Collocation Least-squares Polynomial Chaos Method

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Abstract

The polynomial chaos (PC) method has been used in many engineering applications to replace the traditional Monte Carlo (MC) approach for uncertainty quantification (UQ) due to its better convergence properties. Many researchers seek to further improve the efficiency of PC, especially in higher dimensional space with more uncertainties. The intrusive PC Galerkin approach requires the modification of the deterministic system, which leads to a stochastic system with a much bigger size. The non-intrusive collocation approach imposes the system to be satisfied at a set of collocation points to form and solve the linear system equations. Compared with the intrusive approach, the collocation method is easy to implement, however, choosing an optimal set of the collocation points is still an open problem. In this paper, we first propose using the low-discrepancy Hammersley/Halton dataset and Smolyak datasets as the collocation points, then propose a least-squares (LS) collocation approach to use more collocation points than the required minimum to solve for the system coefficients. We prove that the PC coefficients computed with the collocation LS approach converges to the optimal coefficients. The numerical tests on a simple 2-dimensional problem show that PC collocation LS results using the Hammersley/Halton points approach to optimal result.

1. INTRODUCTION

Scientific computing involves computer simulations to imitate physical and/or chemical phenomena. The purpose is not only gain a better understanding of the nature, but also make predictions with the model. Because of the imperfect human understanding towards nature, uncertainties need to be included in the model. In recent years, uncertainty quantification (UQ) research has attracted lots of attention. The traditional Monte Carlo (MC) [1] sampling technique was popular due to its conceptual simplicity and ease of implementation. However, since its convergence is slow ($1/\sqrt{n}$), it is not an optimal choice for large scale simulations that require long CPU runtime. The polynomial chaos (PC) method uses a spectral approximation to represent uncertainties in the system. The concept originates from Wiener's homogeneous chaos [2], and was further developed by Ghanem and co-workers [3]. Karniadakis and Xiu [4] generalized and expanded the PC method by including the orthogonal polynomial basis from the Askey-scheme class. This expansion provides more flexibility for PC to model non-Gaussian uncertainties. So far, PC has been applied successfully in many engineering applications. It works best for a small number of uncertainties with large degree of uncertainty.

Most of the PC implementations use the Galerkin approach where the original deterministic system needs to be modified. For large scale models, the modification work is both complicated and time consuming. The non-intrusive collocation idea was initially introduced as the Stochastic Response Surface Method (SRSM) [5] and the Deterministic Equivalent Modeling Method (DEMM) [6] that impose systems to be satisfied at a given set of points by treating the system as a blackbox. Both the collocation PC [7] and the Non-Intrusive Polynomial Chaos (NIPC) method [8] use the same number of random collocation points as the number of the PC coefficients. In this paper, we first explore the low discrepancy dataset as the collocation points, then propose a collocation least-squares (LS) approach that uses more collocation points than the number of the PC coefficients. The paper is organized as follows: the PC collocation approach and the low-discrepancy datasets are introduced in section 2. The collocation LS approach is introduced, and theoretical support is provided in section 3. The numerical test results are presented in Section 4. Conclusions are drawn in section 5.

2. PC COLLOCATION APPROACH

A general second-order random process $X(\theta) \in L_2(\Omega, \mathcal{F}, P)$ can be represented as:

$$X(\theta) = \sum_{i=0}^{\infty} c^i \Phi^i(\xi(\theta)),$$

where θ is a random event, and $\Phi^i(\xi(\theta))$ are polynomial functionals defined in terms of the multi-dimensional random

variable $\xi(\theta) = (\xi_1(\theta), \ldots, \xi_n(\theta))$ with the joint probability density function $w(\xi)$. The family $\{\Phi^i\}$ satisfies the orthogonality relations:

$$\langle \Phi^i, \Phi^j \rangle = 0 \quad \text{for} \quad i \neq j,$$

where the inner product on the Hilbert space of random functionals is the ensemble average $\langle \cdot, \cdot \rangle$:

