

ERROR ESTIMATES FOR THE ANOVA METHOD WITH POLYNOMIAL CHAOS INTERPOLATION: TENSOR PRODUCT FUNCTIONS*

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Abstract. We focus on the analysis of variance (ANOVA) method for high dimensional function approximation using Jacobi polynomial chaos to represent the terms of the expansion. First, we develop a weight theory inspired by quasi-Monte Carlo theory to identify which functions have low effective dimension using the ANOVA expansion in different norms. We then present estimates for the truncation error in the ANOVA expansion and for the interpolation error using multielement polynomial chaos in the weighted Korobov spaces over the unit hypercube. We consider both the standard ANOVA expansion using the Lebesgue measure and the anchored ANOVA expansion using the Dirac measure. The optimality of different sets of anchor points is also examined through numerical examples.

Key words. anchored ANOVA, effective dimension, weights, anchor points, integration error, truncation error

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NOTATION.

c, c_k : points in one dimension

$\mathbf{c}$: point in high dimension

$\mathbf{c}^k$: optimal anchor points in different norms

D_s : mean effective dimension

d_s : effective dimension

$f_{\{i\}}$: i th first-order terms in analysis of variance (ANOVA) decomposition

$f^{(i)}$: function of the i th dimension of a high dimensional tensor product function

G_i : i th Genz function

$I(\cdot)$: integration of the function “.” over $[0, 1]^N$ or $[0, 1]$

$\mathcal{I}_{N,\nu}f$: truncated ANOVA expansion with only terms of order lower than $\nu + 1$

$\mathcal{I}_{N,\nu,\mu}f$: multielement approximation of $\mathcal{I}_{N,\nu}f$ with tensor products of μ th order polynomials in each element

$L^2(\cdot)$: space of square integrable functions over the domain “.”; the domain will be dropped if no confusion occurs

$L^\infty(\cdot)$: space of essentially bounded functions over the domain “.”; the domain will be dropped as above

N : dimension of a high dimensional function

w_k : sampled points from a uniform distribution on $[0, 1]$

μ : polynomial order

ν : truncation dimension

τ_k : mean of the function $f^{(k)}$; λ_k^2 : variance of the function $f^{(k)}$

$\sigma^2(\cdot)$: variance of the function “.”

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1. Introduction. Functional ANOVA refers to the decomposition of an N -dimensional function f as follows [9]:

$$(1.1) \quad f(x_1, x_2, \dots, x_N) = f_\phi + \sum_{j_1=1}^N f_{\{j_1\}}(x_{j_1}) + \sum_{j_1 < j_2}^N f_{\{j_1, j_2\}}(x_{j_1}, x_{j_2}) \\ + \dots + f_{\{j_1, \dots, j_N\}}(x_{j_1}, \dots, x_{j_N}),$$

where f_ϕ is a constant and f_S are $|S|$ -dimensional functions called the $|S|$ -order terms. (Here $|S|$ denotes the cardinality of the index set S with $S \subseteq \{1, 2, \dots, N\}$.)

The terms in the ANOVA decomposition over the domain $[0, 1]^N$ (we consider this a hypercube for simplicity in this paper) are

$$(1.2a) \quad f_\phi = \int_{[0,1]^N} f(\mathbf{x}) d\mu(\mathbf{x}),$$

$$(1.2b) \quad f_S(\mathbf{x}_S) = \int_{[0,1]^{-S}} f(\mathbf{x}) d\mu(\mathbf{x}_{-S}) - \sum_{T \subsetneq S} f_T(\mathbf{x}_T),$$

where $-S$ is the complement set of the nonempty set S with respect to $\{1, 2, \dots, N\}$.

We note that there are different types of ANOVA decomposition associated with different measures; here we focus on two types. In the first, we use the Lebesgue measure, $d\mu(x) = \rho(x) dx$ ($\rho(x) = 1$ in this paper), and we will refer to it as *standard* ANOVA expansion. In the second, we use the Dirac measure, $d\mu(x) = \delta(x - c) dx$ ($c \in [0, 1]$), and we will refer to it as *anchored* ANOVA expansion. Recall that $\int_0^1 f(x) d\mu(x) = f(c)$ if $d\mu(x) = \delta(x - c) dx$.

