma_{\mathbf{y}(t)}$ are the variance of each component $y^i(t)$, $1 \le i \le q$ of $\mathbf{y}(t)$.

3. Examples

In this section we will provide several examples with the aim of showing the higher accuracy of the extended adaptive gPC method than compared with the adaptive gPC method. As usual, comparison will be shown by computing the expectation and standard deviation of the solution. The two first examples act as tests since exact expressions for the mean and standard deviation functions are available, whereas approximations of these moments will be carried out applying both the extended adaptive gPC and gPC methods. We will highlight differences between both methods computing the relative error with respect to the exact value to the mean and the standard deviation. In the first example, only one model input parameter is assumed to be random, i.e., the order of the chaos is $s = 1$. This randomness is considered by means of a non-polynomial mapping of itself. The second example is more elaborated; we will assume that three model input parameters are random being included by different non-polynomial mappings of themselves. The last example deals with a system of nonlinear random differential equations for which, an exact solution is not available, thus the usefulness of extended adaptive gPC is completely manifested.

Example 1. *Let us consider the random IVP*

$$\left.\begin{array}{rcl} \dot{y}(t) & = & \mathrm{e}^{A} y(t), \\ y(0) & = & 1, \end{array}\right\} \tag{21}$$

where A is assumed to be a beta RV of parameters $\alpha = 2$ and $\beta = 5$, $A \sim Be(2;5)$. Hence, $0 < A(\omega) < 1$, for every $\omega \in \Omega$. According to the notation introduced in the previous section *regarding extended adaptive gPC, now we have*

$$q=1,\quad h=s=1,\quad \zeta_1=A,\quad \xi_1=r_1(\zeta_1)=\mathrm{e}^{\zeta_1},\quad \boldsymbol{\nu}=\xi_1. \tag{22}$$

Notice that mapping r_1 is strictly increasing. We have taken $p=9$ as the maximum degree of the polynomial canonical basis for the RV ξ_1. Thus according to (9) *one gets*

$$C^9_{\xi_1}=\{1,\xi_1,(\xi_1)^2,\dots,(\xi_1)^9\}. \tag{23}$$

Using the inner product (7)*, which now has the following specific form*

$$\langle g_1(\xi_1),g_2(\xi_1)\rangle_{\xi_1}=\int_0^{\mathrm{e}} g_1(\xi_1)g_2(\xi_1)\,\frac{f_{\zeta_1}(\ln(\xi_1))}{\xi_1}\,\mathrm{d}\xi_1,\qquad f_{\zeta_1}(\ln(\xi_1))=30(1-\ln(\xi_1))^4\ln(\xi_1)\,, \tag{24}$$

and, after applying the Gram-Schmidt process, one obtains the corresponding orthogonal basis

$$\Xi^9_{\xi_1}=\{\phi^1_0(\xi_1),\phi^1_1(\xi_1),\phi^1_2(\xi_1),\dots,\phi^1_9(\xi_1)\}\,. \tag{25}$$

As $h=s$, orthogonal bases $\Xi^9_{\xi_1}$ and $\Xi=\{\Phi_k\}$, where the solution $y(t)$ of IVP (21) *has been represented, coincide. As a consequence, the auxiliary system of differential equations has been constructed using the inner product* (17)–(18) *defined by* (24).

Notice that in this test example, the exact solution SP is given by $y(t)=\mathrm{e}^{\mathrm{e}^{A}t}$, thus taking into account (4) *expressions for the mean and the standard deviation can be computed as follows:*

$$\mathbb{E}[y(t)]=\mathbb{E}[\mathrm{e}^{\mathrm{e}^{A}t}]=30\int_0^1 \mathrm{e}^{\mathrm{e}^{a}t}a(1-a)^4\,\mathrm{d}a\,, \tag{26}$$

and

$$\sigma[y(t)]=+\sqrt{\mathbb{E}\left[(y(t))^2\right]-(\mathbb{E}[y(t)])^2}\ \ \textit{where}\ \ \mathbb{E}\left[(y(t))^2\right]=\mathbb{E}[\mathrm{e}^{2\mathrm{e}^{A}t}]=30\int_0^1 \mathrm{e}^{2\mathrm{e}^{a}t}a(1-a)^4\,\mathrm{d}a\,. \tag{27}$$

In Figures 1 and 2, the relative errors of the approximations obtained by gPC and the proposed extension of adaptive gPC for the mean and standard deviation of $y(t)$ using, in both cases, different orders P with respect to the exact values are shown. For instance, the relative errors for the mean, $\mathrm{RelErr}\,(\mathbb{E}[y(t)])$*, and the standard deviation,* $\mathrm{RelErr}\,(\sigma[y(t)])$*, of the approximations for the mean, $\mu^P_{\mathrm{gPC}}(t)$, and for the standard deviation, $\sigma^P_{\mathrm{gPC}}(t)$, by gPC method of order P, have been computed as follows*

$$\mathrm{RelErr}\,(\mathbb{E}[y(t)])=\left|\frac{\mathbb{E}[y(t)]-\mu^P_{gPC}(t)}{\mathbb{E}[y(t)]}\right|,\quad \mathrm{RelErr}\,(\sigma[y(t)])=\left|\frac{\sigma[y(t)]-\sigma^P_{gPC}(t)}{\sigma[y(t)]}\right|. \tag{28}$$

The graphs show that extended adaptive gPC provides more accurate results than gPC. The higher the order, the better the approximation. Notice that the relative error for extended adaptive gPC with $P=9$ has not been plotted because for $P=7$ it provides better results than gPC for $P=9$.

