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A new multi-element non-intrusive method based on agglomerative clustering for bifurcative dynamical systems

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Abstract:

A multi-element non-intrusive generalised polynomial chaos method is developed to approximate state variable of a bifurcative dynamical system. It rely on a partitioning of the stochastic space along discontinuities of any shapes, efficient even when the discontinuities are running partially, and allowing the use of a low degree of approximation. An agglomerative clustering method is implemented in a space defined by the values of the quantity of interest (QOI) and of its derivatives with respect to the stochastic parameters. The stochastic space is first properly sampled. Then, at every instant, several partitions of the stochastic space are tested and the best one is selected as the one minimizing the maximum of the cross-validation errors of the local surrogate models. Once the local models are obtained and the stochastic space is correctly sliced, a neural network classifier is learned to determine in which element a sample is for further evaluations at the considered instant. The method uses the same samples for the space partitioning and for the training of the local models with regression thus reducing the computational cost. The long-time integration problem is countered and the stochastic space can be split according to the discontinuity induced by the potential bifurcation. The results of the method are advantageously compared to those obtained with the direct use of a Gradient Tree Boosting algorithm at every instant and the classical Pseudo projection method for a system leading to a bifurcation.

Key words: Uncertainty Quantification, Multi-Element, Polynomial Chaos, Agglomerative clustering, Machine learning, neural network

1 Introduction

This article aims to present the development of a non intrusive Multi-element g-PC method able to approximate the evolution of a state variable of a dynamical system which will have potential bifurcative behaviours. In our context, the QOI will be a state variable \( x \) of an Ordinary Differential Equation (ODE), depending on \( d \) uncertainties, called the input parameters, and packed in the vector \( \vec{a} \). The method can be easily generalised to ODE systems with many state variables and to Partial Differential Equation systems. In our study, \( x \) follows a stochastic ODE system:

\[
\dot{x}(t, \vec{a}) = f(x, t, \vec{a}) ,
\]
where $f$ is a linear or a non-linear operator and $t$ is the time variable. We assume that the input parameters are independent and follow a classical probability density function (p.d.f.). In that way, $\vec{a}$ is following the p.d.f.:

$$\rho(\vec{a}) = \prod_{i=1}^{d} \rho_i(a_i),$$

(2)

where $\rho_i$ is the p.d.f. of $a_i$.

Classically, the non-intrusive g-PC expansion approximates the stochastic dependence of the state variable at every instant as a sum of orthogonal polynomials, using interpolation [13, 6], pseudo-spectral projection [12, 5], or regression methods [1, 2] to find the chaos coefficients:

$$\tilde{x}(t, \vec{p}) = \sum_{j=1}^{M} c_j(t) \Phi_j^{(d)}(\vec{p}),$$

(3)

$$\Phi_{\alpha}^{(d)}(\vec{p}) = \prod_{i=1}^{d} \Phi_{\alpha_i}^{(1)}(p_i),$$

(4)

$$M = \frac{(n + d)!}{n!d!},$$

(5)

where $n$ is the chosen truncation degree of the series and the $\phi_{\alpha}$ are the chosen multivariate orthogonal polynomials. In our study, we propose to use regression on the multivariate orthogonal polynomials basis being the product of every monovariate polynomials corresponding to the p.d.f. of each input parameters through the Wiener-Askey scheme [14]. $\vec{p}$ is the vector of normalised input parameters where every $p_i$ has the same type of stochastic distribution than its corresponding $a_i$ but varies in an normalised interval contained in the support of the polynomials. As there is a one-to-one mapping between every $a_i$ and its corresponding $p_i$, we will now refer to the vector of input parameters as being $\vec{p}$.

Classically, the non-intrusive method is conducted independently at every considered instants $t_k$ to find the chaos coefficients $c_j(t_k)$. Standard g-PC with a sufficiently high truncation degree is able to accurately approximates any smooth QOI. However, its accuracy is affected by the so-called 'long-integration problem' and by the possible occurrence of discontinuities [11]. The former is the fact that the state variable will have a more and more complicated behaviour as the time goes by. With a standard g-PC model with fixed truncation degree, the surrogate model will then become less and less accurate. Moreover, when we are in presence of discontinuities, occurring when the state variable has a bifurcative behaviour or when the dynamical system is discontinuous itself, the polynomial nature of the chaos series will induce the Gibbs phenomenon, oscillations which will not vanish when the truncation degree is increased.