All ANOVA terms are mutually orthogonal with respect to the corresponding measure. That is, for every term f_S ,

$$\int_0^1 f_S(\mathbf{x}_S) d\mu(x_j) = 0 \quad \text{if } j \in S; \quad \int_{[0,1]^N} f_S(\mathbf{x}_S) f_T(\mathbf{x}_T) d\mu(\mathbf{x}) = 0 \quad \text{if } S \neq T.$$

Recently, the ANOVA method has been used in solving partial differential equations (PDEs) and stochastic PDEs (SPDEs). Griebel [9] gave a review of the ANOVA method for high dimensional approximation and used the ANOVA method to construct finite element spaces to solve PDEs. Todor and Schwab [20] employed the anchored ANOVA in conjunction with a sparsifying polynomial chaos method and studied its convergence rate based on the analyticity of the stochastic part of the underlying solution to SPDEs. Foo and Karniadakis [6] applied the anchored ANOVA to solve elliptic SPDEs, highlighting its efficiency for high dimensional problems. Bieri and Schwab [2] considered the convergence rate of the truncated anchored ANOVA in polynomial chaos methods and stochastic collocation methods for analytic functions. Cao, Chen, and Gunzburger [4] used the anchored ANOVA to investigate the impact of uncertain boundary conditions on solutions of nonlinear PDEs and on optimization problems. Yang et al. [27] demonstrated the effectiveness of an adaptive ANOVA algorithm in simulating flow problems with 100 dimensions.

In numerical solutions for SPDEs, tensor product functions are mostly used since mutual independence among stochastic dimensions is assumed. For the same reason, many test functions and functions in finance are of the tensor product form; see [4, 14, 23]. The basic problem therein is how well we can approximate high dimensional tensor product functions with a truncated ANOVA expansion and what the proper

interpolation of the retained terms is. Thus, the objective of the current paper is to provide rigorous error estimates for the truncation error of the ANOVA expansion for *continuous* tensor product functions and also for the interpolation error associated with the discrete representation of the ANOVA terms. This discretization is performed based on the multielement Jacobi polynomial chaos [21], hence the convergence of the discrete ANOVA representation depends on four parameters: the anchor point $\mathbf{c}$ (anchored ANOVA), the truncation dimension ν that determines the truncation of the ANOVA expansion, the Jacobi polynomial chaos order μ , and the size of the multielements h .

The paper is organized as follows. In the next section we apply the weight theory, based on quasi-Monte Carlo (QMC) theory, characterizing the importance of each dimension that will allow us to determine the effective dimension both for the standard ANOVA and for the anchored ANOVA. In section 3 we derive error estimates for the anchored ANOVA for *continuous* functions, while in section 4 we provide similar estimates for the standard ANOVA. In section 5 we present more numerical examples for different test functions, and we conclude in section 6 with a brief summary. The appendix includes details of proofs.

2. Weights and effective dimension for tensor product functions. The order at which we truncate the ANOVA expansion is defined as the *effective dimension* [16, 3, 22, 14] provided that the difference between the ANOVA expansion and the truncated one in a certain measure is very small. (See (2.3) below for a definition.) Caflisch, Morokoff, and Owen [3] have explained the success of the QMC approach using the concept of effective dimension; see also [16, 18, 19, 13, 14, 15, 22, 25].

2.1. Standard ANOVA. It can be readily shown that the variance of f is the sum of the variances of the standard ANOVA terms, i.e.,

$$(2.1) \quad \sigma^2(f) = \int_{[0,1]^N} f^2(\mathbf{x}) d\mathbf{x} - \left(\int_{[0,1]^N} f(\mathbf{x}) d\mathbf{x} \right)^2 = \sum_{\emptyset \neq S \subseteq \{1,2,\dots,N\}} \int_{[0,1]^{|S|}} f_S^2(\mathbf{x}_S) d\mathbf{x}_S,$$

or in compact form

$$(2.2) \quad \sigma^2(f) = \sum_{\emptyset \neq S \subseteq \{1,2,\dots,N\}} \sigma_S^2(f_S).$$

The *effective dimension* of f (in the superposition sense, [3]) is the smallest integer d_s satisfying

$$(2.3) \quad \sum_{0 < |S| \leq d_s} \sigma_S^2(f_S) \geq p\sigma^2(f),$$

where $S \subset \{1,2,\dots,N\}$. This implies that we neglect terms in the ANOVA decomposition with more than d_s th order terms. Here p is a constant, $0 < p < 1$, but closer to 1, with, e.g., $p = 0.99$ in [3]. We call N the nominal dimension, i.e., the dimensionality of the function f .