Example 2. *Let us consider the random IVP*

$$\left.\begin{array}{rcl}\dot{y}(t) & = & Cy(t)+\mathrm{e}^{-B}(y(t))^2,\\ y(0) & = & -\frac{1}{100}\sin(A),\end{array}\right\} \tag{29}$$

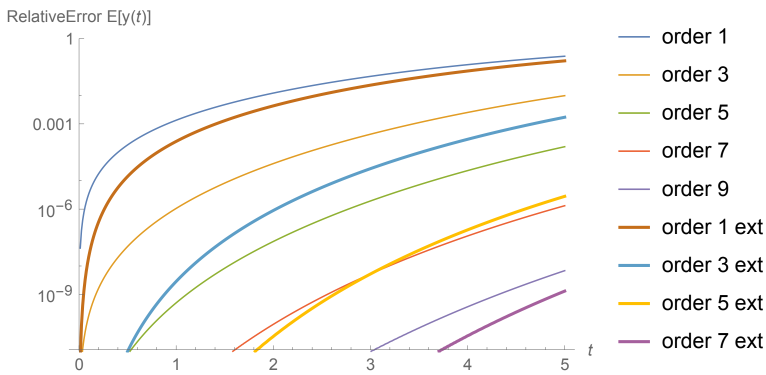

Figure 1: Comparison between relative errors for the mean using adaptive gPC (label: order P) and extended adaptive gPC (label: order P ext) using different orders of truncation $P = 1, 3, 5, 7, 9$ in the Example 1.

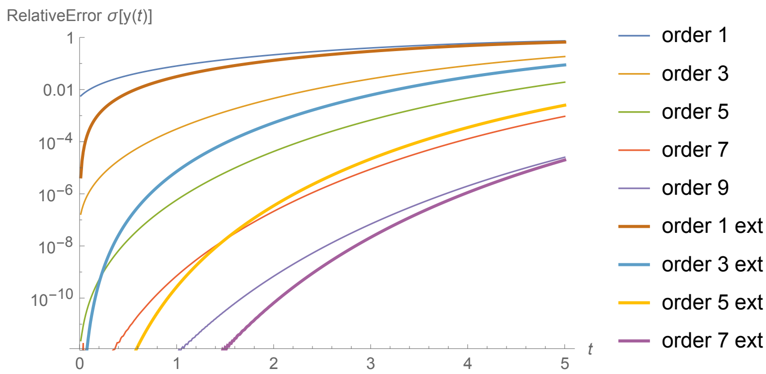

Figure 2: Comparison between relative errors for the standard deviation using gPC (label: order P) and extended adaptive gPC (label: order P ext) using different orders of truncation $P = 1, 3, 5, 7, 9$ in the Example 1.

where A is a beta RV of parameters $\alpha = 2$ and $\beta = 3$, $A \sim Be(2;3)$, B is an exponential RV of parameter $\lambda = 1$, $B \sim Exp(\lambda = 1)$ and, C is a uniform RV on the interval $[1,2]$, $C \sim Un([1,2))$.

Following the notation introduced in the theoretical development, in the current context one gets

$$
\begin{gathered}
q = 1, \quad h = 2, \quad s = 3, \quad \zeta_1 = A, \quad \zeta_2 = B, \quad \zeta_3 = C, \\
\xi_1 = r_1(\zeta_1) = \sin(\zeta_1), \quad \xi_2 = r_2(\zeta_2) = \exp(-\zeta_2), \quad \boldsymbol{\nu} = (\xi_1, \xi_2, \zeta_3).
\end{gathered} \tag{30}
$$

We have taken $p = 5$ as the common maximum degree of the polynomial canonical bases for RV's ξ_1, ξ_2 and ζ_3, therefore according to (9) *one gets*

$$
C^5_{\xi_i} = \{1, \xi_i, (\xi_i)^2, \ldots, (\xi_i)^5\}, \;\; i = 1,2; \qquad C^5_{\zeta_3} = \{1, \zeta_3, (\zeta_3)^2, \ldots, (\zeta_3)^5\}. \tag{31}
$$

In order to orthogonalize $C^5_{\xi_i}$, $i = 1,2$, we define the following inner products in agreement with (7)

$$
\begin{aligned}
\langle g_1(\xi_1), g_2(\xi_1)\rangle_{\xi_1} &= \int_0^{\sin(1)} g_1(\xi_1) g_2(\xi_1) \, \frac{f_{\zeta_1}(\arcsin(\xi_1))}{\sqrt{1-(\xi_1)^2}} \, \mathrm{d}\xi_1, \\
\langle g_1(\xi_2), g_2(\xi_2)\rangle_{\xi_2} &= \int_0^{1} g_1(\xi_2) g_2(\xi_2) \, \frac{f_{\zeta_2}(-\ln(\xi_2))}{\xi_2} \, \mathrm{d}\xi_2,
\end{aligned} \tag{32}
$$

where

$$
f_{\zeta_1}(\arcsin(\xi_1)) = 12 \arcsin(\xi_1)(1 - \arcsin(\xi_1))^2, \quad f_{\zeta_2}(-\ln(\xi_2)) = \xi_2 . \tag{33}
$$