Multi-element (ME) methods [11, 3, 4, 9] were developed to answer to these issues. ME methods consists on dividing the parameter space $\mathcal{P}$ into $N_E$ non overlapping elements $E_i$ and then train local surrogate models. We have
The global piecewise model is then expressed by

\[
\tilde{x}(t, \vec{p}) = \sum_{i=1}^{N_E} \tilde{x}_i(t, \vec{p}) I_{E_i}(\vec{p}) = \sum_{i=1}^{N_E} \left( \sum_{j=1}^{M_i} c_{ij}(t) \Phi_j^{(d)}(\vec{p}) \right) I_{E_i}(\vec{p}),
\]

with \( M_i \) the number of modes of the local g-PC model \( \tilde{x}_i \). \( I_{E_i}(\vec{p}) \) is the indicator function of the element \( E_i \) satisfying

\[
I_{E_i}(\vec{p}) = \begin{cases} 
1 & \text{if } \vec{p} \in E_i, \\
0 & \text{otherwise}.
\end{cases}
\]

The ME methods differ in the way the \( E_i \) are determined and in the way the coefficients \( c_{ij} \) are obtained at every considered instant. The classical ME-PCM non-intrusive method [3] consists on dividing the parameter space into smaller and smaller hypercubes, and then to use stochastic collocation methods to determine every \( c_{ij}(t_k) \). This division of the space permits to contain the discontinuity in some of the hypercubes and to use lower degree local models to approximate local pieces of the quantity of interest. The long-integration problem is then tackled without increasing the truncation degree of the series, reducing the impact of the ‘curse of dimensionality’ expressed by equation 5. More recent technics [4, 9] permit to split the parameter space into elements following the shape of the discontinuities using edge detector or Bayesian inference. But these methods only takes into account the presence of discontinuities and do not aim to simplify the study of the quantity of interest with lower degrees as before. In this article, we present a new ME non-intrusive g-PC approach, giving an accurate approximation of the state variable when it is continuous and smooth, continuous but more irregular and when it is discontinuous towards the input parameters.

2 Algorithm

The algorithm presented in this article is a generalisation of the non-time dependent method developed in [10], for time dependent state variables. Figure 1 sums up the algorithm.

The stochastic parameter space \( \mathcal{P} \) is first sampled. In our method, we will use a Sobol sequence to have samples covering the parameter space with a low discrepancy. The deterministic dynamical system is then integrated on all of these samples. We now have a set of values of \( x(t, \vec{p}) \) at each considered instants \( t_k \) for each considered training samples \( \vec{p}_i \). The key idea of the algorithm is to use agglomerative clustering on the samples represented in a well-chosen abstract space taking in to account the derivatives
of the state variable at the considered instant towards the input parameters in order to define efficiently the elements $E_i$ of the partition. At each instant, several partitions of the space, containing from $N_{E_{\text{min}}}$ to $N_{E_{\text{max}}}$ elements will be tested and if the most accurate partition leads to local models which are accurate enough, this partition will be kept and we will go to the next time step. To evaluate the accuracy of a partition, we will define the selection error $E$. $E$ is going to be the maximum of the Predicted Sum of Square (PRESS) error of every local models (one by element) of the partition. This error is used in [2] the context of non-intrusive gPC (not in a ME approach). The PRESS error is easily obtained as an analytical expression exists in the context of linear regression [8]. Moreover, for every training of every local models, the optimal truncation degree is selected as the one minimising this PRESS error. The selection error is then the maximum of the cross-validation errors of the local models with optimal degree.