In this paper, we consider tensor product functions and define the weights similarly to QMC error theory [18, 5, 22, 24]. Specifically, in QMC theory, there are two different approaches in determining the weights. In [18], they first choose the weights and subsequently determine the sampling points (QMC sequences) based on Korobov spaces via minimization of the error bounds, where the error bounds are set

up via the ANOVA decomposition; see also [5, 22]. In contrast, in [24] the weights are determined according to sensitivity indices by using the so-called matching strategy. In the current work, we utilize the weights differently in that we use them to characterize the classes of functions which can be well approximated with truncated ANOVA expansion and multielement methods in different norms. Our approach can be applied only to tensor product functions.

When tensor product functions are considered, the importance of each term can be evaluated from the first-order terms in standard ANOVA expansion. We define the tensor product function $f(\mathbf{x}) = f^{(1)}(x_1) \otimes \cdots \otimes f^{(N)}(x_N) =: \otimes_{k=1}^N f^{(k)}(x_k)$, where $f^{(k)}(x_k)$ are univariate functions in the x_k -directions. In this situation, the ANOVA terms and the corresponding variances are

$$f_S = \otimes_{k \in S} (f^{(k)}(x_k) - \tau_k) \cdot \prod_{k \notin S} \tau_k, \quad \sigma_S^2(f_S) = \prod_{k \in S} \lambda_k^2 \prod_{k \notin S} \tau_k^2,$$

where the means and the variances of the one-dimensional functions are

$$\tau_k = \int_0^1 f^{(k)}(x_k) dx_k < \infty, \quad \lambda_k^2 = \int_0^1 (f^{(k)}(x_k) - \tau_k)^2 dx_k < \infty, \quad k = 1, 2, \dots, N.$$

Note that the relative importance of each S term (compared to the zeroth-order term f_ϕ) can be estimated in the following way:

$$\frac{\sigma_S^2(f_S)}{\prod_{k=1}^N \tau_k^2} = \prod_{k \in S} \frac{\lambda_k^2}{\tau_k^2},$$

which are products of ratios for the first-order terms. This motivates us to define the weights γ_k^A as

$$(2.4) \quad \gamma_k^A = \frac{\lambda_k^2}{\tau_k^2} \quad \text{if } \tau_k \neq 0, \quad k = 1, 2, \dots, N.$$

These weights can be considered as a special case of the weights presented in [22, 5]. For a low effective dimension, the majority of the weights should be strictly less than one.¹

In the standard ANOVA expansion, the effective dimension, denoted by d_s , is directly related to the truncation error. By definition we have, denoting the term $\sum_{|S| \leq d_s} f_S$ by $\mathcal{I}_{N,d_s} f$, that

$$(2.5) \quad \|f - \mathcal{I}_{N,d_s} f\|_{L^2}^2 \leq (1-p)(\|f\|_{L^2}^2 - (I(f))^2),$$

where $\|f\|_{L^2}^2 = (I(f))^2 + \sigma^2(f)$ and $I(f) = \int_{[0,1]^N} f dx$. Hence, we have

$$\frac{\|f - \mathcal{I}_{N,d_s} f\|_{L^2}}{\|f\|_{L^2}} \leq \sqrt{1-p} \left(1 - \prod_{k=1}^N (1 + \gamma_k^A)^{-1}\right)^{\frac{1}{2}} < \sqrt{1-p}.$$

This estimate represents the worst case since we approximate $(1 - \prod_{k=1}^N (1 + \gamma_k^A)^{-1})^{\frac{1}{2}} \approx 1$, while in practice it can be much smaller than one, as shown in Example 2.2 below.

¹Note that this definition of weights is not applicable if $\tau_k = 0$.