Whereas, set $C^5_{\zeta_3}$, is orthogonalized using the following inner product

$$
\langle g_1(\zeta_3), g_2(\zeta_3)\rangle_{\zeta_3} = \int_1^2 g_1(\zeta_3) g_2(\zeta_3) \, \mathrm{d}\zeta_3 . \tag{34}
$$

The Gram-Schmidt orthogonalization method permits to obtain the orthogonal bases

$$
\Xi^5_{\xi_i} = \{\phi^i_0(\xi_i), \phi^i_1(\xi_i), \phi^i_2(\xi_i), \ldots, \phi^i_5(\xi_i)\}, \;\; i = 1,2; \quad \Xi^5_{\zeta_3} = \{\phi^3_0(\zeta_3), \phi^3_1(\zeta_3), \phi^3_2(\zeta_3), \ldots, \phi^3_5(\zeta_3)\}. \tag{35}
$$

Finally, the polynomials of the basis $\Xi = \{\Phi_k\}$, where the solution $y(t)$ of IVP (29) *has been represented are defined by the tensor product*

$$
\Phi_k(\boldsymbol{\nu}) = \phi^1_{p_1}(\xi_1)\phi^2_{p_2}(\xi_2)\phi^3_{p_3}(\zeta_3), \qquad \boldsymbol{\nu} = (\xi_1, \xi_2, \zeta_3). \tag{36}
$$

In accordance to (17)–(18) *and* (32)–(34)*, the auxiliary system of differential equations has been constructed using the inner product*

$$
\langle g_1(\boldsymbol{\nu}), g_2(\boldsymbol{\nu})\rangle_{\boldsymbol{\nu}} = \int_1^2 \int_0^1 \int_0^{\sin(1)} g_1(\xi_1,\xi_2,\zeta_3) g_2(\xi_1,\xi_2,\zeta_3) \, \frac{f_{\zeta_1}(\arcsin(\xi_1))}{\sqrt{1-(\xi_1)^2}} \, \frac{f_{\zeta_2}(-\ln(\xi_2))}{\xi_2} \, \mathrm{d}\xi_1 \, \mathrm{d}\xi_2 \, \mathrm{d}\zeta_3. \tag{37}
$$

The solution SP of random IVP (29) *is given by*

$$
y(t) = -\frac{c \sin(A) \mathrm{e}^{B+Ct}}{\sin(A)\mathrm{e}^{Ct} - \sin(A) + 100\mathrm{e}^{B} C}. \tag{38}
$$

By applying (4)*, the mean and the standard deviation of the exact solution can be computed in the same way that was shown in Example 1. These values have been used to compute the* *relative errors for the mean and the standard deviation of the approximations obtained by gPC and extended adaptive gPC methods using different orders P. The results have been plotted in Figure 3 (relative error for the mean) and Figure 4 (relative error for the standard deviation). From them, it is observed that the accuracy of extended adaptive gPC is higher than gPC.*

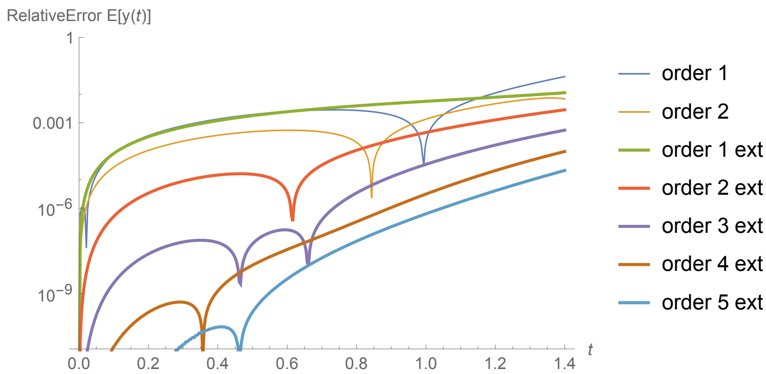

Figure 3: Comparison between relative errors for the mean using adaptive gPC (label: order P) and extended adaptive gPC (label: order P ext) using different orders of truncation $P = 1, 2, 3, 4, 5$, in the Example 2.

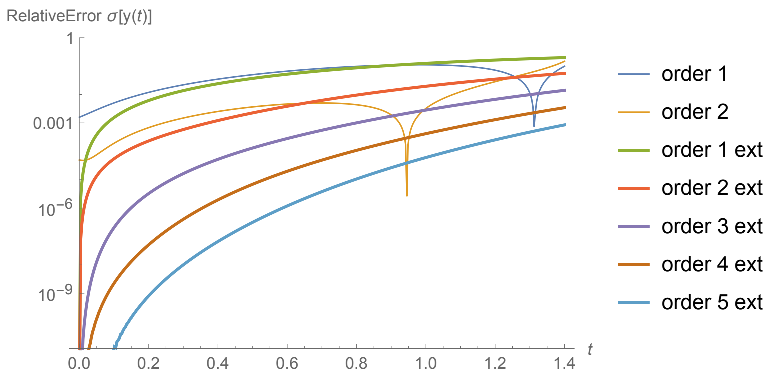

Figure 4: Comparison between relative errors for the standard deviation using adaptive gPC (label: order P) and extended adaptive gPC (label: order P ext) using different orders of truncation $P = 1, 2, 3, 4, 5$, in the Example 2.