To partition the space at the time step $t_k$, every training samples will be represented by a point of coordinates $(x(t_k, \vec{p}), \partial x/\partial p_1(t_k, \vec{p}), ..., \partial x/\partial p_d(t_k, \vec{p}))$ where the first coordinates is normalised to lie in $[-1, 1]$ and then the other are normalised to lie in $[-1, 1]^d$. In that way, we will need to calculate the derivatives of the QOI towards the input parameters at every instants. To calculate the derivatives at one instant, a linear regression is done for each samples with its closer neighbours. The optimal number of neighbours is chosen as being the one minimising the PRESS error, the tested number of neighbours varying from $N_{\text{neigh}} = 2d$ to $N_{\text{neigh}} = 5d$. Then, once we have the coordinates of the samples in the wanted space, we will use agglomerative clustering to determine the elements $E_i$. Gathering samples in this space will tend to partition the space according to discontinuities (as the value of the state variable at the considered instant is present in the coordinates) and will gather zones with close derivatives (as the values of the partial derivatives are present in the coordinates). Moreover, in order to reduce the chances to have elements which are not composed of one unique piece, the clustering will take into account a connectivity between the samples represented by a point of coordinates $(p_1, ..., p_d)$. The connectivity diagram will be realised by doing a Delaunay diagram between the samples. Once the optimal partition is selected (as the one minimising the selection error), a test is computed. If this error is lower than a given threshold, the partition is accepted. A neural network is then trained to know on which element a sample is and then which local model to use to evaluate the surrogate model on this sample at the instant $t_k$. If the test is not satisfied, we can add more samples to the sequence and update the information matrix, the connectivity diagram and the derivatives calculus in order to try a new set of partitions with more samples. For the next time step, the previous partition is first tested and local models in these elements are trained with the value of the state variable at this time step. If the selection error is below the threshold, we can move on the next time step, and the same neural network will be used for this instant. If the selection error is higher than the threshold, new partitions are tested following the procedure described above.

The input of the neural network classifier corresponding to an instant $t_k$ is a sample we want to know in which element it is located. The output is a set of probabilities that this sample is located in each $E_i$ of the optimal partition of the instant. Misclassifying a sample would lead to high errors as polynomials models are usually highly diverging outside of their training domains. Moreover, in the ‘gap’ zones in between the samples located to the boundaries of the elements, polynomials can also diverge, as this is an unknown zone where there is no training sample. In that way, a caution procedure is developed. If for a given sample, the highest probability to be located in a given element $E_i$ is less than $1 - \theta_p$, $\theta_p \in [0, 1]$, the sample is not going to be evaluated as we are not sure in which element it is or if it lies in the unknown zone. The lower $\theta_p$ will be, the more we will ignore samples, but the more we will reduce chances to lie in a ‘gap’ zone where local models are highly diverging.
3 Application

3.1 Bifurcative system

To show the performances of the method, we test its accuracy on the approximation of the state variable of the following dynamical system

\[ \dot{x}(t) = a(x(t)^2 - b^2), \]  

with \( x(t = 0) = 0 \) and where \( a \) and \( b \) are following uniform distribution respectively in \([-0.5, 0.75]\) and in \([0.5, 1]\).
The dynamical system has 3 equilibria : \( x_e = 0 \) if \( a = 0 \), \( x_e = b \) which is only stable if \( a < 0 \), and \( x_e = -b \) which is only stable if \( a > 0 \). The solution of the system is \( x(t, a, b) = b \tanh(-abt) \). The function is well highlighting the appearance of the discontinuity towards the stochastic parameters \((a, b)\).

At early instants, the surface is smooth. As the time goes by, the function is still continuous but become less and less smooth. When \( t \) tends to infinity, the state is discontinuous towards the input parameters:

\[
x(t \to \infty, a, b) = \begin{cases} 
  b & \text{if } a < 0 \\
  -b & \text{if } a > 0 \\
  0 & \text{if } a = 0 
\end{cases}
\]  

(11)

At early instants, the method will not induce any partition of the space, thus being equivalent to a standard g-PC non intrusive method using regression. At medium instants, we can figure out that the method will determine a minimum of 3 elements : the two side forming hyperplanes and the slope in the middle which become sharper and sharper as the time goes by. When the time will tend to infinity, the method will tend to determine 2 elements, the two side hyperplanes of equation \( x(a, b) = -b \) and \( x(a, b) = b \).

This partition permits to have a physical interpretation of the state variable, describing the development of the bifurcation in addition of constructing an accurate piecewise model. Using the classical ME method [3] would not have been efficient, as it would have split the parameter space into two hyperrectangles according to the hyperplane of equation \( a = 0.75 \), middle of the initial hyperrectangle. The method will then split the parameter space again and again, containing the quasi-discontinuity into thin hyperrectangles after a high number of split. It would finally give an accurate piecewise model, but with an important number of elements compared to our method. Using the edge detection partition method [4] at every instants could have also been possible. When the bifurcation has fully developed the discontinuity, the results obtained with this method and the one developed in this article would give similar results. At medium instants, the edge detector could have interpreted the sharp slope as a discontinuity if the resolution parameter is set to be low. However, in this case, the partition of the space would have been less efficient, only splitting the parameter space into 2 elements according to a hyperplane close to the one of equation \( a = 0 \).