We can also derive the following inequality, which we will use later. From the definition of weights, we have $\|f - \mathcal{I}_{N,d_s} f\|_{L^2}^2 = (I(f))^2 \sum_{m=d_s+1}^N \sum_{|S|=m} \prod_{k \in S} \gamma_k^A$. According to (2.5), we have an equivalent definition of the effective dimension

$$(2.6) \quad \sum_{m=d_s+1}^N \sum_{|S|=m} \prod_{k \in S} \gamma_k^A \leq (1-p) \left(\prod_{k=1}^N (1 + \gamma_k^A) - 1 \right).$$

When a function is of tensor product, a similar but simpler expression for the effective dimension, the *mean effective dimension* [14], can be derived in terms of the weights:

$$(2.7) \quad D_s = \frac{\sum_{k=1}^N \frac{\gamma_k^A}{\gamma_k^A + 1}}{1 - \prod_{k=1}^N \frac{1}{\gamma_k^A + 1}} = \frac{N - \sum_{k=1}^N \frac{1}{\gamma_k^A + 1}}{1 - \prod_{k=1}^N \frac{1}{\gamma_k^A + 1}}$$

if $\tau_k \neq 0$ for all $k = 1, 2, \dots, N$.

It is worth mentioning that d_s , by the definition (2.3), can be only an integer while the mean effective dimension D_s can be a noninteger, which may have some advantages in practice. As an illustration, we consider in Example 2.1 a Sobol function with effective dimension $d_s = 2$ corresponding to $p = 0.99$, which suggests that we need $\binom{1000+2}{2} = 500500$ second-order terms to reach the 0.99 threshold. On the other hand, the mean effective dimension is $D_s = 1.06$, which suggests that many fewer second-order terms are required.

Example 2.1. Consider the Sobol function $f(\mathbf{x}) = \otimes_{k=1}^{1000} \frac{|4x_k - 2| + a_k}{1 + a_k}$ with $a_k = k^2$. By (2.3) and (2.7), $d_s = 2$ and $D_s = 1.06$. In this case, we employ the following procedure to find the most important terms in the standard ANOVA and investigate how one can reach the 0.99 of the variance of this function. First, compute the weights γ_k^A ($k = 1, 2, \dots, N$) by (2.4), and then compute the ratios

$$r_k = \frac{\gamma_k^A}{1 + \sum_{i=1}^N \gamma_i^A}.$$

Set a threshold ϵ and let $M = \max_{1 \leq k \leq N} \{k | r_k \geq \epsilon\}$. Then, compute $r_{i,j}$ ($i, j = 1, \dots, M$):

$$r_{i,j} = \frac{\gamma_i^A \gamma_j^A}{1 + \sum_{i=1}^N \gamma_i^A + \sum_{k,l=1}^M \gamma_k^A \gamma_l^A}.$$

Set a threshold η and denote $K = \max_{1 \leq i \leq M} \{i | r_{i,i+1} \geq \eta\}$. Hence, $\frac{K(K+1)}{2}$ second-order terms are required. We note that the number of second-order terms for $d_s = 2$, $\binom{1000+2}{2} = 500500$, is several orders of magnitude larger than the number of terms listed in the last column of Table 2.1. We also note that all first-order terms contribute 98.39 percent of variance for this 1000 dimensional Sobol function.

Next, we present three more examples in order to appreciate the utility of weights.

Example 2.2. Compare the Genz function G_5 [8] and a function g_5 we define here as follows:

$$G_5 = \otimes_{j=1}^N \exp(-c_j |x_j - w_j|), \quad g_5 = \otimes_{j=1}^N \exp(-c_j (x_j - w_j)).$$

Here $c_i = \exp(0.2i)$, $N = 10$, and

$$(w_1, \dots, w_{10}) = (0.695106, 0.851463, 0.413355, 0.410178, \\ 0.226185, 0.7078, 0.478756, 0.183078, 0.0724332, 0.483279),$$

where w_i are sampled from uniform distribution random variables on $[0, 1]$ [8].

TABLE 2.1

Second-order terms needed in the truncated standard ANOVA expansion for small relative variance error: Sobol function with $a_k = k^2$, $\sigma^2(f) = 1.0395e - 01$.