$$\langle f, g \rangle = \int f(\xi)\, g(\xi)\, w(\xi) d\xi.$$

If the uncertainties in the model are independent random variables $\xi = (\xi_1, \cdots, \xi_n)$ with a joint probability distribution $w(\xi) = w^{(1)}(\xi_1) \cdots w^{(n)}(\xi_n)$, then a multi-dimensional orthogonal basis is constructed from the tensor products of one-dimensional polynomials $\{P_m^{(k)}\}_{m \geq 0}$ orthogonal with respect to the density $w^{(k)}$ [7]:

$$\Phi^i(\xi_1, \cdots \xi_n) = P_{i_1}^{(1)}(\xi_1) P_{i_2}^{(2)}(\xi_2) \cdots P_{i_n}^{(n)}(\xi_n).$$

In this case, the evaluation of n-dimensional scalar products is reduced to n independent one-dimensional scalar products. In practice, a truncated PC expansion with S terms is used [3]. Denote the number of random variables by n, and the maximum degree of the polynomials by p, S is given by (1):

$$S = \frac{(n+p)!}{(n!\, p!)}. \tag{1}$$

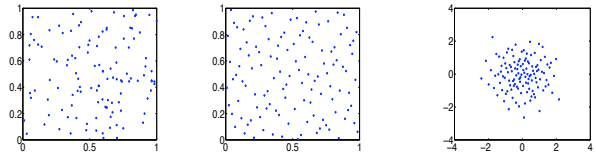
With the growth of the polynomial order and the number of random variables, the total number of terms in the expansion increases rapidly. Using PC expansion, the original deterministic system is replaced by a stochastic system for the PC coefficients, and the uncertainty information is embedded in these coefficients.

In order to solve for these coefficients, one can use the Galerkin approach to project the system on the space spanned by the orthogonal polynomials. Another approach is to impose the expanded system to be satisfied at a set of points, hence the collocation approach [9]. The collocation approach treats the system as a blackbox. The only requirement for the choices of the collocation points is that the system matrix is well-conditioned. This requirement leads to the conventional choice of random collocation points [8, 10]. Although it is convenient to use the random collocation points, an accurate and consistent solution generated by the randomly chosen collocation points is not guaranteed for each run. Moreover, the alignment or clustering of the data points sometimes cause the rank deficiency for the system matrix. In this paper, we consider the low-discrepancy dataset-Hammersley/Halton dataset.

The low discrepancy sequences [11] have been explored in the area of the quasi-Monte Carlo integration with large number of variables. The commonly used datasets include Hammersley points [12], Halton points [13] and Sobol points [14]. The Hammersley and Halton points are closely related, sometimes they are referred to as the Hammersley/Halton points. Halton dataset has a hierarchical structure and is useful for incremental hierarchical data sampling. Comparisons of these datasets were made in [15] for numerical integration purposes.

In general, for the same sample size, HSS sample is more representative of the random distribution than the random generated samples. In the case of a different distribution, such as the Gaussian distribution, the points are more clustered to represent the PDF of the associated random variable. Figure 1 (a) and 1 (b) show the comparison of the random points and the uniformly distributed Hammersley points. The Hammersley points for Gaussian distribution is shown in Figure 1 (c).

Figure 1. Comparison of random points, uniform Hammersley points and Gaussian Hammersley points.



(a) Random pts (b) Unif. Hamm. (c) Gaussian Hamm.

Another dataset we are interested is the Smolyak dataset which is generated from the high order interpolation context where Lagrange interpolation basis is used [16]: The optimal choice for 1-dimensional interpolation uses the Chebyshev points. In higher dimensions, however, the full tensor product becomes infeasible, since the number of interpolation points grows exponentially fast with the increase in the number of dimensions. This is the so-called "curse of dimensionality".

The Smolyak algorithm [17] is designed to handle the "curse of dimensionality". Instead of using a full tensor product for multi-dimensional interpolation, the algorithm chooses the representative polynomials from the lower dimensions to form the higher-order interpolation polynomial.

