Failure Case for the Smolyak Sparse Quadrature for gPC Expansion

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1 Introduction

Let $(\Omega, \mathcal{F}, \rho)$ be a complete N-variate probability space. We consider the algorithms for expanding a quantity of interest $u(Y)$ as a function of uncertain independent input parameters $Y = (y_1, \cdots, y_n, \cdots, y_N)$ in a generalized polynomial chaos expansion using orthonormal Gaussian polynomials $\phi_i^{(n)}(y_n)$. These Gaussian polynomials are orthonormal with respect to their corresponding individual monovariate probability space $(\Omega_n, \mathcal{F}_n, \rho_n)$. The expansion is given by

$$u(Y) \approx \tilde{u}(Y) = \sum_{k \in \Lambda} c_k \Phi_k(Y), \tag{1}$$

where k is a multivariate index, Λ is a set of N-variate indices corresponding to polynomial orders, and Φ_k are a set of orthonormal multidimensional polynomials given by

$$\Phi_k(Y) = \prod_{n=1}^{N} \phi_{k_n}(y_n). \tag{2}$$

We assume Λ can be constructed adaptively. The admissability condition for new indices k into Λ is

$$k - e_j \in \Lambda \forall 1 \leq j \leq N \tag{3}$$

where e_j is a unit vector in the direction of j.
The scalar coefficients c_k in Eq. 1 can be obtained via the orthonormality of Φ_k as

$$c_k = \int_\Omega \rho(Y) u(Y) \Phi_k(Y) dY \equiv \mathcal{I}\big(u \cdot \Phi_k\big). \tag{4}$$

We approximate the integral using Smolyak-like sparse quadrature. Using the notation for a single-dimension quadrature operation

$$\int \rho(x) f(x) dx = \mathcal{I}(f) \approx \sum_{\ell=1}^{L} w_\ell f(x_\ell) \equiv q^L(f), \tag{5}$$

the sparse quadrature is given by

$$\mathcal{I}\big(u \cdot \Phi\big) \approx \mathcal{S}[u \cdot \Phi] \equiv \sum_{\hat{k} \in \Lambda} s_{\hat{k}} \bigotimes_{n=1}^{N} q^{L_n}\big(u(Y)\Phi_k(Y)\big). \tag{6}$$

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The quadrature coefficient $s_{\hat{k}}$ is given by

$$s_{\hat{k}} = \sum_{j \in \{0,1\}^N, i+j \in \Lambda} (-1)^{|j|_1}, \quad |j|_1 = \sum_{n=1}^{N} j_n. \tag{7}$$

We demonstrate here that for a particular simple response $u(Y)$ and index set Λ, the Smolyak algorithm does not accurately integrate all the quadrature coefficients.

2 Case

For demonstration, we consider the quantity of interest

$$u(x, y) = x^2 y^2, \tag{8}$$

with x and y uniformly distributed from -1 to 1. In this case, we use orthonormalized Legendre polynomials for the expansions polynoials ϕ.
For expansion polynomials, we consider as an example the following polynomial set,

(8,0)								
(7,0)								
(6,0)								
(5,0)								
(4,0)								
(3,0)	(3,1)							
(2,0)	(2,1)	(2,2)						
(1,0)	(1,1)	(1,2)	(1,3)					
(0,0)	(0,1)	(0,2)	(0,3)	(0,4)	(0,5)	(0,6)	(0,7)	(0,8)

Because it includes the index set point (2,2), we expect this expansion to exactly represent the original quantity of interest when coefficients c_k are calculated correctly.

3 Analytic

First, we demonstrate the correct, analytic performance of the gPC expansion. The polynomial coefficients c_k are given by Eq. 4. Each coefficient integrates to zero with the exception of the following:

$$c_{(0,0)} = \frac{1}{9}, \tag{9}$$

$$c_{(0,2)} = c_{(2,0)} = \frac{2}{9\sqrt{5}}, \tag{10}$$

$$c_{(2,2)} = \frac{4}{45}. \tag{11}$$

Reconstructing the original model from the expansion, as expected we recover the original model exactly.

