On Spectral Approximations with Nonstandard Weight Functions and Their Implementations to Generalized Chaos Expansions

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Received: 27 July 2017 / Revised: 29 January 2019 / Accepted: 30 January 2019 / Published online: 12 February 2019
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Abstract
In this manuscript, we analyze the expansions of functions in orthogonal polynomials associated with a general weight function in a multidimensional setting. Such orthogonal polynomials can be obtained, e.g., by Gram–Schmidt orthogonalization. However, in most cases, they are not eigenfunctions of some singular Sturm–Liouville problem, as is the case for known polynomials, such as the Jacobi polynomials. Therefore, the standard convergence theorems do not apply. Furthermore, since in general multidimensional cases the weight functions are not a tensor product of one-dimensional functions, the orthogonal polynomials are not a product of one-dimensional orthogonal polynomials, as well. This work provides a way of estimating the convergence rate using a comparison lemma. We also present a spectrally convergent, multidimensional, integration method. Numerical examples demonstrate the efficacy of the proposed method. We also show that the use of non-standard weight functions can allow for efficient integration of singular functions. We demonstrate the use of this method to uncertainty quantification problem using Generalized Polynomial Chaos Expansions in the case of dependent random variables, as well.

Keywords GPC · Generalized chaos expansions · Spectral methods · Orthogonal polynomials · Integration methods · Collocation methods

1 Introduction
Orthogonal polynomials play a key role in approximation theory in weighted-\(L^2\) spaces. Given a set \(\Omega \subseteq \mathbb{R}^d\) and a weight function \(w : \Omega \rightarrow [0, \infty)\), one can define a weighted-\(L^2\) space, \(L^2_w(\Omega)\), with an inner product induced by this weight function

\[
\langle f, g \rangle_w := \int_{\Omega} f(z)g(z)w(z)dz
\]
In order to approximate a function $f \in L^2_w(\Omega)$, one can represent it as a series of polynomials that are orthogonal with respect to $\langle f, g \rangle_w$. The required approximation is obtained by truncating the series.

In the case where the weight function is classical (such as the constant or Gaussian weight functions) one can associate with the weight function a family of classical polynomials. For example, the orthogonal polynomials which are associated with the constant or Gaussian weight functions are the Legendre and Hermite polynomials, respectively. Moreover, these families of polynomials are eigenfunctions of known singular Sturm–Liouville problems. As a result, important properties such as the rate of convergence can be proved using the corresponding Sturm–Liouville operator. Moreover, it can be shown that the rate of convergence of such approximations depends on the smoothness of the approximated function. For more details see e.g. [1,5,7,15,18]. As a result of these properties, classical orthogonal polynomials have been proven to be a valuable tool in approximation theory and numerical analysis. An important application of such spectral approximations appears in the field of uncertainty quantification (UQ). This application motivated the current work and is described in the following discussion. However, we note that all the results described in this manuscript relate to questions in spectral approximations in general and are not limited to UQ.

Consider the PDE:

$$u_t(x, t, Z) = \mathcal{L}(u), \quad x \in \Sigma, \ t \in [0, T), \ Z \in \Omega \subset \mathbb{R}^d$$

$$\mathcal{B}(u) = 0, \quad x \in \partial \Sigma, \ t \in [0, T), \ Z \in \Omega \subset \mathbb{R}^d$$

$$u(t = 0) = u_0$$

(2)

where $Z = (z_1, \ldots, z_d)$ are random variables. A simple example of such a situation is the location of the transition layer in the solutions of Burgers equation, where the random variables are a perturbation in the boundary value. Another example is the heat equation in a domain whose properties are not exactly known. This problem can be modeled by a heat conduction coefficient which depends on random variables. In this case, the problem is to find the temperature or heat flux, at a given point, or the whole boundary. Equation (2) is a formulation of uncertainty quantification problems which arise in many applications in science and engineering, See e.g. [6,10,19,19–24].

Several methods were developed to analyze these problems, among which are Monte Carlo and Sampling-Based Methods, Perturbation Methods, Moment Equations and Generalized Polynomial Chaos. In the GPC method the solution to (2), $u(x, t, Z)$, which is an unknown random variable is expressed as a function of the random variables $Z$, whose distributions are known. Thus, $u(x, t, Z)$ can be expanded in orthogonal polynomials in $Z$. If $u(x, t, Z)$ is smoothly dependent on $Z$, and $d$ is small, typically less than six, the GPC expansion is highly efficient due to a spectral rate of convergence, see e.g. [20]. The standard assumption is that the random variables are mutually independent, see e.g. [20]. More generally, the classical GPC theory in the multi-dimensional setting relies on the fact that the multivariate weight function can be decomposed into a product of one-dimensional weight functions

$$w(Z) = \prod_{j=1}^{d} w_j(z_j)$$
As a result, the integral of an integrable function \( f : \Omega \rightarrow \mathbb{R} \) can be calculated by applying Fubini’s theorem
\[
\int_{\Omega} f(Z)w(Z)dZ = \int w_1(z_1) \int w_2(z_2) \ldots \int w_d(z_d) f(Z)dz_d \ldots dz_1.
\]

For each inner product
\[
(u, v)_{w_j} = \int u(z_j)v(z_j)dz_j
\]
a set of one-dimensional orthogonal polynomials can be associated and the basis for the expansion in the whole \( \Omega \) is a tensor product of these one-dimensional polynomials. Important properties, such as the rate of convergence and cubature integration formulas, are governed by the properties of the 1-D expansions.

This assumption makes the expansion and its analysis much simpler as the polynomial basis is a tensor product of one-dimensional orthogonal polynomials. There are situations, however, in which the random variables are not independent. In such cases, the decomposition of the multivariate weight function can not be carried out. An example of such a situation is temperature and relative humidity. As the temperature changes the relative humidity changes as well. Drying processes are strongly dependent on both the temperature and the relative humidity, see [11].

There are two common approaches to address the dependence problem. The first one is to transform the problem into an independent variables problem using, for example, the Rosenblatt transformation, [14]. This transformation, however, may be ill-conditioned. The second approach is to consider the problem in an epistemic uncertainty framework, see e.g. [2,8,9]. Since the exact distributions are not used in this approach, the convergence rate may be slow.

In the case of dependent variables, \( w(Z) \) is indeed a genuine \( d \) dimensional function which cannot be decomposed into a product of one-dimensional functions. Though a set of orthogonal polynomials is defined on \( \Omega_Z \) and they can be found, e.g. using the Gram–Schmidt process, the convergence rate is not easily obtained by integration by parts (as in the classical one dimensional case) and requires additional assumptions regarding the properties of the weight function, see e.g. [25].

Even in the 1-D case, it can be difficult to evaluate the rate of convergence for a general weight function when there is no singular Sturm–Liouville problem associated with it.

**Remark** As we’ve mentioned before, these are questions in spectral approximations and are not limited to GPC expansions.

In this paper, we analyze the expansion of functions in the set of orthogonal polynomials associated with \( w(Z) \) in \( \Omega \). We evaluate the convergence rate using a comparison to a known distribution. We also propose a heuristic way to derive cubature integration formulas. The paper is constructed as follows: in Sect. 2 we analyze the convergence rate of the orthogonal polynomial expansion. We present a Lemma which enables to determine the convergence rate by comparing it to an expansion with a known convergence rate. In Sect. 3 we present a spectrally accurate integration method in multidimensional domains. In Sect. 4 we present the implementation of the proposed method in a GPC setting. Concluding remarks are presented in Sect. 5.
2 Convergence Rate

Let

\[ f(Z) = \sum_{|v|=0}^{\infty} \hat{f}(v) P_v(Z) \]  

(3)

where \( v = (v_1, \ldots, v_d) \), \( v_j \geq 0 \) is a multi-index and \( \{P_v(Z)\}_{|v|=0}^{\infty} \) is a set of orthonormal polynomials. In the context of uncertainty quantification, presented above, \( Z = (z_1, \ldots, z_d)^T \) is a vector of random variables. The same question, however, holds for approximation problems in which \( Z = (z_1, \ldots, z_d)^T \in \Omega \subset \mathbb{R}^d \).