There are two implementations of the Smolyak algorithm. One uses the Chebyshev points in 1-dimension, which generates the Clenshaw-Curtis formula. The other option uses Gaussian points (zeros of the orthogonal polynomials with respect to a weight ρ), which leads to the Gaussian formula. The optimality of these constructions over the traditional tensor product is discussed in [18].

Using the Smolyak algorithm, a polynomial interpolation of a d-dimensional function is given by a linear combination of the tensor product polynomials:

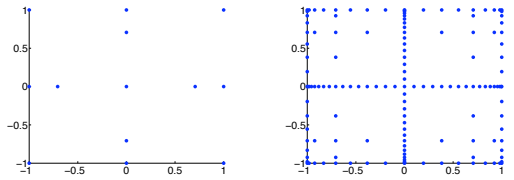
$$\mathcal{I}(f) \equiv A(q,d) = \sum_{q-d+1 \le |i| \le q} (-1)^{q-|i|_1} \binom{d-1}{q-|i|} \cdot (\mathcal{U}^{i_1} \otimes \cdots \otimes \mathcal{U}^{i_d}),$$

in which d is the number of dimensions, q is the order of the algorithm, and $q-d$ is called the level of interpolation.

The nested data set guarantees that the higher degree polynomials reproduce all polynomials of the lower degrees.

Figure 2 illustrates the 2-dimensional Clenshaw-Curtis sparse grids for level 2 and level 5 constructions.

Figure 2. 2-D Smolyak points.



(a) level 2 (13 points) (b) level 5 (145 points)

The Smolyak sparse grids can be used in both the PC collocation method as the collocation dataset, and in the high-order interpolation approaches. However, there are disadvantages of using the Smolyak sparse grids as the collocation points for PC collocation. First, the number of points is restricted by the algorithm, as can be seen in Table 1; second, in higher dimensions, the alignment of the data points causes rank deficient of the system matrix easily. In this case, data points constructed at a higher level should be used.

Table 1. Number of 2D Smolyak points for different construction levels.

level	No. of Smolyak points
1	5
2	13
3	29

3. COLLOCATION LEAST-SQUARES METHOD

In the PC collocation approach, typically, one requires $Q = S$ collocation points in order to solve for S unknowns. Here we explore the setting where $Q > S$, hence the least-squares (LS) problem. In the following we show that PC LS collocation solution converges to the theoretical LS solution for a large number of collocation points.

Consider a function $f \in \mathbb{L}^2(\Omega)$. We seek to approximate f by another function p in a finite dimensional subspace $\mathbb{P}$ of $\mathbb{L}^2(\Omega)$. Let $\Phi_1, \ldots, \Phi_S$ be a basis of this subspace. The LS solution finds $p \in \mathbb{P}$ to minimize:

$$\min_{p\in\mathbb{P}} \int_\Omega \Big[f(\xi) - p(\xi)\Big]^2 \mathbf{w}(\xi) d\xi = \int_\Omega \Big(f(\xi) - \sum_{i=0}^{S-1} a_i \Phi_i(\xi)\Big)^2 \mathbf{w}(\xi) d\xi \qquad (2)$$

Specifically, let $p(\xi) = \sum_{i=0}^{S-1} a_i \Phi_i(\xi)$. The optimal LS coefficients can be calculated by taking the derivative of the error function with respect to the coefficients a_i and setting them to zero (3):

$$\begin{aligned} \frac{d}{da_i} = 0 \quad &\Longrightarrow \quad \sum_{m=0}^{S-1} a_m \Theta_{im} = \gamma_i, \\ \text{where } \Theta_{im} = \mathbb{I},\ \gamma_i \quad &= \quad \int_\Omega f(\xi)\Phi_i(\xi)\mathbf{w}(\xi)d\xi \\ \Longrightarrow a_i \quad &= \quad \int_\Omega f(\xi)\Phi_i(\xi)\mathbf{w}(\xi)d\xi \end{aligned} \qquad (3)$$