Figure 2 shows the accuracy of the method on the temporal evolution of the mean and of the variance of \( x \). The mean and the variance at every instants were calculated on a set of 1000 randomly chosen samples. The relative error of the considered variable \( m \) (in our case, the mean or the variance of \( x \)) and its approximation (in our case, the mean or the variance of \( \bar{x} \), \( \bar{x} \) being the approximation of \( x \) with the considered method) is defined as

\[
e_{\text{relative}} = \frac{|m - \bar{m}|}{m}.
\]  

(12)

The results of the method (labelled ‘Method’) are compared with the results obtained with the use of the standard \( g - PC \) non-intrusive approach Pseudo-Spectral Projection at every considered instants (labelled ‘PSP’) and with the use of a Gradient Tree Boosting regressor algorithm computed at every instant and tuned by hand (labelled ‘GTB’). At every instant, the coefficient of determination \( R^2 \) of the GTB regressor with the chosen parameters was higher than 99%. The GTB was computed with the scikit-learn toolkit [7]. For ‘PSP’ method, a truncature degree \( n = 15 \) was taken. The collocation points were
taken to correspond to a Gauss-Legendre grid of \((n + 1)^2\) samples. To be fair in the comparison, a Sobol sequence of 256 samples was generated for the training of the models of 'Method' and for the training of 'GTB'. For 'Method', a value of \(\theta = 0.005\) for the selection error threshold was taken and no sample was added. The caution procedure is not added in this application \((\theta_p = 1)\).

The 'PSP' curve is well highlighting the 'long-time integration problem' described above. When the state variable is smooth, the method is very accurate. However, when the state variable becomes less and less smooth, the accuracy highly deteriorates. 'GTB' method gives an accurate approximation, but as 'GTB' gives by definition a step function model, the slopes are approximated in a stepwise fashion, thus impacting the approximation of the variance but not of the mean. In this example, our method is shown to be more efficient than standard g-PC or Gradient-Tree boosting regression. We can see on figure 2, two jumps in the curves. These jumps correspond to new partitions of the parameter space, due to the fact that the selection error (based on cross-validation results of each local models on their training samples) is becoming larger than the threshold \(\theta = 0.005\) at \(t = 15s\) and \(t = 29s\). The number of elements are respectively: \(N_E = 1\) for early instants \((t < 15s)\), \(N_E = 4\) for medium instants \((t \geq 15s\) and \(t < 29s)\) and \(N_E = 5\) for the last instants \((t \geq 29s\) and \(t \leq 50s)\). At early instants, the most accurate model is obtained by doing no partition of the parameter space, as the state variable is very smooth. When the state variable become not smooth enough to satisfy the criterion, the space is split into 4 elements, 2 containing the hyperplanes and 2 approximating the sharp slope (sharper when \(b\) has higher values). When \(t \leq 29s\), the discontinuity is not fully developed yet, but the slope is so sharp that only a few training samples are not located in one of the 2 hyperplanes. The algorithm gathers these samples into 3 elements, thus leading to \(N_E = 5\).

4 Conclusion

The method is shown as producing an accurate piecewise surrogate model to approximate a state variable with a bifurcative behaviour. As the development of the discontinuity is not direct, there are instants where the state variable is continuous but not smooth enough to have an accurate standard g-PC model of low degree. Moreover, as the state variable is not discontinuous yet at these instants, method based on edge detection or bayesian inference are not well adapted. The method presented in this article is able to approximate the state variable at every instants, as the classical ME method \([3]\), but with an efficient splitting of the parameter space, following the same kind of logic as in \([4, 9]\). It has only been tested on a system containing a simple bifurcation in low dimension but it will be tested on a larger set of applications in a further work. It is worthy to note that the addition procedure of the method could be ameliorated. Indeed, as shown in \([3]\), the value of the previous piecewise model could be used on the new samples instead of integrating the system on the new samples in order to reduce computational cost. Moreover, a more efficient procedure could be to add more samples in the elements having a high cross-validation error, where the information is needed and not to only add samples uniformly with the Sobol sequence.
Figure 2 – Comparison of the three methods by approximating the accuracy of the statistic moments of $x$. The number of samples $N_{samples} = 256$ is the same for the three methods and the same sampling is used for the training of the GTB model and for the piecewise model of the method developed in this article. (a) Temporal evolution of the mean. (b) Relative error on the mean. (c) Temporal evolution of the variance. (d) Relative error on the variance.
Références