Example 3. *This last example is devised to test the accuracy of extended adaptive gPC method in dealing with RDE's whose solution is highly oscillatory. In contrast to previous examples, where linear and nonlinear scalar RDE's were considered, now we will apply the method to the following nonlinear system of differential equations*

$$\left.\begin{array}{rclrcl} \dot{x}_1(t) & = & x_2(t)x_3(t), & x_1(0) & = & \alpha + 0.01\cos(A), \\ \dot{x}_2(t) & = & x_1(t)x_3(t), & x_2(0) & = & 1, \\ \dot{x}_3(t) & = & -2x_1(t)x_2(t), & x_3(0) & = & 1, \end{array}\right\} \tag{39}$$

where uncertainty is considered in the first initial condition $x_1(0)$. *We will assume that A is a uniform RV on the interval* $[0,\pi]$, $A \sim U([0,\pi])$, *and* α *is a deterministic parameter. Depending on the values taken by* α *parameter, the solution of this system has very different (oscillatory) behaviour. Hereinafter, we will analyse the following values:* $\alpha = 0.5$ *and* $\alpha = 0.85$.

In accordance with the notation introduced in the previous section, we have

$$q = 3, \quad h = s = 1, \quad \zeta_1 = A, \quad \xi_1 = r_1(\zeta_1) = \alpha + 0.01\cos(\zeta_1), \quad \boldsymbol{\nu} = \xi_1. \tag{40}$$

In this case, the mapping r_1 *is strictly decreasing. We have taken* $p = 3$ *as the maximum degree of the polynomial canonical basis for the RV* ξ_1. *Thus the basis is the set* $C^3_{\xi_1}$ *defined by* (23). *Whereas, the inner product* (7), *now takes the form*

$$\langle g_1(\xi_1), g_2(\xi_1)\rangle_{\xi_1} = \frac{1}{\pi}\int_{-0.01+\alpha}^{0.01+\alpha} g_1(\xi_1)g_2(\xi_1)\,\frac{1}{\sqrt{0.01^2-(\xi_1-\alpha)^2}}\,\mathrm{d}\xi_1\,. \tag{41}$$

This inner product permits to apply the Gram-Schmidt process in order to build an orthogonal basis, $\Xi^3_{\xi_1} = \{\phi^1_i(\xi_1),\ 0 \le i \le 3\}$. *Since* $h = s$, *orthogonal bases* $\Xi^3_{\xi_1}$ *and* $\Xi = \{\Phi_k\}$, *where the vector solution* $(x_1(t), x_2(t), x_3(t))$ *of IVP* (39) *has been represented, coincide. This entails that the auxiliary system of differential equations has been constructed using the inner product* (17)–(18) *defined by* (41).

In contrast to what happens in the two previous examples, a closed-form solution to the non-linear system (39) *is not available now. In order to analyse the quality of the approximations provided by extended adaptive gPC, we will take advantage of the fact that an invariant associated to system* (39) *can be determined in an exact manner. This invariant will be also computed by extended adaptive gPC and then, compared against its exact value.*

Notice that multiplying the first equation of (39) *by* $x_1(t)$*; the second one by* $x_2(t)$*; the third one by* $x_3(t)$ *and then, adding the three resulting equations one gets*

$$\sum_{i=1}^{3} x_i(t)\dot{x}_i(t) = x_1(t)x_2(t)x_3(t) + x_1(t)x_2(t)x_3(t) - 2x_1(t)x_2(t)x_3(t) = 0, \tag{42}$$

or equivalently

$$\sum_{i=1}^{3}\frac{\mathrm{d}}{\mathrm{d}t}\left((x_i(t))^2\right) = \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{3}(x_i(t))^2\right) = 0. \tag{43}$$

Let us take the expectation operator in the above expression

$$\mathbb{E}\left[\frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{3}(x_i(t))^2\right)\right] = \frac{\mathrm{d}}{\mathrm{d}t}\left(\sum_{i=1}^{3}\mathbb{E}\left[(x_i(t))^2\right]\right) = 0. \tag{44}$$

Notice that interchange of time differentiation and expected value is allowed, since the domain of the random variable is compact and all involved functions are continuous. Then

$$\mathcal{I}_\alpha = \sum_{i=1}^{3}\mathbb{E}\left[(x_i(t))^2\right], \quad \textit{for all } t, \tag{45}$$

is an invariant to the system (39). *Thus, the* $\mathcal{I}_\alpha$ *value does not change over time t. In particular, as the initial conditions are known,* $\mathcal{I}_\alpha$ *value can be calculated exactly from initial conditions*

$$\mathcal{I}_\alpha = \mathbb{E}\left[(x_1(0))^2\right]+\mathbb{E}\left[(x_2(0))^2\right]+\mathbb{E}\left[(x_3(0))^2\right] = \frac{1}{\pi}\int_0^\pi (\alpha+0.01\cos(a))^2\,\mathrm{d}a+1+1 = 2.00005+\alpha^2. \tag{46}$$