The question is how fast \( \hat{f}(v) \to 0 \) as \( |v| \to \infty \). For the 1-D classical polynomials, such as Jacobi polynomials, there is an underlying singular Sturm–Liouville problem, and the “spectral convergence” (i.e an exponential decay of the coefficients) results from it. In the multidimensional case or in the case of non-standard weight functions, there is no similar theory, see e.g. [25]. Therefore, we analyze the rate of convergence by comparison to known weight functions.

2.1 Main Lemma

**Lemma**  Let \( V \) be an infinite dimension linear vector space and \( \mathcal{H}_1 \) and \( \mathcal{H}_2 \) be two separable Hilbert spaces defined on \( V \) with inner products \( \langle \cdot, \cdot \rangle_1 \) and \( \langle \cdot, \cdot \rangle_2 \), respectively. Let \( \{\phi_j^k\}_{j \geq 0} \) be an orthogonal basis of \( \mathcal{H}_k \) with respect to \( \langle \cdot, \cdot \rangle_k \) and suppose that

\[ \text{span} \{\phi_j^k\}_{0 \leq j \leq N} = \text{span} \{\phi_j^1\}_{0 \leq j \leq N} = V_N, \quad \forall N \in \mathbb{N} \]  

(4)

and

\[ \|v\|_2 \leq C \|v\|_1, \quad \forall v \in \mathcal{H}_1 \]  

(5)

where \( C > 0 \) is a constant that is independent of \( v \).

Let \( P_k^N \) be the projection operators onto \( \text{span} \{\phi_j^k\}_{0 \leq j \leq N} \) with respect to the inner product \( \langle \cdot, \cdot \rangle_k \), \( k = 1, 2 \) and \( Q_k^N = I - P_k^N \) their complementary projection operators. Then, For all \( v \in \mathcal{H}_1 \),

\[ \|Q_k^N v\|_2 \leq C \|Q_1^N v\|_1 \]  

(6)

and

\[ \|P_2^k v - P_1^N v\|_2 \leq C \|Q_1^N v\|_1 \]  

(7)

Note that \( v \in \mathcal{H}_1 \), \( v = P_1^N v + Q_1^N v \) in the sense that \( \|v - (P_1^N v + Q_1^N v)\|_1 = 0 \). Similarly, \( v \in \mathcal{H}_2 \), \( v = P_2^N v + Q_2^N v \) in the sense that \( \|v - (P_2^N v + Q_2^N v)\|_2 = 0 \). Therefore \( \forall v \in \mathcal{H}_1 \),

\[ \|v - (P_1^N v + Q_1^N v)\|_2 \leq C \|v - (P_1^N v + Q_1^N v)\|_1 = 0, \text{ due to } (5). \]

**Proof**  Let \( v \in \mathcal{H}_1 \). Since, as pointed above, \( v = P_1^N v + Q_1^N v = P_2^N v + Q_2^N v \) then \( v \in \|\cdot\|_2 \).

By using (5) we obtain the following estimate:

\[ C^2 \|Q_1^N v\|_1^2 \geq \|Q_1^N v\|_2^2 = \|P_2^N v - P_1^N v\| + Q_2^N v\|_2^2 \]  

(8)
Since \( P_N^2 z - P_N^1 z \in V_N \) and \( Q_N^2 z \in V_N^{1,2} \), where \( V_N^{1,2} \) is the orthogonal subspace of \( V_N \) in \( H_2 \). Then

\[
C^2 \left\| Q_N^1 v \right\|_1^2 \geq \left\| P_N^2 v - P_N^1 v \right\|_2^2 + \left\| Q_N^2 v \right\|_2^2
\]

which leads to (6) and (7).

**Remark** In the case of comparing two sets of orthogonal polynomials, condition (4) is trivially satisfied. Therefore, the conclusion is that the convergence rate of the expansion in orthogonal polynomials \( \{ \varphi_n \}_{n=0}^{\infty} \), derived from a bounded weight function \( W(Z) \) (of the inner product) is, at least, of the same order as the expansion in Legendre polynomials.

In example 4, below, we consider a non smooth or singular function, \( f(z) \), can be presented as a product

\[
f(z) = w(z) \cdot f_{\text{smooth}}(z)
\]

where \( w(z) \) is singular. In this case, \( f_{\text{smooth}}(z) \) can be expanded in a set of non-standard orthogonal polynomials with respect to the weight function \( w(z) \) and the lemma provides a bound on the rate of convergence of such approximations.

### 2.2 Numerical Examples

In this section, we demonstrate the claims of the Lemma using several numerical examples.

**Example 1** In this example we compare the rate of decay of the projection coefficients of the functions \( f(z) = \sin(10z) + \cos(8z) \), \( g(z) = (z + 1/2)^3 \mid z + 1/2 \mid \) and \( h(z) = |z + 1/2| \).

We compare the expansions of this function with respect to Legendre-type polynomials (\( w_1(z) = 1/2 \)) and Gegenbauer orthogonal polynomials (\( w_2(z) = 3/4 (1 - z^2) \)). The latter were obtained via Gram–Schmidt orthogonalization (although these are classical polynomials, Gram–Schmidt orthogonalization was used, as dictated by the general approach). The plots of the logarithm of the coefficients are presented in Figs. 1, 2 and 3, respectively. Since \( f(z) \) is analytic, \( g(z) \in C^3[-1, 1] \) and \( h(z) \in C[-1, 1] \) the decay rates of their coefficients are significantly different. However the comparison between the Legendre-type expansion and the expansion in the polynomials associated with \( w_2(z) \) indicates that the decay rates are very much alike.

We also note that the norm that is induced by \( w_2(z) \) is dominated by the norm induced by \( w_1(z) \) and, therefore, the conditions of the lemma are satisfied.

**Example 2** In this example we compare the rate of decay of the projection coefficients of the same functions, \( f(z) = \sin(10z) + \cos(8z) \), \( g(z) = (z + 1/2)^3 \mid z + 1/2 \mid \) and \( h(z) = |z + 1/2| \).

We compare the expansions of this function with respect to Chebychev polynomials (\( w_1(z) = 1/\sqrt{1 - z^2} \)) and non-standard orthogonal polynomials (\( w_2(z) = 1/(2\sqrt{1 - |z|}) \)) which were obtained via Gram–Schmidt orthogonalization. The plots of the logarithm of the coefficients are presented in Figs. 4, 5 and 6, respectively. As in the previous example, the decay rates are almost identical. Here as well, the norm that is induced by \( w_2(z) \) is dominated by the norm induced by \( w_1(z) \).