4 Smolyak

In order to be sufficient in a general sense, we desire the Smolyak sparse quadrature algorithm to perform as accurately as the analytic case for this polynomial quantity of interest case. We begin by evaluating the values of the quadrature coefficients $s_{\hat{k}}$. These are all zero with the exception of the following:

$$s_{(0,3)} = s_{(3,0)} = -1, \tag{12}$$

$$s_{(0,8)} = s_{(8,0)} = 1, \tag{13}$$

$$s_{(1,2)} = s_{(2,1)} = -1, \tag{14}$$

$$s_{(1,3)} = s_{(3,1)} = 1, \tag{15}$$

$$s_{(2,2)} = s_{(2,2)} = 1. \tag{16}$$

Using the quadrature order rule $L = k_n + 1$, we will need points and weights for Legendre quadrature orders 1, 2, 3, 4 and 9. The points and weights are listed here for convenience.

Quadrature Order	Points	Weights
1	0	2
2	± 0.5773502691896257	1
3	± 0.7745966692414834	0.5555555555555556
	0	0.8888888888888888
4	± 0.8611363115940526	0.3478548451374538
	± 0.3399810435848563	0.6521451548625461
9	± 0.9681602395076261	0.0812743883615744
	± 0.8360311073266358	0.1806481606948574
	± 0.6133714327005904	0.2606106964029354
	± 0.3242534234038089	0.3123470770400029
	0	0.3302393550012598

There are nine distinct tensor quadratures necessary to construct the Smolyak-like quadrature set, four of which are duplicated because of symmetry. This results in the following Smolyak-like quadrature set:

Tensor	Points
(1)×(4) = (4)×(1)	(0, ± 0.8611363115940526)
	(0, ± 0.3399810435848563)
(1)×(9) = (9)×(1)	(0, ± 0.9681602395076261)
	(0, ± 0.8360311073266358)
	(0, ± 0.6133714327005904)
	(0, ± 0.3242534234038089)
	(0, 0)
(2)×(3) = (3)×(2)	(± 0.5773502691896257, ± 0.7745966692414834)
	(± 0.5773502691896257,0)
(2)×(4) = (4)×(2)	(± 0.5773502691896257, ± 0.8611363115940526)
	(± 0.5773502691896257, ± 0.3399810435848563)
(3)×(3) = (3)×(3)	(± 0.7745966692414834, ± 0.7745966692414834)
	(± 0, ± 0.7745966692414834)
	(± ± 0.7745966692414834, 0)
	(0, 0)

The weights for each ordered set are the product of the weights for each individual point within the set.

We use this quadrature to evaluate Eq. 4. We truncate the values to four digits in tables below, but retain machine precision throughout the calculations. In the calculation tables below, the first two columns are the ordered set (x, y) that make up a realization of the input space. The third and fourth columns are the quadrature weights corresponding to each individual point in the ordered set. The fifth column is the Smolyak quadrature coefficient shown in Eq. 12. The sixth column is the evaluation of the quantity of interest for the provided realization of x and y. The seventh and eighth columns are the orthonormal Legendre polynomials evaluated at their respective realization (quadrature points). Finally, the last column is a product comprising a single term in the quadrature summation.

4.1 c_k, $k = (2,2)$

We first consider the coefficient for $k = (2,2)$ in Table 1.