In Figure 5 (top) we show the computation of the invariant $\mathcal{I}_\alpha$ for $\alpha = 0.5$ by extended adaptive gPC. Notice that, according to (46), its exact value is $\mathcal{I}_{0.5} = 2.25005$. From this representation, we observe that the approximation obtained by extended adaptive gPC in the time interval $t \in [0, 50]$ is very accurate. This can be confirmed in Figure 5 (bottom) where the relative error for the computation of $\mathcal{I}_{0.5}$ by extended adaptive gPC is represented in the interval $t \in [0, 50]$. Notice that the maximum error order is about 10^{-7}. An analogous representation is presented in Figure 6 for the invariant $\mathcal{I}_{0.85} = 2.72255$. We again observe that extended adaptive gPC provides very good approximations.

Once extended adaptive gPC has been validated through the computation of the invariant $\mathcal{I}_\alpha$ for $\alpha \in \{0.5, 0.85\}$, we will construct approximations for the mean, $\mathbb{E}[x_1(t)]$, $\mathbb{E}[x_2(t)]$, $\mathbb{E}[x_3(t)]$, and, the standard deviation, $\sigma[x_1(t)]$, $\sigma[x_2(t)]$, $\sigma[x_3(t)]$, of the solution SP of (39) for each one of these values of α parameter. Since standard deviation of each one of the components of the solution has small values, for the sake of clarity, in Figures 7–8, we show separately the results for the means and standard deviations, respectively, in the case $\alpha = 0.5$. Whereas, in the case $\alpha = 0.85$, Figures 9–11 show together the approximations of the mean plus/minus standard deviation, $\mathbb{E}[x_i(t)] \pm \sigma[x_i(t)]$, for each one of the components of the solution, $x_i(t)$, $1 \le i \le 3$. In all the cases we observe that the solution has highly oscillatory behaviour in average with variability increasing significantly as time increases.

4. Conclusions

Recently, a novel technique to solve systems of random differential equations, referred to as adaptive gPC (generalized polynomial chaos), has been developed by the authors, in collaboration with other colleagues, [6]. The application of adaptive gPC is limited to systems whose equations depend polynomially on unknowns and random input parameters. Although polynomial dependence is often found in many applications, specially in epidemiological models, generalizations of adaptive gPC are required to deal with another class of models. In this paper a new version of adaptive gPC has been developed taking advantage of RVT (random variable transformation) technique. Through several illustrative examples it is demonstrated the superiority of the extended adaptive gPC against the version presented in [6]. These examples cover a variety of situations including linear and nonlinear scalar random differential equations and a nonlinear system of random differential equations whose solution is highly oscillatory. In addition, in all these examples uncertainty is assumed to be represented by nonlinear expressions. To validate the numerical approximations obtained for the mean and the standard deviation of the solution by extended adaptive gPC, in the first test examples they are compared with the ones corresponding to their exact results.

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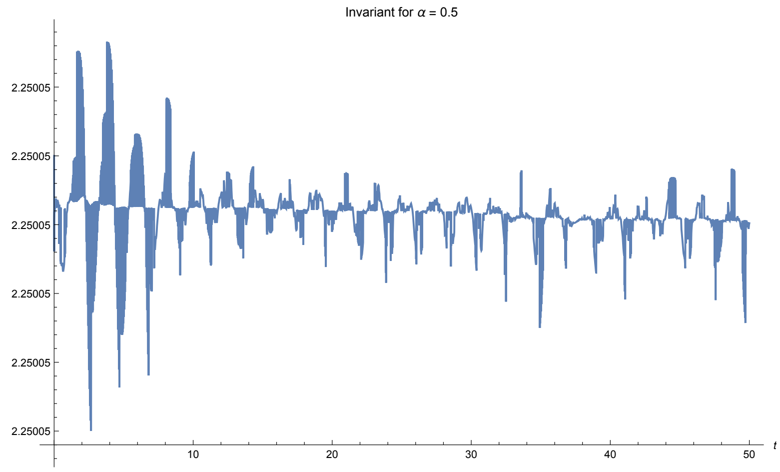
Conflict of Interest Statement

The authors declare that there is no conflict of interests regarding the publication of this article.