For a numerical approach, we approximate the integral in (2) by MC formula at Q points $\xi^j \in \Omega$ ($j = 1, \ldots, Q$):

$$\int_\Omega (f(\xi) - p(\xi))^2 \mathbf{w}(\xi) d\xi \approx \frac{1}{Q} \sum_{j=1}^{Q} \Big[\Big(f(\xi^j) - \sum_{i=0}^{S-1} a_i \Phi_i(\xi^j) \Big)^2 \mathbf{w}(\xi^j) \Big] \qquad (4)$$

The minimum of (2) is replaced by the minimum of (4). In order to find the optimal values of a_i, we take the derivatives with respect to a_i and set them to zero to obtain:

$$\begin{aligned} \sum_{m=0}^{S-1} \widehat{a_m}\widehat{\Theta_{im}} \quad &= \quad \widehat{\gamma_i}, \quad \text{where} \\ \widehat{\Theta_{im}} \quad &= \quad \sum_{j=1}^{Q} \Phi_m(\xi^j)\Phi_i(\xi^j)\mathbf{w}(\xi^j), \\ \widehat{\gamma_i} \quad &= \quad \sum_{j=1}^{Q} f(\xi^j)\Phi_i(\xi^j)\mathbf{w}(\xi^j). \end{aligned} \qquad (5)$$

Define the collocation matrix:

$$\tilde{A}_{ji} = \tilde{\Phi}_i(\xi^j) = \Phi_i(\xi^j)\sqrt{\mathbf{w}(\xi^j)} \quad i = 0, \ldots S-1, \quad j = 1, \ldots Q,$$

and $\tilde{f}(\xi^j) = f(\xi^j)\sqrt{\mathbf{w}(\xi^j)}$, we have:

$$\widehat{\Theta_{im}} = \big(\tilde{A}^T\tilde{A}\big)_{im} \quad \text{and} \quad \widehat{\gamma_i} = (\tilde{A}^T \cdot \tilde{f})_i.$$

The relation (5) finds the coefficients a_i by solving the linear system:

$$\tilde{A}^T \tilde{A} \cdot \hat{a} = \tilde{A}^T \cdot \tilde{f}.$$

Numerically, $\hat{a}$ is obtained by solving the system $\tilde{A} \cdot \hat{a} = \tilde{f}$. In LS sense, $\tilde{A}$ will be a Q-by-S matrix, with $Q > S$.

In (5), the left-hand-side involves the MC approximation for $\langle \Phi_m, \Phi_i \rangle$, which contains the approximation error ε_{mi}. The right-hand-side involves the MC approximation for $\langle f, \Phi_i \rangle$, which contains the approximation error δ_i. So the numerical LS solution $\hat{a}_i$ for:

$$\underbrace{(\Theta + \varepsilon)}_{\hat{\Theta}} \cdot \hat{a} = \underbrace{(\gamma + \delta)}_{\hat{\gamma}}$$

is bounded by the following (note that $\Theta = \mathbb{I}$, the identity matrix):

$$\frac{||a - \hat{a}||}{||a||} \leq cond(\Theta) \left[\frac{||\varepsilon||}{||\Theta||} + \frac{||\delta||}{||\gamma||} \right] = ||\varepsilon|| + \frac{||\delta||}{||\gamma||}.$$

With the increasing of Q, the MC ensemble numbers, the numerical integration errors $\frac{||\varepsilon||}{||\Theta||}$ and $\frac{||\delta||}{||\gamma||} \to 0$, therefore, $\hat{a} \to a$.

4. NUMERICAL RESULTS

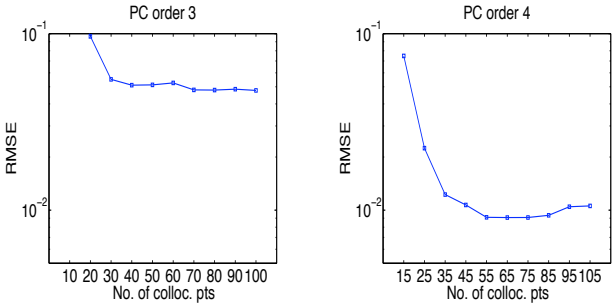
To illustrate the collocation LS approach, consider a simple 2-dimensional nonlinear function of the random variable ξ_1 and ξ_2 (6):

$$f = \cos(\xi_1 + \xi_2) \times e^{\xi_1 \xi_2}, \qquad \xi_1, \xi_2 \in [0, 1]. \tag{6}$$