ϵ	η	Error	Relative error	Terms required
1e-04	1e-08	3.3270e-05	3.2006e-04	21
1e-04	1e-07	4.6856e-05	4.5076e-04	15
1e-04	1e-06	1.2148e-04	1.1687e-03	6
1e-04	1e-05	2.3682e-04	2.2783e-03	3
1e-04	1e-04	5.5905e-04	5.3781e-03	1

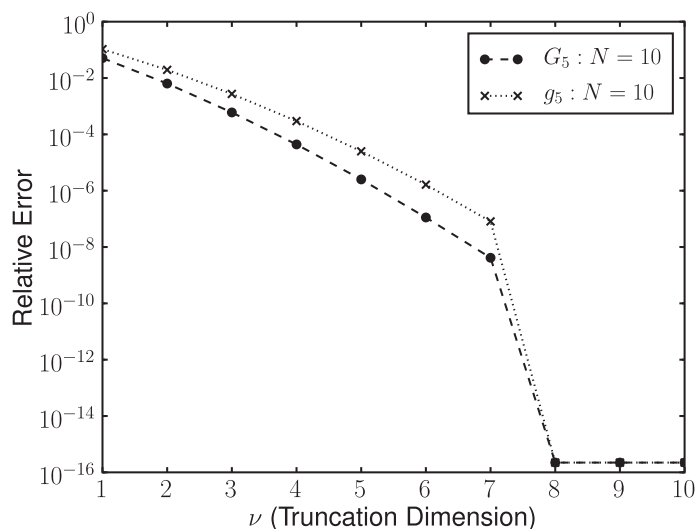


FIG. 2.1. Relative error $\frac{\|f - \mathcal{I}_{N,\nu}(f)\|_{L^2}}{\|f\|_{L^2}}$ versus truncation dimension ν with nominal dimension $N = 10$ for G_5 and g_5 .

TABLE 2.2

Weights for G_5 and g_5 with $N = 10$.

k	$\gamma_k^A(G_5)$	$\gamma_k^A(g_5)$
1	2.3859 e-2	5.5246 e-2
2	2.8857 e-2	3.7167 e-2
3	7.2403 e-3	2.4974 e-2
4	4.9209 e-3	1.6768 e-2
5	6.8950 e-3	1.1257 e-2
6	3.5777 e-3	7.5484 e-3
7	1.2794 e-3	5.0624 e-3
8	2.4467 e-3	3.3945 e-3
9	2.1451 e-3	2.2759 e-3
10	3.8402 e-4	1.5258 e-3

Note that g_5 is much *smoother* than G_5 , but the truncation error for g_5 is worse than that for G_5 , as shown in Figure 2.1. This is because G_5 has smaller weights, as shown in Table 2.2. In Figure 2.1, there is a sudden drop since the terms of 8, 9, and 10 orders are contributing little, noting that $\sum_{|S|=7} \sigma_S^2(G_{5S}) = 1.2594e - 15$ and $\sum_{|S|=8}^{10} \sigma_S^2(G_{5S}) < 1.4246e - 18$. (This phenomenon happens in Figure 2.2 as well, where smaller weights lead to earlier sudden drops.)

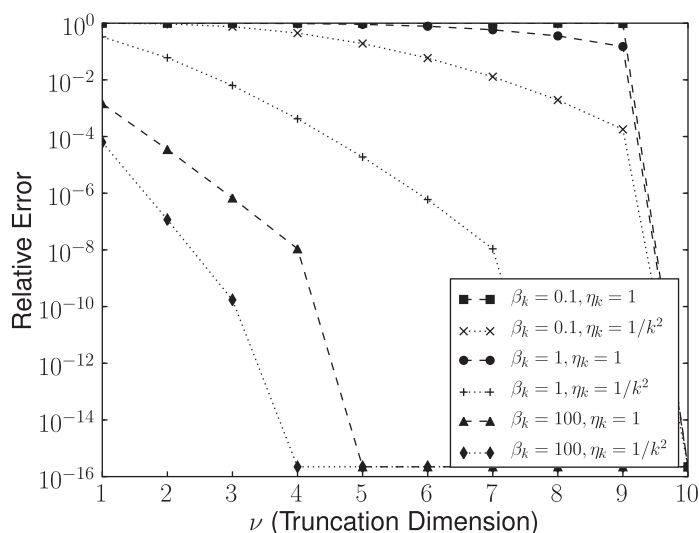


FIG. 2.2. Relative error $\frac{\|f - \mathcal{I}_{N,\nu}(f)\|_{L^2}}{\|f\|_{L^2}}$ versus truncation dimension ν with nominal dimension $N = 10$ for the Bernoulli function.