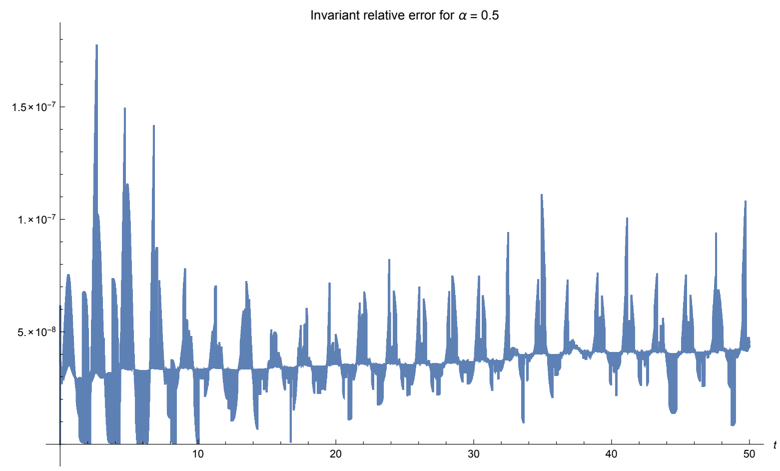
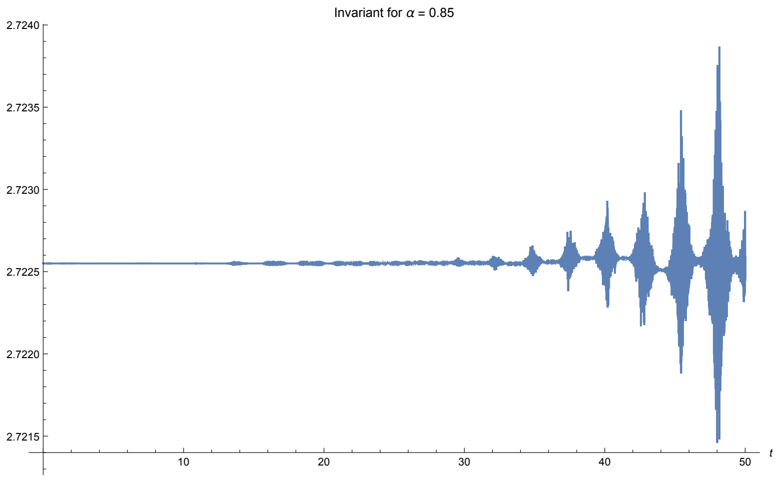


Figure 5: Computation of the invariant $\mathcal{I}_\alpha$ for $\alpha = 0.5$ by extended adaptive gPC (top). Relative error associated to the computation of $\mathcal{I}_{0.5}$ by extended adaptive gPC (bottom). Both have been computed in the time interval $t \in [0, 50]$ in the context of Example 3.



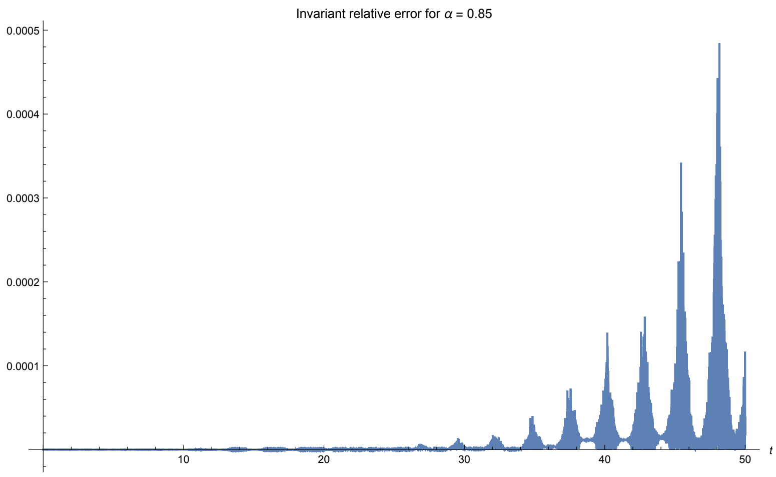


Figure 6: Computation of the invariant $\mathcal{I}_\alpha$ for $\alpha = 0.85$ by extended adaptive gPC (top). Relative error associated to the computation of $\mathcal{I}_{0.85}$ by extended adaptive gPC (bottom). Both have been computed in the time interval $t \in [0, 50]$ in the context of Example 3.