For the PC collocation approach: first, the system states x and y are expanded using order 3 Legendre basis, which results 10 unknown system coefficients. The PC collocation approach is applied to solve for these unknown coefficients. We tested Halton datasets that contain $10, 20, \ldots, 100$ points. The hierarchical Halton dataset has a feature that the smaller number of the dataset is a subset of the larger number dataset. The RMSE is shown in Figures 3 (a) and 3 (b) for PC order 3 and 4 respectively. From the graph, we observe that the best possible number of the collocation points is around 30-40 for order 3 and 45-55 for order 4. The numerical example shows that the collocation LS method converges to the true solution with the increasing of the collocation points. The slight increases of the last three test cases in 3 (b) are caused by the numerical errors. The figures also show that the RMSE decreases with the PC order increase. We find that the optimal number of collocation points should be about 3-4 times of the PC modes S.

Lagrange interpolation at the Smolyak points is implemented for the 2-dimensional test function (6). We build

Figure 3. The RMSE decreases with the increase of the number of collocation points for both PC order 3 and 4.

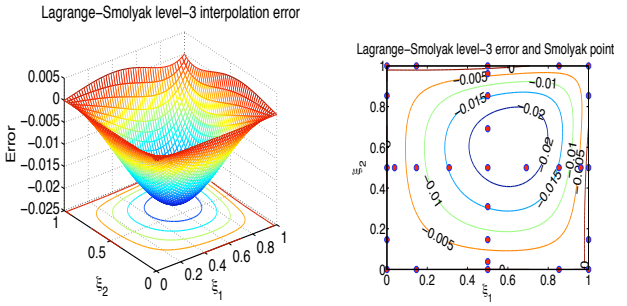


(a) PC-3 Colloc. test (b) PC-4 Colloc. test

level-2 and level-3 interpolation, which requires 13 and 29 Smolyak points, respectively.

The Lagrange interpolation error plots and contour plots for Smolyak level-3 (29 points) are shown in Figure 4 (a) and (b), respectively.

Figure 4. Lagrange-Smolyak interpolation level-3 error and Contour plot.

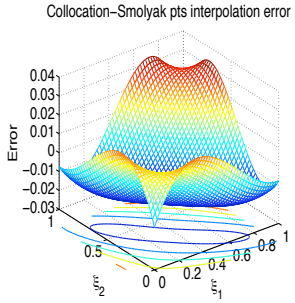


(a) Lag. err. (b) Err. contour and lv3 pts

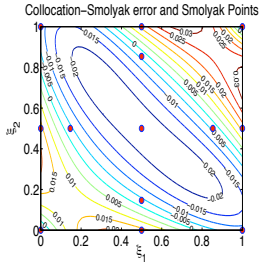
The PC order 3 collocation LS approach with different sets of collocation points are displayed in Figure 5. The optimal coefficients are computed by analytically taking the derivative with respect to the coefficients, setting them to zero and solving for them. Comparing Figure 5 (a), (c) with (e), the PC collocation LS approach generates similar results for both Smolyak and Hammersly/Halton collocation datasets. However, the error contour plot using the Hammersley dataset resembles the optimal coefficients result, as can be seen from 5 (d) and (e).

Detailed information is listed in Table 2. As can be seen from the table, when we increase the number of collocation points from 13 to 29 for both Hammersley dataset and the Smolyak dataset, the RMSE error decreases. The last 2 rows in the table show the high-order Lagrange interpolation RMSE error. Although the Lagrange interpolation is a minimax approach (implemented under the assumption that the maximum error is minimized), and we can reduce the RMSE error by building a higher level interpolation, the implemen-

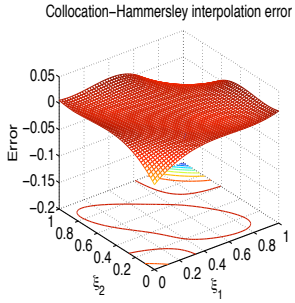
Figure 5. PC order 3 collocation error with different collocation data sets.