**Example 3** In this 2-D example we compare the rate of decay of the projection coefficients for the function \( f(z_1, z_2) = \sin(4(z_1 + z_2)) + \cos(6(z_1 - z_2)) \).
We compare the expansions with respect to Legendre polynomials ($w_1(z_1, z_2) = 1/4$) and non-standard orthogonal polynomials ($w_2(z_1, z_2) = (2/9) (\chi_Q(z_1, z_2) + 1)$), where $\chi_Q(z_1, z_2)$ is the indicator function of the set.

$$Q = \left\{ (z_1, z_2) \left| -\frac{1}{2} \leq z_1 \leq \frac{1}{2}, \quad -\frac{1}{2} \leq z_2 \leq -z_1 \right. \right\}$$

As before, the latter were obtained via Gram–Schmidt orthogonalization. The plot of the logarithm of the coefficients is presented in Fig. 7. Note that although $w_2(z_1, z_2)$ is discontinuous, the decay rates of the coefficients are almost identical and that the peaks correspond to the same indexes, i.e. to polynomials which are generated by orthogonalization of the same monomials. The linear fits, generated by the last four peaks (polynomials 145, 181, 221 and 265) for $w_1$ and $w_2$ are $-0.024211589198446N + 1.255763616975428$ and $-0.024225507106957N + 1.252771892243472$, respectively.
Fig. 3 Comparison between the coefficients of the expansions of \( h(x) = |x + \frac{1}{2}| \) in \( a \) Legendre polynomials and \( b \) the orthogonal polynomials associated with \( w_2(x) = \frac{3}{4} \left( 1 - x^2 \right) \)

Fig. 4 Comparison between the coefficients of the expansions of \( f(z) = \sin(10z) + \cos(8z) \) in \( a \) Chebychev polynomials and \( b \) the orthogonal polynomials associated with \( w_2(z) = \frac{1}{2\sqrt{1-|z|}} \)

We also calculate the coefficients of the expansion of

\[
g(z_1, z_2) = [\sin(4(z_1 + z_2)) + \cos(6(z_1 - z_2))] \cdot \frac{2}{9} (x_Q(z_1, z_2) + 1)
\]

in 2-D Legendre-type polynomials \( (w_1(z_1, z_2) = \frac{1}{4}) \). Since \( g \) is discontinuous the decay rate of the coefficients is much lower, see Fig. 8. This example illustrates the potential use of nonstandard weight functions as a tool for obtaining fast coefficient decay rates for discontinuous or singular functions. In this case, instead of expanding, or integrating, \( g \) directly one can use the discontinuous part, \( \frac{2}{9} (x_Q(z_1, z_2) + 1) \) as a weight function and obtain a much higher convergence rate, see Fig. 7b. This idea is not new. The use of expansions in Chebyshev, or Jacobi polynomials in order to get high convergence rates for integrating functions with singularities near the boundaries in the 1-D case was demonstrated e.g. in
Example 4 - L-shaped domain: We utilize the proposed approach for approximating the function

\[ f(z_1, z_2) = \cos(z_1 + z_2) \cdot \left( z_1^2 + z_2^2 \right)^{\frac{1}{4}} \]  

(10)

on the L-shaped domain \( \Omega = \Omega_1 \cup \Omega_2 \), where

\[ \Omega_1 = \{ (z_1, z_2) | -1 < z_1 < 1, \quad -1 < z_2 < 0 \} \]
\[ \Omega_2 = \{ (z_1, z_2) | 0 < z_1 < 1, \quad -1 < z_2 < 1 \} \]

(11)

With respect to the standard \( L^2(\Omega) \) norm. Here, the approximated function can be written as

\[ f(z_1, z_2) = f_R(z_1, z_2) \cdot f_S(z_1, z_2) \]  

(12)

Fig. 5 Comparison between the coefficients of the expansions of \( g(z) = \left( z + \frac{1}{2} \right)^3 \left( |z| + \frac{1}{2} \right) \) in a Chebychev polynomials and b the orthogonal polynomials associated with \( w_2(z) = 1/(2\sqrt{1-|z|}) \)

Fig. 6 Comparison between the coefficients of the expansions of \( h(z) = |z + \frac{1}{2}| \) in a Chebychev polynomials and b the orthogonal polynomials associated with \( w_2(z) = 1/(2\sqrt{1-|z|}) \)

[3]. The lemma, however, provides the theoretical background for the use of a larger class of weight functions in multidimensional settings.
where $f_R(z_1, z_2) = \cos(z_1 + z_2)$ is a regular function and $f_S(z_1, z_2) = (z_1^2 + z_2^2)^{\frac{1}{2}} = w(z_1, z_2)$ can be regarded as a bounded and positive weight function on $\Omega$. Moreover, the partial derivatives of $f_S$ are unbounded near the origin. Thus, the origin is a point of weak singularity of $f$. Similar models frequently appear in heat transfer or elasticity problems, e.g [17].

The approximation was done by decomposing $\Omega$ into a finite collection of equal squares $\{\Omega_j\}_{j=1}^{27}$ and constructing local approximations, $H_j : \Omega_j \rightarrow \mathbb{R}$, which define a global approximating function, $H$, by

$$H(z_1, z_2) = H_j(z_1, z_2); \quad (z_1, z_2) \in \Omega_j$$

(13)
We compare the following two approaches, for a given choice of the degree of the local approximation, $N_j$:

(1) The ‘classical’ approach: the approximating functions, $H_j$, is constructed by using classical Legendre-type polynomials on $\Omega_j$ with respect to the inner product

$$
\langle g, l \rangle_{v_j} := \iint_{\Omega_j} g(z_1, z_2) l(z_1, z_2) \, dz_1 \, dz_2
$$

$$
v_j(z_1, z_2) := \frac{1}{d_j}; \quad d_j := \mu(\Omega_j)
$$

where $\mu$ denotes the standard Lebesgue measure on $\mathbb{R}^2$. The error on the square, $E_j := \|f - H_j\|_{L^2(\Omega_j)}$, can be bounded by using convergence results for classical orthogonal polynomials. The total $L^2(\Omega)$ error is calculated by summation over the local errors.

(2) The modified approach: the approximation on $\Omega_j$ is carried out with respect to the following inner product on $\Omega_j$

$$
\langle g, l \rangle_{w_j} := \iint_{\Omega_j} g(z_1, z_2) l(z_1, z_2) \, dz_1 \, dz_2
$$

$$
w_j(z_1, z_2) := \frac{w(z_1, z_2)}{d_j}; \quad d_j := \iint_{\Omega_j} w(z_1, z_2) \, dz_1 \, dz_2
$$

where $f_S$ plays the role of a weight function. Let $P_{N_j} f_R$ be the polynomial $L^2_{w_j}(\Omega_j)$—approximation of $f_R$ with respect to the polynomial basis that is generated by orthogonalization, $\{\Psi_k\}_{|k| \leq N_j}$. Thus, we have the following representation

$$
P_{N_j} f_R = \sum_{|k| \leq N_j} \hat{f}_{Rk} \Psi_k; \quad \hat{f}_{Rk} = \langle f_R, \Psi_k \rangle_{w_j}.
$$

Hence, we define

$$
H_j(z_1, z_2) := P_{N_j} f_R(z_1, z_2) \cdot f_S(z_1, z_2); \quad (z_1, z_2) \in \Omega_j
$$

The local error on $\Omega_j$ is $E_j := \|f - H_j\|_{L^2(\Omega_j)}$ and the total error is obtained by summation over the squares.

**Remark** Generating non-standard orthogonal polynomials for a non-classical weight function is a costly procedure. Thus, a more advanced approach is to use the approximations of the second type only for elements that are adjacent to the singularity.

We postpone the formal error analysis of the latter approach for future work which will also include a comparison to the full h-p approximation method. In this example, we used local approximations by cubic polynomials.