TABLE 2.3

Ratios of the sum of the variances of f_S up to $|S| = \nu$ over the variance of the function: comparison between G_5 and g_5 .

ν	1	2	3	4
$\frac{\sum_{0 < S \leq \nu} \sigma_S^2(G_{5,S})}{\sigma^2(G_5)}$	0.9691861	0.99951933	0.99999573	0.99999998
$\frac{\sum_{0 < S \leq \nu} \sigma_S^2(g_{5,S})}{\sigma^2(g_5)}$	0.9362764	0.99784671	0.99995787	0.99999950

Table 2.3 shows the ratios of the sum of the variances of the subset S up to $|S| = \nu$ over the variances of the functions G_5 and g_5 . Notice that the effective dimension for both functions is 2. It is worth noting that the relative error is much smaller than 0.1 in Figure 2.1, as we pointed out earlier.

Example 2.3. Next we consider a function in a weighted Korobov space (see section 3):

$$(2.8) \quad f(\mathbf{x}) = \otimes_{k=1}^N (\beta_k + 2\pi^2 \eta_k B_2(\{x_k - y_k\}))$$

with $B_2(x) = x^2 - x + \frac{1}{6}$ the Bernoulli polynomial of order 2 and $\{\cdot\}$ denoting the fractional part of a real number “.”. The means and variances are $\tau_k = \beta_k$, $\lambda_k^2 = \frac{\pi^4}{45} \eta_k^2$. Taking $\beta_k = 1$ for every k leads to $\gamma_k^A = \frac{\lambda_k^2}{\beta_k^2} = \frac{\pi^4}{45} \eta_k^2$, which are not equal to the weights $\frac{2\pi^2 \eta_k}{\beta_k} = 2\pi^2 \eta_k^2$ for the weighted Korobov space (see Remark 3.3).

Clearly, $\eta_k = 1$ for every k leads to γ_k^A larger than 1. In this case, each dimension is important, so this case results in a high effective dimension. For example, when $N = 100$, $d_s = 71$; also $d_s = 109$ when $N = 200$ and $d_s = 161$ when $N = 500$. However, if η_k is smaller than 1, then a low effective dimension can be expected. For example, when $\eta_k = \frac{1}{k^2}$, the effective dimension is 2, even if N is very large. Typical results for different choices of β_k, η_k are shown in Figure 2.2 for $N = 10$.

TABLE 2.4
 $(\beta_k, \eta_k), k = 1, \dots, N, N = 10$, and corresponding effective dimensions d_s .

(β_k, η_k)	$(0.1, 1/k^2)$	$(0.1, 1.0)$	$(100, 1/k^2)$	$(100, 1.0)$	$(1.0, 1/k^2)$	$(1.0, 1.0)$
d_s	6	10	1	1	2	10

Note that for high β_k and small η_k the weight is very small, close to 0, which implies low effective dimension of the standard ANOVA expansion; see Table 2.4.

Example 2.4 (a counterexample). Here we consider tensor products of monomials, $f = \otimes_{k=1}^{10} x_k^n$, and aim to use the “weight” theory to obtain the maximum monomial order n when using the standard ANOVA. We have for the mean and variance in each dimension that

$$\tau_k = \int_0^1 x_k^n dx_k = \frac{1}{n+1}, \quad \lambda_k^2 = \int_0^1 \left(x_k^n - \frac{1}{n+1} \right)^2 dx_k = \frac{n^2}{(2n+1)(n+1)^2}.$$

The weights γ_k^A here are $\frac{n^2}{2n+1}$, where $k = 1, \dots, 10$. Thus, for the weights to be smaller than 1, n has to be less than 3, which is a severe restriction. So even for a smooth function, as the monomial x^3 is in each dimension, the effective dimension may not be small. For example, the relative variance error with ANOVA terms up to sixth order is only 0.5239.