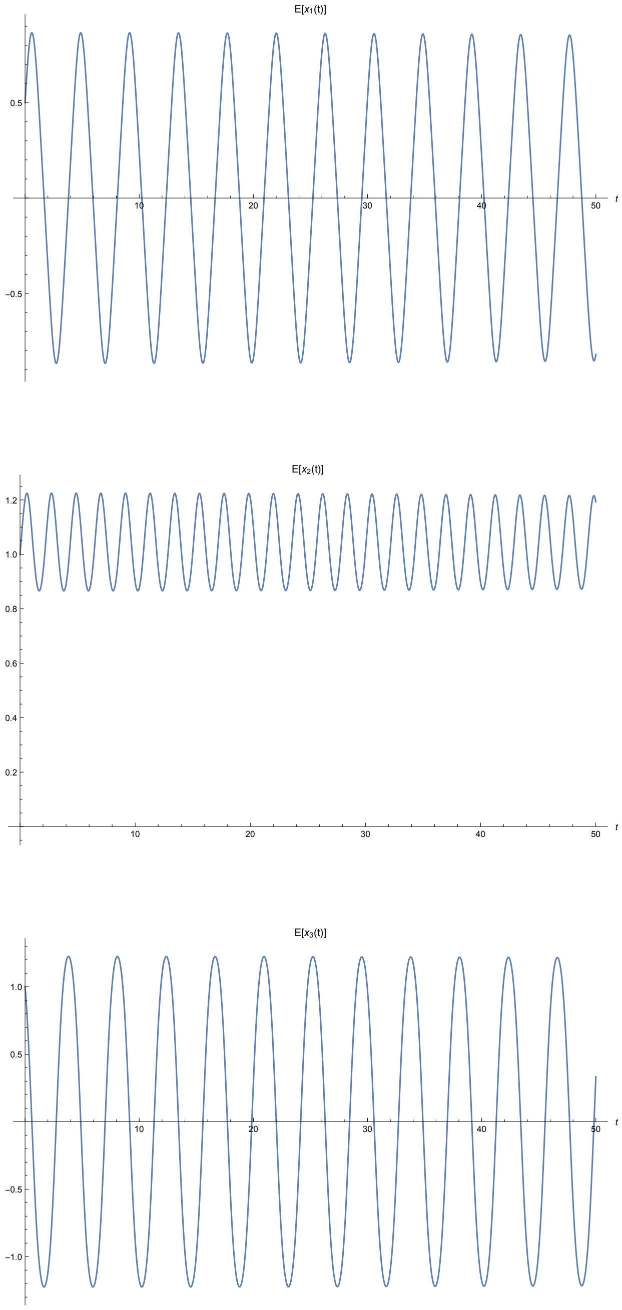


Figure 7: Approximations for the expectation of the solution $(x_1(t), x_2(t), x_3(t))$ of nonlinear system (39) with $\alpha = 0.5$ by extended adaptive gPC on the interval $0 \le t \le 50$ in the Example 3.

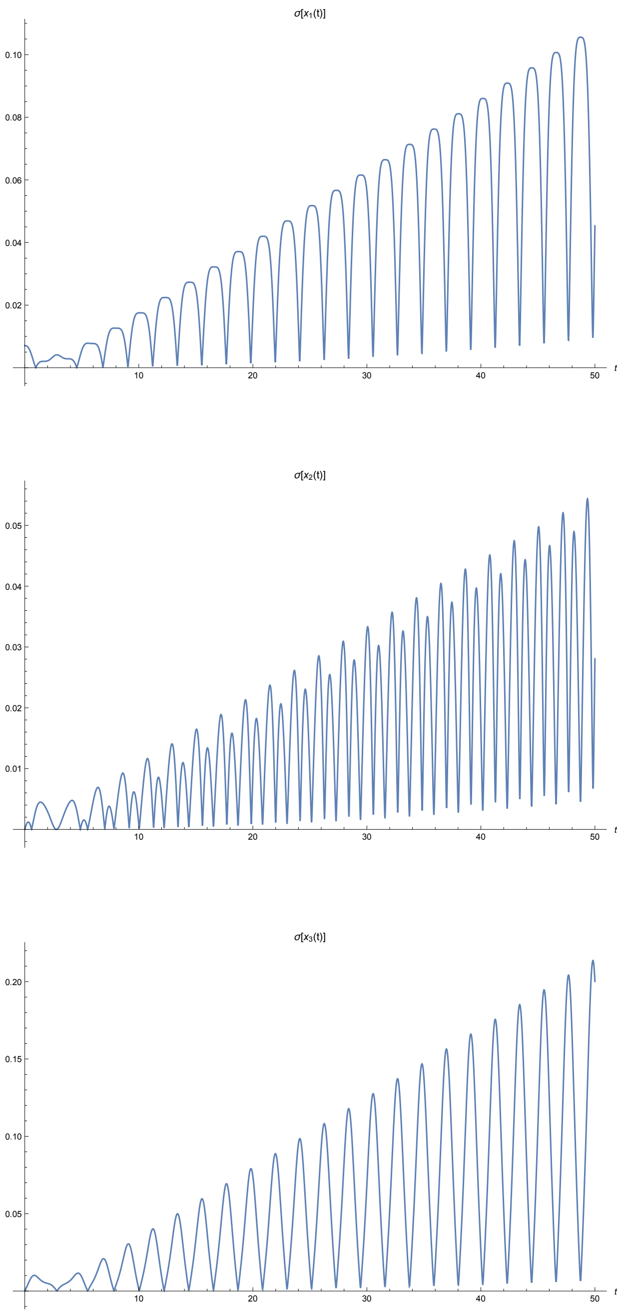


Figure 8: Approximations for the standard deviation of the solution $(x_1(t), x_2(t), x_3(t))$ of nonlinear system (39) with $\alpha = 0.5$ by extended adaptive gPC on the interval $0 \leq t \leq 50$ in the Example 3.