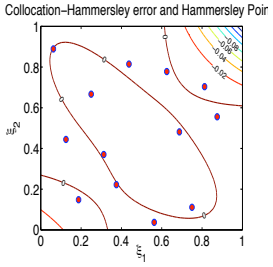
(a) Colloc. err. (Smolyak level 2 (13 pts))



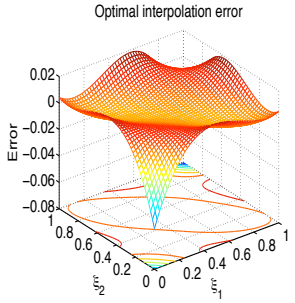
(b) Err. contour and Smo. pts



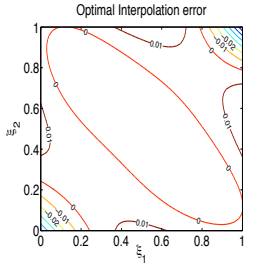
(c) Colloc. err. (Hammersley (13 pts))



(d) Err contour and Hamm. pts



(e) Opt. PC-3 err.



(f) Opt. PC-3 err. contour

tation is not trivial. The collocation results are better approximation to the optimal result since the collocation approach minimize the overall error.

Next we assess the robustness of these approaches when numerical noises are present in function values, which is always the case for large-scale models. We introduce 2% of random normal noise for both the Lagrange and PC collcoation cases. The RMSE and the maximum absolute errors are displayed in Table 3.

From the error data, we see that the collocation method with the Smolyak dataset is less sensitive than the Lagrange interpolation method, and has a smaller error. Another fact to notice when comparing the collocation and Lagrange interpolation method is that building the high level Lagrange interpolation with Smolyak algorithm is very tedious, which also involves the function evaluation. However, for PC collocation method, the basis can be built beforehand and used later on. In a case where the function is not smooth, the PC collocation method has more advantages than the Lagrange interpolation.

Table 2. RMSE and maximum absolute error comparison for PC collocation method with Hammersley points, Smolyak points, and optimal interpolation for PC order 3. Lagrange interpolation with Smolyak points results are also listed.

	RMSE	Max abs. err.
PC-3 - Hamm. 13 pts	1.11×10^{-1}	1.58×10^{-1}
PC-3 - Smo. 13 pts	1.11×10^{-1}	3.27×10^{-2}
PC-3 - optimum	5.69×10^{-2}	6.84×10^{-2}
PC-3 - Hamm. 29 pts	7.11×10^{-2}	8.05×10^{-2}
PC-3 - Smo. 29 pts	8.27×10^{-2}	2.71×10^{-2}
Lag.- Smo.(lv2-13 pts)	9.28×10^{-1}	2.28×10^{-1}
Lag.- Smo.(lv3-29 pts)	8.49×10^{-2}	2.43×10^{-2}

Table 3. With 2 % random normal noise added, RMSE and maximum absolute error comparison for Lagrange interpolation with Smolyak points, PC collocation method with Smolyak points for PC order 4 expansion.

	RMSE	Max abs. err.
Lag.- Smo.(lv3-29 pts)	3.38×10^{-1}	1.11×10^{-1}
PC col. (4) -Smo. 29 pts	1.19×10^{-1}	5.25×10^{-2}

5. CONCLUSIONS

We propose a collocation LS approach with the Hammersley/Halton dataset as collocation points. We show that this method converges to the optimal LS solution. Numerical tests show that the high order interpolation using Langrange with Smolyak points has similar accuracy as the PC approach, but the collocation LS approach is more flexible, and the collocation sets are easier to generate. We expect to implement the collocation LS approach to large scale real model simulation in the future for UQ purpose.

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