2.2. Anchored ANOVA. In the anchored ANOVA expansion it is not so clear how to define the weights and in which norm. Also, the choice of the anchor points is important to the efficiency of the anchored ANOVA truncation. Motivated by the fact that smaller weights lead to smaller relative variance errors, we may define weights in different norms, starting with the L^∞ -norm. Specifically, we define the weights as follows:

$$(2.9) \quad \gamma_k^\infty = \frac{\|f^{(k)} - f^{(k)}(c_k)\|_{L^\infty}}{|f^{(k)}(c_k)|} \quad \text{when} \quad f(\mathbf{c}) = \prod_{k=1}^N f^{(k)}(c_k) \neq 0.$$

THEOREM 2.5. *If there exists $p_{\bar{\nu}} \in (0, 1)$ such that*

$$\sum_{m=\bar{\nu}+1}^N \sum_{|S|=m} \prod_{k \in S} \gamma_k^\infty \leq (1 - p_{\bar{\nu}}) \left(\prod_{k=1}^N (1 + \gamma_k^\infty) - 1 \right),$$

then the relative error of the truncated anchored ANOVA expansion can be bounded by

$$(2.10) \quad \frac{\|f - \mathcal{I}_{N, \bar{\nu}} f\|_{L^\infty}}{\|f\|_{L^\infty}} \leq (1 - p_{\bar{\nu}}) \left(\prod_{k=1}^N (1 + \gamma_k^\infty) - 1 \right) \left(\prod_{k=1}^N \frac{|f^{(k)}(c_k)|}{\|f^{(k)}\|_{L^\infty}} \right).$$

The weights (2.9) are minimized if all the $f^{(k)}$ are nonnegative or nonpositive and the anchor point $\mathbf{c}^2 = (c_1^2, c_2^2, \dots, c_N^2)$ is chosen such that

$$f^{(k)}(c_k^2) = \frac{1}{2} \max_{x_k \in [0, 1]} f^{(k)}(x_k) + \frac{1}{2} \min_{x_k \in [0, 1]} f^{(k)}(x_k), \quad k = 1, 2, \dots, N.$$

For the proof of this theorem and all other proofs in this subsection, please refer to the appendix.

Remark 2.6. From the weights definition (2.9), it holds that

$$\left\| f^{(k)} - f^{(k)}(c_k) \right\|_{L^\infty} \leq \gamma_k^\infty \left| f^{(k)}(c_k) \right| \leq \gamma_k^\infty \left\| f^{(k)} \right\|_{L^\infty}.$$

If we assume, as in [2], that $\|\partial_{x_k} f^{(k)}\|_{L^\infty} \leq \rho_k \|f^{(k)}\|_{L^\infty}$, then

$$\left\| f^{(k)} - f^{(k)}(c_k) \right\|_{L^\infty} \leq \left\| \partial_{x_k} f^{(k)} \right\|_{L^2} \leq \left\| \partial_{x_k} f^{(k)} \right\|_{L^\infty} \leq \rho_k \left\| f^{(k)} \right\|_{L^\infty}.$$

In other words, ρ_k in [2] plays the role of weight γ_k^∞ in our approach.

We may define the weights with respect to integration as follows:

$$\gamma_k^{int} = \frac{\left| \int_{[0,1]} f^{(k)} dx - f^{(k)}(c_k) \right|}{\left| f^{(k)}(c_k) \right|} \quad \text{when} \quad f(\mathbf{c}) = \prod_{k=1}^N f^{(k)}(c_k) \neq 0.$$

Of course, if we choose $f^{(k)}(c_k^3) = \int_{[0,1]} f^{(k)} dx$, then we are simply using the standard ANOVA expansion and $\gamma_k^{int} = 0$. In order to avoid this trivial choice, the weights can be defined as in [10], i.e.,

$$\gamma_k^Q = \frac{\left| Q_k(f^{(k)}) - f^{(k)}(c_k) \right|}{\left| f^{(k)}(c_k) \right|} \quad \text{when} \quad f(\mathbf{c}) = \prod_{k=1}^N f^{(k)}(c_k) \neq 0,$$

where Q_k is a quadrature rule used for numerical integration. Note that the best choice for anchor points then satisfies $f^{(k)}(c_k^4) = Q_k(f^{(k)})$ for any k .

