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 $Y = (y_1, \dots, y_n, \dots, y_N)$ 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

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

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

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

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

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

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

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

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

We demonstrate here that for a particular index set Λ , the Smolyak algorithm does not accurately integrate the quadrature coefficients.

2 Case

For demonstration, we consider the quantity of interest

$$u(x,y) = x^2 y^2, (8)$$

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.

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:

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

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

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

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:

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

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

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

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

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

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	0.555555555555556	
	0	0.88888888888888	
4	± 0.8611363115940526	0.3478548451374538	
	$\pm\ 0.3399810435848563$	0.6521451548625461	
9	± 0.9681602395076261	0.0812743883615744	
	$\pm\ 0.8360311073266358$	0.1806481606948574	
	$\pm\ 0.6133714327005904$	0.2606106964029354	
	$\pm\ 0.3242534234038089$	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	
$(1)\times(4) = (4)\times(1)$	$(0, \pm 0.8611363115940526)$	
	$(0, \pm 0.3399810435848563)$	
$(1)\times(9) = (9)\times(1)$	$(0, \pm 0.9681602395076261)$	
	$(0, \pm 0.8360311073266358)$	
	$(0, \pm 0.6133714327005904)$	
	$(0, \pm 0.3242534234038089)$	
	(0, 0)	
$(2)\times(3) = (3)\times(2)$	$(\pm \ 0.5773502691896257, \pm \ 0.7745966692414834)$	
	$(\pm\ 0.5773502691896257,0)$	
$(2)\times(4) = (4)\times(2)$	$(\pm\ 0.5773502691896257, \pm\ 0.8611363115940526)$	
	$(\pm 0.5773502691896257, \pm 0.3399810435848563)$	
$(3)\times(3) = (3)\times(3)$	$(\pm 0.7745966692414834, \pm 0.7745966692414834)$	
	$(\pm 0, \pm 0.7745966692414834)$	
	$(\pm \pm 0.7745966692414834, 0)$	
	(0, 0)	

We use this quadrature to evaluate Eq. 4. Because u(x=0,y)=u(x,y=0)=0, quadrature points containing a zero value for either x or y will not be shown here. We also truncate the points to four digits here, but retain them all throughout the calculations. We first consider the coefficient for (2,2):

Point	Weight s	$\int_{\mathbb{R}} \left \ u(x_{\ell}, y_{\ell}) \right $	$\phi_2^{(1)}(x_\ell)\phi_2^{(2)}(y_\ell)$	$u(x_{\ell}, y_{\ell}) \cdot \phi_2^{(1)}(x_{\ell}) \phi_2^{(2)}(y_{\ell}) \cdot s_{\hat{k}} \cdot \text{ weight}$
(-0.5774, -0.7746)	-			
(-0.5774, 0.7746)	-	L		
(0.5774, -0.7746)	-	L		
(0.5774, 0.7746)	-	L		
(-0.7746, -0.5774)	-	L		
(-0.7746, 0.5774)	-	L		
(0.7746, -0.5774)	-	L		
(0.7746, 0.5774)	-	L		
(-0.5774, -0.8611)	1			
(-0.5774, -0.3400)	1			
(-0.5774, -0.3400)]			
(-0.5774, 0.3400)]			