Points (x)	(y)	Weights w_x	w_y	s_k	$u(x,y)$	$\phi_{k_1}(x)$	$\phi_{k_2}(y)$	$u(x,y) \cdot \Phi_k(x,y) \cdot w_x w_y \cdot s_k$
0.0000	-0.8611	2.0000	0.3479	-1	0.0000	-1.1180	1.3692	0.0000
0.0000	-0.3400	2.0000	0.6521	-1	0.0000	-1.1180	-0.7303	0.0000
0.0000	0.3400	2.0000	0.6521	-1	0.0000	-1.1180	-0.7303	0.0000
0.0000	0.8611	2.0000	0.3479	-1	0.0000	-1.1180	1.3692	0.0000
-0.8611	0.0000	0.3479	2.0000	-1	0.0000	1.3692	-1.1180	0.0000
-0.3400	0.0000	0.6521	2.0000	-1	0.0000	-0.7303	-1.1180	0.0000
0.3400	0.0000	0.6521	2.0000	-1	0.0000	-0.7303	-1.1180	0.0000
0.8611	0.0000	0.3479	2.0000	-1	0.0000	1.3692	-1.1180	0.0000
0.0000	-0.9682	2.0000	0.0813	1	0.0000	-1.1180	2.0259	0.0000
0.0000	-0.8360	2.0000	0.1806	1	0.0000	-1.1180	1.2263	0.0000
0.0000	-0.6134	2.0000	0.2606	1	0.0000	-1.1180	0.1439	0.0000
0.0000	-0.3243	2.0000	0.3123	1	0.0000	-1.1180	-0.7654	0.0000
0.0000	0.0000	2.0000	0.3302	1	0.0000	-1.1180	-1.1180	0.0000
0.0000	0.3243	2.0000	0.3123	1	0.0000	-1.1180	-0.7654	0.0000
0.0000	0.6134	2.0000	0.2606	1	0.0000	-1.1180	0.1439	0.0000
0.0000	0.8360	2.0000	0.1806	1	0.0000	-1.1180	1.2263	0.0000
0.0000	0.9682	2.0000	0.0813	1	0.0000	-1.1180	2.0259	0.0000
-0.9682	0.0000	0.0813	2.0000	1	0.0000	2.0259	-1.1180	0.0000
-0.8360	0.0000	0.1806	2.0000	1	0.0000	1.2263	-1.1180	0.0000
-0.6134	0.0000	0.2606	2.0000	1	0.0000	0.1439	-1.1180	0.0000
-0.3243	0.0000	0.3123	2.0000	1	0.0000	-0.7654	-1.1180	0.0000
0.0000	0.0000	0.3302	2.0000	1	0.0000	-1.1180	-1.1180	0.0000
0.3243	0.0000	0.3123	2.0000	1	0.0000	-0.7654	-1.1180	0.0000
0.6134	0.0000	0.2606	2.0000	1	0.0000	0.1439	-1.1180	0.0000
0.8360	0.0000	0.1806	2.0000	1	0.0000	1.2263	-1.1180	0.0000
0.9682	0.0000	0.0813	2.0000	1	0.0000	2.0259	-1.1180	0.0000
-0.5774	0.7746	1.0000	0.5556	-1	0.2000	0.0000	0.8944	0.0000
-0.5774	0.0000	1.0000	0.8889	-1	0.0000	0.0000	-1.1180	0.0000
-0.5774	-0.7746	1.0000	0.5556	-1	0.2000	0.0000	0.8944	0.0000
0.5774	0.7746	1.0000	0.5556	-1	0.2000	0.0000	0.8944	0.0000
0.5774	0.0000	1.0000	0.8889	-1	0.0000	0.0000	-1.1180	0.0000
0.5774	-0.7746	1.0000	0.5556	-1	0.2000	0.0000	0.8944	0.0000
0.7746	-0.5774	0.5556	1.0000	-1	0.2000	0.8944	0.0000	0.0000
0.0000	-0.5774	0.8889	1.0000	-1	0.0000	-1.1180	0.0000	0.0000
-0.7746	-0.5774	0.5556	1.0000	-1	0.2000	0.8944	0.0000	0.0000
0.7746	0.5774	0.5556	1.0000	-1	0.2000	0.8944	0.0000	0.0000
0.0000	0.5774	0.8889	1.0000	-1	0.0000	-1.1180	0.0000	0.0000
-0.7746	0.5774	0.5556	1.0000	-1	0.2000	0.8944	0.0000	0.0000
-0.5774	-0.8611	1.0000	0.3479	1	0.2472	0.0000	1.3692	0.0000
-0.5774	-0.3400	1.0000	0.6521	1	0.0385	0.0000	-0.7303	0.0000
-0.5774	0.3400	1.0000	0.6521	1	0.0385	0.0000	-0.7303	0.0000
-0.5774	0.8611	1.0000	0.3479	1	0.2472	0.0000	1.3692	0.0000
0.5774	-0.8611	1.0000	0.3479	1	0.2472	0.0000	1.3692	0.0000