The domain decomposition and the numbering of the subdomains $\Omega_j$ are shown in Fig. 9. The errors in each element for local approximations of various degree are summarized in Appendix A, Tables 1 and 2. The total error over all elements is presented in Fig. 10. The local error for approximation on each element is shown in Figs. 11 and 12. We also present the approximation error for element number 13, which is adjacent to the singularity, see Fig. 13. These results show that the singularity of $f$ at the origin causes the approximation errors in the Legendre-type polynomials expansion to be approximately 2.5 orders of magnitude larger than the errors in expansion using non-standard polynomials.
Fig. 9 L-Shaped—Example 3—Domain Decomposition and the numbering of the subdomains $\Omega_j$

log$_{10}$(Total Error) vs. Degree

Degree of Local Approximation

Fig. 10 L-Shaped—Example 3—Total Error

Fig. 11 L-Shaped—Example 3—Legendre Polynomials, deg = 4, Local Error
Fig. 12 L-Shaped—Example 3—Non-standard Polynomials, degree = 4, Local Error

Fig. 13 L-Shaped—Example 3—Element 13, Local Error

3 Numerical Integration: A Heuristic Approach

Since it is rarely possible to symbolically integrate arbitrary functions, it is essential to provide an approach for constructing numerical integration formulas. Unfortunately, unlike the 1-D case, where Gauss quadrature can be used, there is no systematic way of generating such formulas in a multidimensional setting. In this section, we demonstrate a possible approach to finding suitable numerical integration formulas for spectral integration. The proposed approach is based on selection of collocation points that minimize the condition number of the induced cubature formula. This section presents the theoretical framework for this construction, followed by several numerical examples which demonstrate the validity of the described approach. The development of more efficient and robust methods of implementing the presented ideas is postponed for future work.

Let $\Omega \in \mathbb{R}^d$ and $w(z)$ be a weight function on $\Omega$, $f : \Omega \longrightarrow \mathbb{R}$ and $f \in H^p_w(\Omega)$ for $p \geq 1$ where $H^p_w(\Omega)$ is a weighted Sobolev space defined on $\Omega$ with the weight function $w(z)$. 
We use the following notations:

- \( \{\Psi_n(z)\}_{n \geq 0} \) — Orthogonal polynomials on \( \Omega \) with respect to the weighted inner product
  \( \int_{\Omega} f(z) g(z) w(z) dz \).
- \( P_N, Q_N \) — The projection operators that correspond to \( \{\Psi_n(z)\}_{n \geq 0} \).
- Let \( z_0, \ldots, z_M \) be a set of points in \( \Omega \). We denote by \( f \) the vector
  \[
  f = \begin{pmatrix}
  f(z_0) \\
  \vdots \\
  f(z_M)
  \end{pmatrix} \in \mathbb{R}^{M+1}
  \]

**Remark** In this section, and the rest of the manuscript, \( M + 1 \) is the number of polynomials in the constructed basis of the space of polynomials of degree less than or equal to \( N \). In \( d \) dimensions

\[
(M + 1) = \binom{N + d}{d} = O(N^d).
\]

In order to simplify the notations, we make a technical assumption that

\[
\int_{\Omega} w(z) dz = 1,
\]

otherwise, it is always possible to normalize \( w \).

We assume that

\[
\| Q_N f \|_{L^2_w(\Omega)} \leq \text{const} \cdot N^{-p} \cdot \| f \|_{H^p_w(\Omega)}
\]

This results from comparison to a standard weight function (see the main lemma), which we assume is possible. Let \( z_0, \ldots, z_M \in \Omega \) be a set of collocation points. We would like to find a numerical integration formula of the form:

\[
I[g] := \int_{\Omega} g(z) w(z) dz \approx \sum_{j=0}^{M} A_j g(z_j) = \langle A, g \rangle,
\]

where

\[
A = \begin{pmatrix}
A_0 \\
\vdots \\
A_M
\end{pmatrix}.
\]

We denote this numerical integration operator by \( NI[g] = NI_{M+1}^{z_0 \ldots z_M}[g] \).

If the collocation points \( z_0, \ldots, z_M \in \Omega \) are known (for example, the Gauss or Gauss-Lobatto collocation points) then the coefficients vector, \( A \), could be found by demanding that \( NI[g] \) is exact for \( \{\Psi_0, \ldots, \Psi_M\} \). This gives rise to the following system of linear equations

\[
\begin{pmatrix}
\Psi_0 (z_0) & \Psi_0 (z_1) & \cdots & \Psi_0 (z_M) \\
\Psi_1 (z_0) & \Psi_1 (z_1) & \cdots & \Psi_1 (z_M) \\
\vdots & \vdots & \ddots & \vdots \\
\Psi_M (z_0) & \Psi_M (z_1) & \cdots & \Psi_M (z_M)
\end{pmatrix} A = \begin{pmatrix}
\beta_0 \\
0 \\
\vdots \\
0
\end{pmatrix},
\]

where

\[
\beta_0 = \int_{\Omega} 1 w(z) dz = 1.
\]
which can be written as:

\[ RA = \beta, \text{ or } A = R^{-1}\beta \]  \hspace{1cm} (28)

and \( R^{-1} = R^{-1}(z_0, \ldots, z_M) \).

The numerical integration formula is then given by

\[ NI[g] = \langle A, g \rangle = \langle R^{-1}\beta, g \rangle \]  \hspace{1cm} (29)

Following [13] we define the absolute condition number of the numerical integration formula \( NI \), \( \text{by} \)

\[ K_{abs}(NI) := \sup_{\|u\|_2 \leq 1} \left| \langle R^{-1}(z_0, \ldots, z_M)\beta, u \rangle \right| = \| R^{-1}(z_0, \ldots, z_M)\beta \|_2 = \| A \|_2 \]  \hspace{1cm} (30)

The Proposed Approach

For every \( M \in \mathbb{N} \) find a set of collocation points in \( \Omega \), denoted by \( z_0, \ldots, z_M \), such that the condition number, \( K_{abs}(NI) \), is as small as possible. We denote this bound by \( \lambda(M) \), to emphasize the dependence on the number of points. i.e

\[ \| R^{-1}(z_0, \ldots, z_M)\beta \|_2 = \lambda(M) \]  \hspace{1cm} (31)

This is done by using a suitable minimization algorithm on \( \| R^{-1}(z_0, \ldots, z_M)\beta \|_2 \) as a function of \( M + 1 \) variables.

Remarks

- We do not claim that an absolute minimum for \( \| R^{-1}(z_0, \ldots, z_M)\beta \|_2 \) is required for the approach to work. Subsequent analysis and examples will show that as long as \( \lambda(M) \) does not grow too rapidly as \( M \) tends to infinity, this approach will result in spectral convergence of the resulting cubature formulas. Specifically, the analysis will show that if \( \lambda(M) = O(M^\alpha) \) where \( \alpha \) is small with respect to the smoothness of the function, \( p \), then the use of numerical integration, instead of analytic one will allow for convergence, although at a slower rate.

- It is well known that in the multidimensional case, system (26) doesn’t have to be invertible. However, for such collocation points, the condition number is infinite. Therefore, such points are avoided according to our approach (as are points for which the condition number is very large).

- The collocation points can be found in a sequential manner, where in each step the previously found points are fixed and the minimization is carried out with respect to the new (additional) point.

3.1 The Construction Method

The proposed heuristic approach can be summarized as follows:

Given the Orthogonal Polynomials \( \{\psi_j\}_{j \geq 0} \):

1. Normalize \( w \).
2. Construct the matrix \( R \) as a function of \( z_0, \ldots, z_M \) and find \( z_0, \ldots, z_M \) which minimize \( \| R^{-1}(z_0, \ldots, z_M)\beta \|_2 \). This is done numerically using an optimization algorithm.
3. The obtained \( z_0, \ldots, z_M \) are the integration points, \( A = R^{-1}\beta \) are the integration weights and \( NI[g] = \langle A, g \rangle \), See (29).
In simple cases \[ \{ \Psi_j \}_{j \geq 0} \] can be found analytically. Otherwise, they can be computed using Gram Schmidt procedure or via a three term recursion formula based on classical numerical integration schemes. Although this is a costly procedure it is done once as a preprocessing stage.