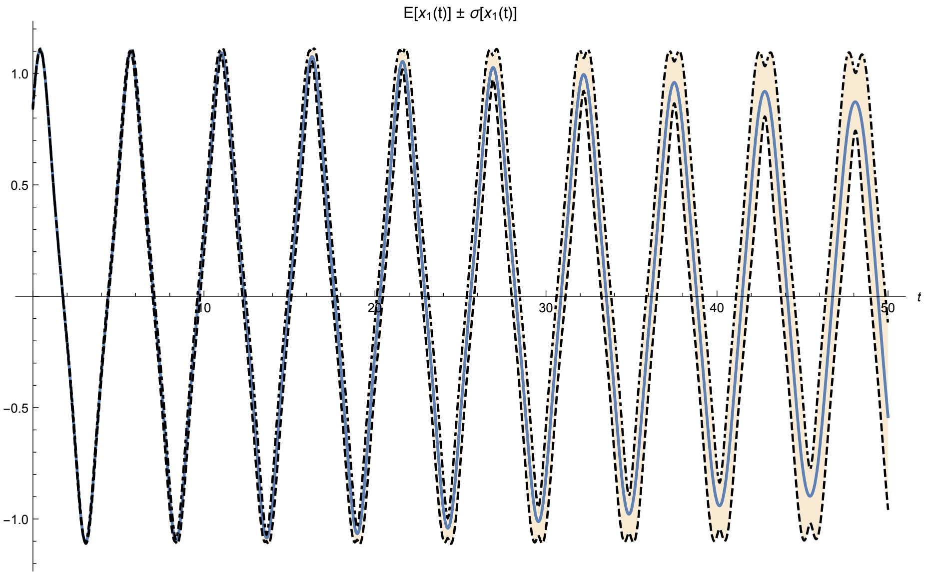


Figure 9: Approximations for the expectation plus/minus standard deviation of the first component $x_1(t)$ of the solution for nonlinear system (39) with $\alpha = 0.85$ by extended adaptive gPC on the interval $0 \leq t \leq 50$ in the Example 3.

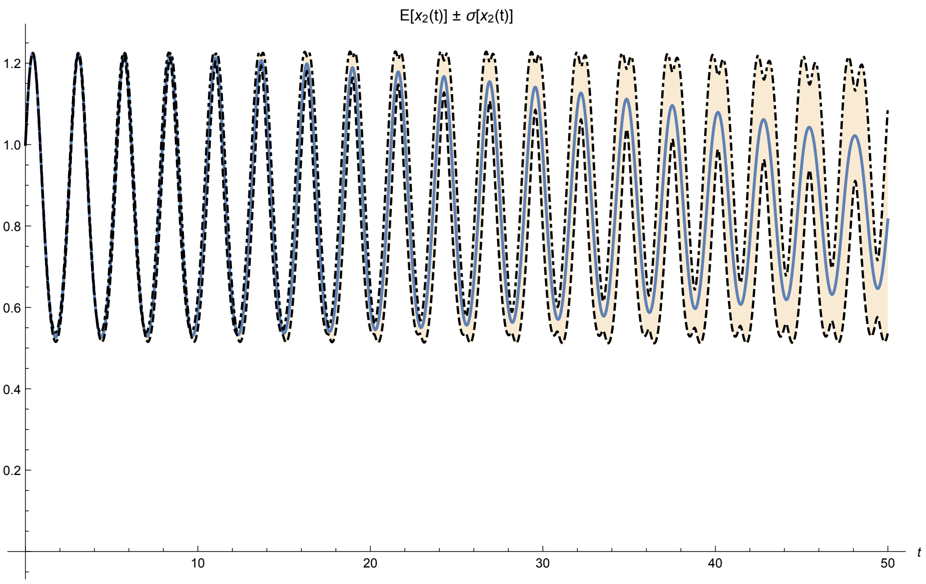


Figure 10: Approximations for the expectation plus/minus standard deviation of the second component $x_2(t)$ of the solution for nonlinear system (39) with $\alpha = 0.85$ by extended adaptive gPC on the interval $0 \leq t \leq 50$ in the Example 3.

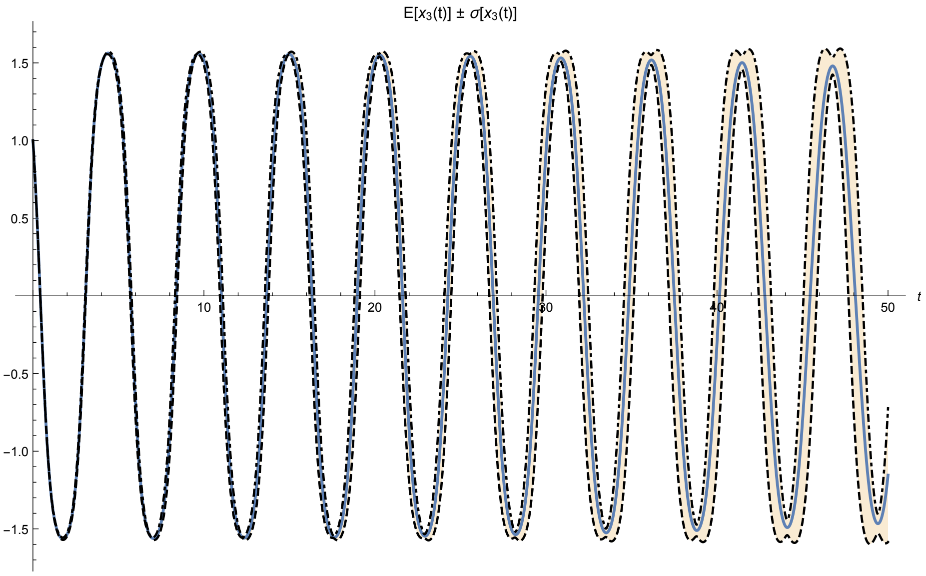


Figure 11: Approximations for the expectation plus/minus standard deviation of the third component $x_3(t)$ of the solution for nonlinear system (39) with $\alpha = 0.85$ by extended adaptive gPC on the interval $0 \leq t \leq 50$ in the Example 3.

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