0.5774	-0.3400	1.0000	0.6521	1	0.0385	0.0000	-0.7303	0.0000
0.5774	0.3400	1.0000	0.6521	1	0.0385	0.0000	-0.7303	0.0000
0.5774	0.8611	1.0000	0.3479	1	0.2472	0.0000	1.3692	0.0000
-0.8611	-0.5774	0.3479	1.0000	1	0.2472	1.3692	0.0000	0.0000
-0.3400	-0.5774	0.6521	1.0000	1	0.0385	-0.7303	0.0000	0.0000
0.3400	-0.5774	0.6521	1.0000	1	0.0385	-0.7303	0.0000	0.0000
0.8611	-0.5774	0.3479	1.0000	1	0.2472	1.3692	0.0000	0.0000
-0.8611	0.5774	0.3479	1.0000	1	0.2472	1.3692	0.0000	0.0000
-0.3400	0.5774	0.6521	1.0000	1	0.0385	-0.7303	0.0000	0.0000
0.3400	0.5774	0.6521	1.0000	1	0.0385	-0.7303	0.0000	0.0000
0.8611	0.5774	0.3479	1.0000	1	0.2472	1.3692	0.0000	0.0000
-0.7746	-0.7746	0.5556	0.5556	1	0.3600	0.8944	0.8944	0.0889
-0.7746	0.0000	0.8889	0.8889	1	0.0000	0.8944	-1.1180	0.0000
-0.7746	0.7746	0.5556	0.5556	1	0.3600	0.8944	0.8944	0.0889
0.0000	-0.7746	0.5556	0.5556	1	0.0000	-1.1180	0.8944	0.0000
0.0000	0.0000	0.8889	0.8889	1	0.0000	-1.1180	-1.1180	0.0000
0.0000	0.7746	0.5556	0.5556	1	0.0000	-1.1180	0.8944	0.0000
0.7746	-0.7746	0.5556	0.5556	1	0.3600	0.8944	0.8944	0.0889
0.7746	0.0000	0.8889	0.8889	1	0.0000	0.8944	-1.1180	0.0000
0.7746	0.7746	0.5556	0.5556	1	0.3600	0.8944	0.8944	0.0889

Table 1: Numeric Integration of c_k, $k = (2, 2)$

Dividing the sum of the last column by $2^N = 4$ yields a machine-precision accurate result for the analytic value of $c_{(2,2)}$ shown in Eq. 9, 0.0888888888888883. This demonstrates that the Smolyak quadrature is suitable for performing the numerical integral.

4.2 c_k, $k = (6, 0)$

We now consider the coefficient for $k = (6, 0)$ in Table 2.

Points (x)	(y)	Weights w_x	w_y	s_k	$u(x,y)$	$\phi_{k_1}(x)$	$\phi_{k_2}(y)$	$u(x,y) \cdot \Phi_k(x,y) \cdot w_x w_y \cdot s_k$
-0.8611	0.0000	0.3479	2.0000	-1.0000	0.0000	-1.3878	1.0000	0.0000
-0.3400	0.0000	0.6521	2.0000	-1.0000	0.0000	0.7402	1.0000	0.0000
0.3400	0.0000	0.6521	2.0000	-1.0000	0.0000	0.7402	1.0000	0.0000
0.8611	0.0000	0.3479	2.0000	-1.0000	0.0000	-1.3878	1.0000	0.0000
0.0000	-0.9682	2.0000	0.0813	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	-0.8360	2.0000	0.1806	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	-0.6134	2.0000	0.2606	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	-0.3243	2.0000	0.3123	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.0000	2.0000	0.3302	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.3243	2.0000	0.3123	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.6134	2.0000	0.2606	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.8360	2.0000	0.1806	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.9682	2.0000	0.0813	1.0000	0.0000	-1.1267	1.0000	0.0000
-0.9682	0.0000	0.0813	2.0000	1.0000	0.0000	1.5548	1.0000	0.0000
-0.8360	0.0000	0.1806	2.0000	1.0000	0.0000	-1.4919	1.0000	0.0000
-0.6134	0.0000	0.2606	2.0000	1.0000	0.0000	0.4999	1.0000	0.0000
-0.3243	0.0000	0.3123	2.0000	1.0000	0.0000	0.6368	1.0000	0.0000
0.0000	0.0000	0.3302	2.0000	1.0000	0.0000	-1.1267	1.0000	0.0000
0.3243	0.0000	0.3123	2.0000	1.0000	0.0000	0.6368	1.0000	0.0000
0.6134	0.0000	0.2606	2.0000	1.0000	0.0000	0.4999	1.0000	0.0000
0.8360	0.0000	0.1806	2.0000	1.0000	0.0000	-1.4919	1.0000	0.0000
0.9682	0.0000	0.0813	2.0000	1.0000	0.0000	1.5548	1.0000	0.0000
-0.5774	0.7746	1.0000	0.5556	-1.0000	0.2000	0.8012	1.0000	-0.0890
-0.5774	0.0000	1.0000	0.8889	-1.0000	0.0000	0.8012	1.0000	0.0000
-0.5774	-0.7746	1.0000	0.5556	-1.0000	0.2000	0.8012	1.0000	-0.0890
0.5774	0.7746	1.0000	0.5556	-1.0000	0.2000	0.8012	1.0000	-0.0890
0.5774	0.0000	1.0000	0.8889	-1.0000	0.0000	0.8012	1.0000	0.0000
0.5774	-0.7746	1.0000	0.5556	-1.0000	0.2000	0.8012	1.0000	-0.0890
0.7746	-0.5774	0.5556	1.0000	-1.0000	0.2000	-1.2403	1.0000	0.1378
0.0000	-0.5774	0.8889	1.0000	-1.0000	0.0000	-1.1267	1.0000	0.0000
-0.7746	-0.5774	0.5556	1.0000	-1.0000	0.2000	-1.2403	1.0000	0.1378
0.7746	0.5774	0.5556	1.0000	-1.0000	0.2000	-1.2403	1.0000	0.1378
0.0000	0.5774	0.8889	1.0000	-1.0000	0.0000	-1.1267	1.0000	0.0000
-0.7746	0.5774	0.5556	1.0000	-1.0000	0.2000	-1.2403	1.0000	0.1378
-0.5774	-0.8611	1.0000	0.3479	1.0000	0.2472	0.8012	1.0000	0.0689
-0.5774	-0.3400	1.0000	0.6521	1.0000	0.0385	0.8012	1.0000	0.0201
-0.5774	0.3400	1.0000	0.6521	1.0000	0.0385	0.8012	1.0000	0.0201
-0.5774	0.8611	1.0000	0.3479	1.0000	0.2472	0.8012	1.0000	0.0689
0.5774	-0.8611	1.0000	0.3479	1.0000	0.2472	0.8012	1.0000	0.0689
0.5774	-0.3400	1.0000	0.6521	1.0000	0.0385	0.8012	1.0000	0.0201
0.5774	0.3400	1.0000	0.6521	1.0000	0.0385	0.8012	1.0000	0.0201
0.5774	0.8611	1.0000	0.3479	1.0000	0.2472	0.8012	1.0000	0.0689
-0.8611	-0.5774	0.3479	1.0000	1.0000	0.2472	-1.3878	1.0000	-0.1193