### 3.2 Analysis

Recall that we denote by \( P_M \Psi f \), \( Q_M \Psi f \) the projection operators corresponding to \( w \). The error of the quadature formula is defined by:

\[
E[f] := I[f] - NI[f], \quad f \in H^p_w(\Omega).
\]  

(32)

Since \( f = P_M \Psi f + Q_M \Psi f \) and \( NI[\cdot] \) is exact for the polynomials \( \{ \Psi_j \}_{j \geq 0} \)

\[
|E[f]| = |I[P_M \Psi f] + I[Q_M \Psi f] - NI[P_M \Psi f] - NI[Q_M \Psi f]| 
= |I[Q_M \Psi f] - NI[Q_M \Psi f]| 
\leq |I[Q_M \Psi f]| + |NI[Q_M \Psi f]| 
\]  

(33)

Now, by orthogonality

\[
|I[Q_M \Psi f]| = \left| \int_{\Omega} (Q_M \Psi f)(x)w(x)dx \right| 
= \left| \int_{\Omega} 1 \cdot (Q_M \Psi f)(x)w(x)dx \right| = 0
\]  

(34)

Evaluating the second term in (33), \( |NI[Q_M \Psi f]| \), is more difficult as it requires to estimate \( |Q_M \Psi f| \) at the nodes \( z_0, \ldots, z_M \) rather than it’s integral norm. It is well know that the sequence \( \| \Psi_j \|_\infty \) can be unbounded as \( j \to \infty \). For example, the \( L_2 \) normalized Legendre polynomials satisfy \( \| P_j \|_\infty = O(\sqrt{j}) \). For general orthogonal polynomials there are no known evaluations of \( \| \Psi_j \|_\infty \). Another approach could be the use of inequalities which bound the maximum norm of polynomials, or some norm of their derivatives, by the norm of these polynomials. Well-known inequalities are the Bernstein and Nikolskii inequalities, see e.g. [4]. However, they are not directly applicable in this setting since, as far as we know, there are no generalizations of these inequalities to several dimensions and to nonstandard weight functions. Therefore, we use the following approach:

- We first show that the Lebesgue measure (denoted by \( \mu \)) of the set in which \( |(Q_M \Psi f)(z)| \) is larger than \( M^{-\theta} \), for an auxiliary parameter \( \theta > 0 \), tends to zero as \( M \to \infty \).
- We then show that when the nodes \( z_0, \ldots, z_M \) are taken in the complement of this set the integration error is small.
- In the second part of the following analysis, there is an implicit assumption that \( \mu(\Omega) < \infty \). In practice, this assumption poses no loss of generality. Indeed, since \( f \in L_{2,w}(\Omega) \) we know (see [16]) that for a ball \( B = B(0, R) \) with a sufficiently large radius

\[
\int_{B^c} |f(z)|^2 w(z)dz \leq \epsilon^2
\]  

(35)
where $\epsilon$ is the machine precision. Thus, it is sufficient to approximate the integral of the function $f(z)$ on the ball $B$ without incurring any loss of accuracy. This follows from

$$
\left| \int_{B_c} f(z) w(z) \, dz \right| = \int_{B_c} |f(z)| \sqrt{w(z)} \, dz \leq \sqrt{\int_{B_c} |f(z)|^2 \, dz} \cdot \sqrt{\int_{B_c} w(z) \, dz} \leq \epsilon
$$

As we’ve mentioned, this is a theoretical analysis of the approach and, thus, the auxiliary parameter $\theta$ does not appear in any of the calculations carried out in practice. Moreover, we assume that $f$ is sufficiently smooth so that such a parameter $\theta$ can be obtained.

Note that

$$
|NI\left[Q_M^\Psi f\right]| \leq \lambda(M) \cdot \sqrt{M} \cdot \max_{0 \leq j \leq M} |(Q_M^\Psi f)(z_j)\|
$$

We now divide the analysis into two cases:

**Case 1** $w(z) \geq \delta > 0$

Let $\theta > 0$. By using Markov’s inequality we obtain

$$
\mu\left( \{z \in \Omega \mid |(Q_M^\Psi f)(z)| > M^{-\theta} \} \right) \leq M^{2\theta} \int_{\Omega} |(Q_M^\Psi f)(z)|^2 \, dz
$$

$$
= \frac{M^{2\theta}}{\delta} \int_{\Omega} |(Q_M^\Psi f)(z)|^2 \, dz \leq \frac{M^{2\theta}}{\delta} \|Q_M^\Psi f\|_{L^2_{\omega}(\Omega)}^2
$$

$$
\leq \frac{M^{2\theta}}{\delta} \text{const} \cdot M^{-2p} \cdot \|f\|_{H^p_{\omega}(\Omega)}^2\approx \text{const} \cdot \frac{N^{2d(\theta-p)}}{\delta} \cdot \|f\|_{H^p_{\omega}(\Omega)}^2
$$

Therefore, if $\theta - p < 0$

$$
\mu\left( \{z \in \Omega \mid |(Q_M^\Psi f)(z)| > M^{-\theta} \} \right) \xrightarrow{N \to \infty} 0
$$

Thus, by selecting the collocation points in the complement of this set (which has measure of at least $1 - \left( N^{2d(\theta-p)} / \delta \cdot \text{const} \cdot \|f\|_{H^p_{\omega}(\Omega)}^2 / \mu(\Omega) \right) )$

$$
|NI\left[Q_M^\Psi f\right]| \leq \lambda(M) \cdot M^{1/2-\theta}
$$

Under the assumption that $\lambda(M) \propto M^\alpha$, we have

$$
|E[f]| \leq \lambda(M) \cdot M^{1/2-\theta} \approx N^{d(\alpha+\frac{1}{2}-\theta)}
$$

Therefore, if $\theta > \alpha + \frac{1}{2}$, the numerical integration formula approximates the exact integration asymptotically as $N \to \infty$. From this analysis it follows that for this approach to be valid it must be the case that $\alpha + \frac{1}{2} < p$ (i.e the approximated function must be sufficiently smooth in comparison to the growth of the condition number).

**Case 2** If there is no positive constant $\delta$ that bounds $w(z)$ from below we use a different approach. For every $n \in \mathbb{N}$ define the following set

$$
S_n = \left\{ z \in \Omega \mid w(z) < \frac{1}{n} \right\}
$$

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The sequence \( \{S_n\}_{n \geq 1} \) is downward monotone with respect to inclusion. Since \( \mu(S_1) \leq \mu(\Omega) < \infty \), by applying the downward monotone convergence theorem, we obtain that

\[
0 = \mu(\{z \in \Omega \mid w(z) = 0\}) = \lim_{n \to \infty} \mu(S_n). \tag{43}
\]

Where we use the fact that \( w(z) \) is a weight function that does not vanish on positive measure sets. Therefore, there exists a number \( N_0 \in \mathbb{N} \) such that

\[
\mu(S_{N_0}) < \eta \tag{44}
\]

For \( \eta > 0 \) small enough. Therefore,

\[
\mu\left( \left\{ z \in \Omega \mid \left| (Q_M^\Psi f)(z) \right| > M^{-\theta}, w(z) < \frac{1}{N_0} \right\} \right) \leq \eta \tag{45}
\]

Moreover,

\[
\left\{ z \in \Omega \mid \left| (Q_M^\Psi f)(z) \right| > M^{-\theta}, w(z) \geq \frac{1}{N_0} \right\} \subset \left\{ z \in \Omega \mid \left| (Q_M^\Psi f)(z) \right| \cdot \sqrt{w(z)} > M^{-\theta} \frac{1}{\sqrt{N_0}}, w(z) \geq \frac{1}{N_0} \right\} \tag{46}
\]

Thus, by using Markov’s inequality and (23) we get the following estimate

\[
\mu\left( \left\{ z \in \Omega \mid \left| (Q_M^\Psi f)(z) \right| > M^{-\theta}, w(z) \geq \frac{1}{N_0} \right\} \right) \leq N_0 \cdot M^{2\theta} \cdot \|Q_M^\Psi f\|_{L_w^2}^2 \leq \text{const} \cdot N_0 \|f\|_{H^2_w(\Omega)}^2 M^{2\theta} M^{-2p} \approx \text{const} \cdot N_0 \|f\|_{H^2_w(\Omega)}^2 N^{2d(\theta-p)} \tag{47}
\]

Finally, by using (45) and (47) we have

\[
\mu\left( \left\{ x \in \Omega \mid \left| (Q_M^\Psi f)(z) \right| > M^{-\theta} \right\} \right) \leq \text{const} \cdot N_0 \|f\|_{H^2_w(\Omega)}^2 M^{2(\theta-p)} + \eta \approx \text{const} \cdot N_0 \|f\|_{H^2_w(\Omega)}^2 N^{2d(\theta-p)} + \eta \tag{48}
\]

Which implies that, if \( \theta < p \), it is possible, in principal, to select points \( \{z_0, \ldots, z_M\} \) that minimize the condition number, and also belong to the set

\[
\left\{ z \in \Omega \mid \left| (Q_M^\Psi f)(z) \right| < M^{-\theta} \right\} .
\]

The rest of the analysis and the conclusions are identical to the previous case.
3.3 Numerical Examples

In this section, we present three examples of numerical integration using the algorithm described above. These examples demonstrate the validity of the described method, under the mentioned assumptions. For simplicity, the optimization was carried out using sequential choice of points via the downhill simplex method, see e.g. [12].

**Example 1**  In this example we tested our approach to finding numerical integration formulas for the weight function \( w(z) = \frac{1}{3}(\chi_Q(z) + 1) \), where \( \chi_Q(z) \) is the indicator function of the set \( Q = \{-\frac{1}{2} \leq z \leq \frac{1}{2} \} \) and the integration domain is \([-1, 1]\). The integration was carried out using the process presented above for the function

\[
f(z) = e^{1.1z} + \cos(1.2z) .
\]

The log10 of the error vs the number of collocation points is presented in Fig. 14a. The spectral convergence can be clearly seen from this plot. The locations of the collocation points are shown in Fig. 14b.

**Example 2**  In this example we integrate the function

\[
f(z_1, z_2) = \sin(1.1(z_1 + z_2)) + \cos(1.2(z_1 - z_2)) .
\]

in the domain \((z_1, z_2) \in [-1, 1]^2\) with the weight function \( w(z_1, z_2) = \frac{2}{9}(\chi_Q(z_1, z_2) + 1) \), where \( \chi_Q(z_1, z_2) \) is the indicator function of the set

\[
Q = \left\{-\frac{1}{2} \leq z_1 \leq \frac{1}{2}, \quad -\frac{1}{2} \leq z_2 \leq -z_1 \right\} .
\]

The log10 of the error vs the number of collocation points is presented in Fig. 15a. The spectral convergence can be clearly seen from this plot. The locations of the collocation points are shown in Fig. 15b.
**Example 3** In this example we integrate the function

\[ f(z_1, z_2) = \sin(1.1(z_1 + z_2)) + \cos(1.2(z_1 - z_2)) , \]  

with the weight function \( w(z_1, z_2) = 2 \) on the triangular domain

\[ \Omega = \{0 \leq z_1 \leq 1, \ 0 \leq z_2 \leq z_1 \} . \]  

The \( \log_{10} \) of the error versus the number of collocation points is presented in Fig. 16a. As in the previous examples, the spectral convergence (exponential decay) can be clearly seen from this plot. The locations of the collocation points are shown in Fig. 16b. We also list the obtained condition numbers corresponding to the first 29 points in “Appendix A”, Table 3. Though it is hard to determine how fast the condition number grows as \( M \) increases, it is less than linear (the slope of the linear least squares regression of \( \log(\text{the condition number}) \) versus \( \log(M) \) is 0.7086).

These examples demonstrate the applicability of this integration method. It should be noted that though the locations of the collocation points look random, they are not. Choosing random points leads to a very large condition number and poor convergence rate.

**4 GPC Example**

In this section, we apply the theory presented above to solving a partial differential equation with stochastic parameters. We consider the following Cauchy problem, which is similar to Example 4.5 in [20].

\[ u_t = a(z_1, z_2)^2 u_{xx} \quad t > 0, \ x \in \mathbb{R} ; \quad u(x, 0) = e^{-x} \quad x \in \mathbb{R} , \]  

where \((z_1, z_2)\) is a random vector with values in \([-1, 1]^2\) and a probability density function

\( w(z_1, z_2) = \frac{2}{9}(\chi_Q(z_1, z_2) + 1) ; \quad Q = \left\{ \frac{1}{2} \leq z_1 \leq \frac{1}{2}, \quad \frac{1}{2} \leq z_2 \leq -z_1 \right\} \)  

(55)
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and \( a(z_1, z_2) = \sqrt{\ln(\cos(z_1 - z_2) + \sin(1.1(z_1 + z_2)) + 4) \right) \). The solution to this Cauchy problem is a function \( u(x, t, z_1, z_2) \) which depends on the time and spatial variable, as well as on the random vector. Our goal is to estimate \( u(0, 1, z_1, z_2) \) by using stochastic collocation based on GPC. The solution to the initial value problem is

\[
    u(0, 1, z_1, z_2) = \cos(z_1 - z_2) + \sin(1.1(z_1 + z_2)) + 4 .
\]  

Denote by \( \{\Phi_k(z_1, z_2)\}_{|k|\geq 0} \) the set of orthogonal polynomials on \([-1, 1]^2\) with respect to \( w(z_1, z_2) \), which were obtained via Gram–Schmidt algorithm. Thus, \( u(0, 1, z_1, z_2) \) can be expanded into a series given by

\[
    u(0, 1, z_1, z_2) = \sum_{|k|=0}^{\infty} \hat{u}_k(0, 1) \Phi_k(z_1, z_2) \tag{57}
\]

where

\[
    \hat{u}_k(0, 1) = (\Phi_k(\cdot, \cdot), u(0, 1, \cdot, \cdot))_w
    = \int_{-1}^{1} \int_{-1}^{1} \Phi_k(z_1, z_2) u(0, 1, z_1, z_2) w(z_1, z_2) \, dz_1 \, dz_2 \tag{58}
\]

For \( N \in \mathbb{N} \) we define

\[
    (P_N u) (0, 1, z_1, z_2) = \sum_{|k|=0}^{N} \hat{u}_k(0, 1) \Phi_k(z_1, z_2) \tag{59}
\]

to be the projection of \( u(0, 1, z_1, z_2) \) on the set of orthonormal polynomials of degree less or equal to \( N \). Instead of using the symbolic projections \( (P_N u) (0, 1, z_1, z_2) \) we approximate \( u(0, 1, z_1, z_2) \) by numerical projections

\[
    (\tilde{P}_N u) (0, 1, z_1, z_2) = \sum_{|k|=0}^{N} \tilde{u}_k(0, 1) \Phi_k(z_1, z_2) , \tag{60}
\]
where the coefficients $\tilde{u}_k(0, 1)$ are obtained by using a numerical integration formula based on $\left(\frac{2N+2}{2}\right)$ collocation points (the number of points is equal to the number of orthogonal polynomials of degree less or equal to $2N$). By the Pythagoras theorem, we have
\[
\| u(0, 1, \cdots) - \left( \tilde{P}_N u \right)(0, 1, \cdots) \|^2_{L^2_{\eta}(\Omega)} = \left\| \left( \tilde{P}_N u - P_N u \right)(0, 1, \cdots) \right\|^2_{L^2_{\eta}(\Omega)} + \left\| (u - P_N u)(0, 1, \cdots) \right\|^2_{L^2_{\eta}(\Omega)}
\]
(61)

The decay rate of the second term can be estimated with the main lemma. Thus, it is sufficient to estimate the behavior of the first term for different values of $N \in \mathbb{N}$. By the Parseval’s equality, we have that the second term is equal to
\[
H(N) := \sum_{|k|=0}^{N} |\tilde{u}_k(0, 1) - \hat{u}_k(0, 1)|^2
\]
(62)

The plot of $H(N)$ vs $N$ on a logarithmic scale is presented in Fig. 17. As can be seen, $H(N)$ decays exponentially with $N$. The outlier in $N = 6$ is probably due to the unsophisticated optimization algorithm used for finding the collocation points. See further discussion in the conclusion section.