-0.3400	-0.5774	0.6521	1.0000	1.0000	0.0385	0.7402	1.0000	0.0186
0.3400	-0.5774	0.6521	1.0000	1.0000	0.0385	0.7402	1.0000	0.0186
0.8611	-0.5774	0.3479	1.0000	1.0000	0.2472	-1.3878	1.0000	-0.1193
-0.8611	0.5774	0.3479	1.0000	1.0000	0.2472	-1.3878	1.0000	-0.1193
-0.3400	0.5774	0.6521	1.0000	1.0000	0.0385	0.7402	1.0000	0.0186
0.3400	0.5774	0.6521	1.0000	1.0000	0.0385	0.7402	1.0000	0.0186
0.8611	0.5774	0.3479	1.0000	1.0000	0.2472	-1.3878	1.0000	-0.1193
-0.7746	-0.7746	0.5556	0.5556	1.0000	0.3600	-1.2403	1.0000	-0.1378
-0.7746	0.0000	0.8889	0.8889	1.0000	0.0000	-1.2403	1.0000	0.0000
-0.7746	0.7746	0.5556	0.5556	1.0000	0.3600	-1.2403	1.0000	-0.1378
0.0000	-0.7746	0.5556	0.5556	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.0000	0.8889	0.8889	1.0000	0.0000	-1.1267	1.0000	0.0000
0.0000	0.7746	0.5556	0.5556	1.0000	0.0000	-1.1267	1.0000	0.0000
0.7746	-0.7746	0.5556	0.5556	1.0000	0.3600	-1.2403	1.0000	-0.1378
0.7746	0.0000	0.8889	0.8889	1.0000	0.0000	-1.2403	1.0000	0.0000
0.7746	0.7746	0.5556	0.5556	1.0000	0.3600	-1.2403	1.0000	-0.1378

Table 2: Numeric Integration of c_k, $k = (6, 0)$

Dividing the sum of the last column by $2^N = 4$ yields the value -0.1007265118224860, but the analytic value for this polynomial coefficient is zero. This demonstrates that Smoyak sparse grid quadrature as outlined above is not suitable for performing the numeric integral.

5 Conclusion

Having outlined an implementation of gPC expansion and Smolyak sparse quadrature algorithms, along with a particular response function, we have demonstrated cases where the Smolyak quadrature both does and does not work well. Because there are numerical integrals the Smolyak algorithm cannot perform well, it seems unsuitable for general integration of polynomial expansion coefficients in arbitrary polynomial sets for gPC expansions.

It is my hope that I have erred at some point, and that the Smolyak algorithm is more suitable than shown here.