Thus, it can be seen that the error which arises from using the numerical integration formula instead of analytic one also decays.

### 5 Summary

In this work, we showed that the convergence rate of expansions in orthogonal polynomials with respect to a ‘general’ weight function $w_2$ can be bounded by the convergence rate of expansions in polynomials associated with respect to weight function $w_1$, as long as $w_2$ is dominated by $w_1$. This result allows the evaluation of the convergence rate even in the case where the orthogonal polynomials are not eigenfunctions of some singular Sturm–Liouville
problem. This result gives the theoretical background for the use of these expansions. We also demonstrated that the use of nonstandard weight functions enables to derive fast convergent expansions of non-smooth functions.

We also presented an approach to derive a multi-dimensional, spectrally accurate, integration method by finding the collocation points which minimize the absolute condition number of the integration formula. Although, for the simplicity of the implementation we used the downhill simplex method, which is not an optimal algorithm, we demonstrated that efficient integration method can be derived even for non-continuous weight functions and non-standard domains. More research is needed in analyzing the properties of this integration method and its implementations. In particular, finding a proper optimization algorithm for obtaining the collocation points.

It should be noted that this integration method is less efficient than the classical Gauss quadrature as an \( M + 1 \) point formula is accurate only for the \( M + 1 \) polynomials which are used, rather than achieving increased algebraic accuracy, as in the case of Gauss integration. However, it can be used even when no Gauss-type quadrature can be derived.

Numerical examples demonstrated the efficacy of the proposed method.

A Appendix: Local Errors for the L-Shaped Domain and Condition Numbers in a Triangular Domain.

Table 1 The error in each subdomain, \( \Omega_j \) for different degree of non-standard polynomials expansions

| Degree/element | 1  | 2  | 3  | 4  |
|---------------|----|----|----|----|
| 1             | 6.01801e−4 | 2.83446e−4 | 1.46762e−4 | 6.86025e−4 |
| 2             | 5.04182e−5 | 6.21132e−5 | 7.00263e−5 | 2.92184e−5 |
| 3             | 1.29901e−6 | 1.20905e−6 | 2.9024e−7  | 1.48222e−6 |
| 4             | 2.88336e−7 | 2.76578e−7 | 6.43554e−8 | 3.39858e−7 |

| Degree/element | 5  | 6  | 7  | 8  |
|---------------|----|----|----|----|
| 1             | 5.45596e−4 | 2.83395e−4 | 5.1755e−4  | 6.86025e−4 |
| 2             | 4.58312e−5 | 6.21132e−5 | 9.49984e−6 | 2.92184e−5 |
| 3             | 1.17826e−6 | 6.05555e−7 | 1.08778e−7 | 1.48222e−6 |
| 4             | 2.51762e−7 | 4.05396e−7 | 1.31404e−8 | 3.88262e−7 |

| Degree/element | 9  | 10 | 11 | 12 |
|---------------|----|----|----|----|
| 1             | 6.01804e−4 | 6.0181e−4 | 6.86025e−4 | 5.1733e−4 |
| 2             | 5.04182e−5 | 5.04181e−5 | 2.92172e−5 | 9.4998e−6 |
| 3             | 1.29902e−6 | 1.2872e−6  | 1.4835e−6  | 1.0866e−6 |
| 4             | 2.21688e−7 | 2.21688e−7 | 3.88264e−7 | 1.3141e−8 |

| Degree/element | 13 | 14 | 15 | 16 |
|---------------|----|----|----|----|
| 1             | 6.11872e−4 | 8.36335e−4 | 8.78226e−4 | 2.8344e−4 |
| 2             | 1.3364e−6  | 1.57323e−5 | 3.72123e−5 | 6.21132e−5 |
### Table 1 continued

| Degree/element | 13     | 14     | 15     | 16     |
|----------------|--------|--------|--------|--------|
| 3              | 1.3318e-7 | 1.8075e-6 | 1.8970e-6 | 6.0137e-6 |
| 4              | 8.0571e-8  | 4.4432e-7  | 4.3589e-7  | 4.0539e-7  |

| Degree/element | 17     | 18     | 19     | 20     |
|----------------|--------|--------|--------|--------|
| 1              | 5.4558e-4  | 6.8602e-4  | 8.3633e-4  | 1.0239e-4  |
| 2              | 4.5831e-5  | 2.9218e-5  | 1.5732e-5  | 2.2136e-6  |
| 3              | 1.1742e-6  | 1.4833e-6  | 1.8075e-6  | 2.2126e-7  |
| 4              | 2.5176e-7  | 3.3985e-7  | 3.2434e-8  | 5.2352e-7  |

| Degree/element | 21     | 22     | 23     | 24     |
|----------------|--------|--------|--------|--------|
| 1              | 1.1306e-4  | 1.4676e-4  | 2.8345e-4  | 8.3633e-4  |
| 2              | 2.1181e-5  | 7.0026e-5  | 6.2111e-5  | 1.5732e-5  |
| 3              | 2.4426e-6  | 2.9033e-7  | 1.2190e-5  | 1.8075e-6  |
| 4              | 5.5725e-7  | 6.4355e-8  | 2.7657e-7  | 4.4332e-7  |

| Degree/element | 25     | 26     | 27     |
|----------------|--------|--------|--------|
| 1              | 8.7822e-4  | 1.1306e-3  | 1.3167e-4  |
| 2              | 3.7213e-5  | 2.1181e-5  | 2.8449e-5  |
| 3              | 1.8970e-6  | 2.4426e-6  | 2.8445e-6  |
| 4              | 4.5397e-7  | 6.5872e-7  | 3.8622e-7  |

### Table 2

The error in each subdomain, $\Omega_j$ for different degree of Legendre-type polynomials expansions

| Degree/element | 1            | 2            | 3            | 4            |
|----------------|--------------|--------------|--------------|--------------|
| 1              | 1.3600e-3    | 1.1679e-3    | 6.4432e-4    | 1.7775e-3    |
| 2              | 4.9884e-5    | 8.4779e-5    | 1.0332e-4    | 1.5179e-4    |
| 3              | 9.5025e-6    | 4.0296e-6    | 1.7648e-6    | 3.5548e-5    |
| 4              | 2.1083e-6    | 8.9406e-7    | 3.9156e-7    | 7.4434e-6    |

| Degree/element | 5            | 6            | 7            | 8            |
|----------------|--------------|--------------|--------------|--------------|
| 1              | 1.6803e-3    | 1.1679e-3    | 4.1791e-3    | 1.7775e-3    |
| 2              | 9.2685e-5    | 8.4779e-5    | 1.1997e-3    | 1.5179e-4    |
| 3              | 8.3363e-6    | 4.0296e-6    | 6.5325e-4    | 3.5548e-5    |
| 4              | 1.8496e-6    | 3.5979e-6    | 3.8022e-4    | 7.4434e-6    |

| Degree/element | 9            | 10           | 11           | 12           |
|----------------|--------------|--------------|--------------|--------------|
| 1              | 1.3600e-3    | 1.3600e-3    | 1.7775e-3    | 4.1791e-3    |
| 2              | 4.9884e-5    | 4.9884e-5    | 1.5197e-4    | 1.1997e-3    |
| 3              | 9.5025e-6    | 9.5025e-6    | 3.5548e-5    | 6.5325e-4    |
| 4              | 2.1083e-6    | 2.1083e-6    | 7.4434e-6    | 3.8022e-4    |
Table 2 continued

| Degree/element | 13          | 14          | 15          | 16          |
|----------------|-------------|-------------|-------------|-------------|
| 1              | 295143e−3   | 8.10902e−4 | 1.1291e−3  | 1.16796e−3 |
| 2              | 1.28745e−3  | 1.95597e−4 | 5.36411e−5 | 8.47799e−5 |
| 3              | 6.76481e−4  | 3.54234e−5 | 9.6454e−6  | 4.0296e−6  |
| 4              | 3.84855e−4  | 8.47482e−6 | 2.3076e−6  | 3.59799e−6 |

| Degree/element | 17          | 18          | 19          | 20          |
|----------------|-------------|-------------|-------------|-------------|
| 1              | 1.68033e−3  | 1.77759e−3 | 8.10902e−4 | 4.94571e−4 |
| 2              | 9.26857e−5  | 1.51793e−4 | 1.95597e−4 | 9.97282e−5 |
| 3              | 8.3363e−6   | 3.35481e−5 | 3.54234e−5 | 1.56367e−5 |
| 4              | 1.84962e−6  | 7.4434e−6  | 8.4748e−6  | 3.7409e−6  |

| Degree/element | 21          | 22          | 23          | 24          |
|----------------|-------------|-------------|-------------|-------------|
| 1              | 9.24513e−4  | 6.44328e−4 | 1.16796e−3 | 1.36001e−3 |
| 2              | 5.30707e−5  | 1.03328e−4 | 8.47799e−5 | 4.98848e−5 |
| 3              | 5.3995e−6   | 1.7648e−6  | 4.02965e−6 | 9.50255e−6 |
| 4              | 1.23179e−6  | 3.91562e−7 | 8.94361e−7 | 2.10813e−6 |

| Degree/element | 25          | 26          | 27          |
|----------------|-------------|-------------|-------------|
| 1              | 1.1291e−3   | 9.2451e−4  | 1.04132e−3 |
| 2              | 5.36411e−5  | 5.30707e−5 | 4.47484e−5 |
| 3              | 9.6454e−6   | 5.3995e−6  | 2.4735e−6  |
| 4              | 2.3076e−6   | 1.231895e−6| 5.9165e−7  |

Table 3 Condition numbers in a triangular domain. The condition number grows less than linear with $M$ (the slope of the linear least squares regression of log(the condition number) versus log($M$) is 0.7086)

| Number of points | Condition number | Number of points | Condition number |
|------------------|------------------|------------------|------------------|
| 2                | 6.25762e−1       | 16               | 1.50603          |
| 3                | 3.37827e−1       | 17               | 2.37553e−1       |
| 4                | 2.96099e−1       | 18               | 1.71286e−1       |
| 5                | 4.39415e−1       | 19               | 1.77015e−1       |
| 6                | 2.07519e−1       | 20               | 6.55397e−1       |
| 7                | 1.58796e−1       | 21               | 5.09683e−1       |
| 8                | 4.55232e−1       | 22               | 1.4648           |
| 9                | 2.95506e−1       | 23               | 2.96243e−1       |
| 10               | 2.96696e−1       | 24               | 2.71367          |
| 11               | 2.85709e−1       | 25               | 5.81762          |
| 12               | 7.21967e−1       | 26               | 2.844            |
| 13               | 1.81206e−1       | 27               | 1.6857           |
| 14               | 1.987e−1         | 28               | 2.84475          |
| 15               | 1.66435e−1       | 29               | 3.32741          |
References

1. Canuto, C., Quarteroni, A.: Approximation results for orthogonal polynomials in sobolev spaces. Math. Comput. 38(157), 67–86 (1982)
2. Chen, X., Park, E.-J., Xiu, D.: A flexible numerical approach for quantification of epistemic uncertainty. J. Comput. Phys. 240, 211–224 (2013)
3. Conte, S.D., De Boor, C.W.: Elementary Numerical Analysis: an Algorithmic Approach. McGraw-Hill Higher Education, New York City, NY (1980)
4. DeVore, R.A., Lorentz, G.G.: Constructive Approximation, vol. 303. Springer, Berlin, Germany (1993)
5. Funaro, D.: Polynomial Approximation of Differential Equations, vol. 8. Springer, Berlin, Germany (2008)
6. Gottlieb, D., Xiu, D.: Galerkin method for wave equations with uncertain coefficients. Commun. Comput. Phys 3(2), 505–518 (2008)
7. Hesthaven, J.S., Gottlieb, S., Gottlieb, D.: Spectral Methods for Time-Dependent Problems, vol. 21. Cambridge University Press, Cambridge, UK (2007)
8. Jakeman, J., Eldred, M., Xiu, D.: Numerical approach for quantification of epistemic uncertainty. J. Comput. Phys. 229(12), 4648–4663 (2010)
9. Li, J., Qi, X., Xiu, D.: On upper and lower bounds for quantity of interest in problems subject to epistemic uncertainty. SIAM J. Sci. Comput. 36(2), A364–A376 (2014)
10. Lin, G., Su, C.-H., Karniadakis, G.E.: Random roughness enhances lift in supersonic flow. Phys. Rev. Lett. 99(10), 104501 (2007)
11. Mujumdar, A.S.: Handbook of Industrial Drying. CRC Press, Boca Raton, Florida (2014)
12. Nelder, J.A., Mead, R.: A simplex method for function minimization. Comput. J. 7(4), 308–313 (1965)
13. Quarteroni, A., Sacco, R., Saleri, F.: Numerical Mathematics, vol. 37. Springer, Berlin, Germany (2010)
14. Rosenblatt, M.: Remarks on a multivariate transformation. Ann. Math. Stat. 23(3), 470–472 (1952)
15. Shen, J., Tang, T., Wang, L.-L.: Spectral Methods: algorithms, Analysis and Applications, vol. 41. Springer, Berlin, Germany (2011)
16. Stein, E.M.: Harmonic Analysis (PMS-43), Volume 43: real-variable Methods, Orthogonality, and Oscillatory Integrals. (PMS-43), vol. 3. Princeton University Press, Princeton, NJ (2016)
17. Szabó, B.A., Yosibash, Z.: Numerical analysis of singularities in two dimensions. Part 2: computation of generalized flux/stress intensity factors. Int. J. Numer. Methods Eng. 39(3), 409–434 (1996)
18. Szeg, G.: Orthogonal Polynomials, vol. 23. American Mathematical Soc., Providence, Rhode Island (1939)
19. Xiu, D.: Fast numerical methods for stochastic computations: a review. Commun. Comput. Phys. 5(2–4), 242–272 (2009)
20. Xiu, D.: Numerical Methods for Stochastic Computations: a Spectral Method Approach. Princeton University Press, Princeton, NJ (2010)
21. Xiu, D., Hesthaven, J.S.: High-order collocation methods for differential equations with random inputs. SIAM J. Sci. Comput. 27(3), 1118–1139 (2005)
22. Xiu, D., Karniadakis, G.E.: Modeling uncertainty in flow simulations via generalized polynomial chaos. J. Comput. Phys. 187(1), 137–167 (2003)
23. Xiu, D., Karniadakis, G.E.: A new stochastic approach to transient heat conduction modeling with uncertainty. Int. J. Heat Mass Transf. 46(24), 4681–4693 (2003)
24. Xiu, D., Tartakovsky, D.M.: Numerical methods for differential equations in random domains. SIAM J. Sci. Comput. 28(3), 1167–1185 (2006)
25. Yuan, X.: Lecture notes on orthogonal polynomials of several variables. Adv. Theory Spec. Funct. Orthogonal Polynomials Nova Sci. Publ. 135, 188 (2004)

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