The error estimate for the case using the weights with respect to integration can also be obtained in the same fashion as in the proof of Theorem 2.5. The relative integration error will be, taking $f^{(k)}(c_k) = (1 - \alpha_k)\tau_k$,

$$\left| \frac{I(\mathcal{I}_{N,\nu} f) - I(f)}{I(f)} \right| = \left| \sum_{m=\nu+1}^N \sum_{|S|=m} \prod_{k \in S} \frac{\alpha_k}{1 - \alpha_k} \prod_{k=1}^N (1 - \alpha_k) \right|.$$

When $|\alpha_k| \ll 1$, $\gamma_k^{int} = \left| \frac{\alpha_k}{1 - \alpha_k} \right| \ll 1$ and then by (2.6),

$$\begin{aligned} \left| \frac{I(\mathcal{I}_{N,\nu} f) - I(f)}{I(f)} \right| &\leq \sum_{m=\nu+1}^N \sum_{|S|=m} \prod_{k \in S} \left| \frac{\alpha_k}{1 - \alpha_k} \right| \prod_{k=1}^N (1 - \alpha_k) \\ &\leq (1 - p_\nu) \left(\prod_{k=1}^N \left(1 + \left| \frac{\alpha_k}{1 - \alpha_k} \right| \right) - 1 \right) \prod_{k=1}^N (1 - \alpha_k), \end{aligned}$$

if p_ν exists, and thus we will have a small relative error.

Similarly, we define weights using the L^2 -norm as

$$(2.11) \quad \gamma_k^{L^2} = \frac{\left\| f^{(k)} - f^{(k)}(c_k) \right\|_{L^2}}{\left| f^{(k)}(c_k) \right|} \quad \text{when} \quad f(\mathbf{c}) = \prod_{k=1}^N f^{(k)}(c_k) \neq 0.$$

THEOREM 2.7. *If there exists $p_{\bar{\nu}} \in (0, 1)$ such that*

$$\sum_{m=\bar{\nu}+1}^N \sum_{|S|=m} \prod_{k \in S} \gamma_k^{L^2} \leq (1 - p_{\bar{\nu}}) \left(\prod_{k=1}^N (1 + \gamma_k^{L^2}) - 1 \right),$$

TABLE 2.5

Relative integration errors for G_5 using different anchor points according to different criteria.

ν	$\epsilon_{\nu, \mathbf{c}^1}(G_5)$	$\epsilon_{\nu, \mathbf{c}^2}(G_5)$	$\epsilon_{\nu, \mathbf{c}^4}(G_5)$	$\epsilon_{\nu, \mathbf{c}^5}(G_5)$
0	4.3118 e-1	9.2379 e-2	2.3196 e-3	8.4200 e-2
1	6.6207 e-2	3.7949 e-3	6.5030 e-7	2.6350 e-3
2	5.2552 e-3	8.8265 e-5	1.2577 e-9	4.1197 e-5
3	2.3796 e-4	1.2680 e-6	3.0718 e-13	3.6539 e-7
4	6.2412 e-6	1.1568 e-8	1.2815 e-13	1.9498 e-9

then the relative error of the truncated anchored ANOVA expansion can be bounded by

$$(2.12) \quad \frac{\|f - \mathcal{I}_{N, \bar{\nu}} f\|_{L^2}}{\|f\|_{L^2}} \leq (1 - p_{\bar{\nu}}) \left(\prod_{k=1}^N (1 + \gamma_k^{L^2}) - 1 \right) \left(\prod_{k=1}^N \frac{|f^{(k)}(c_k)|}{\|f^{(k)}\|_{L^2}} \right).$$

The weights (2.11) are minimized if all the $f^{(k)}$ are nonnegative or nonpositive and the anchor point $\mathbf{c}^5 = (c_1^5, c_2^5, \dots, c_N^5)$ is chosen such that for $k = 1, \dots, N$, $f^{(k)}(c_k^5) = \frac{\lambda_k^2 + \tau_k^2}{\tau_k}$.

Remark 2.8. In Theorem 2.7, the weights, with the choice $\mathbf{c}^5$, are $\gamma_k^{L^2} = (1 + \frac{\tau_k^2}{\lambda_k^2})^{-\frac{1}{2}}$, which reveals that the ratios of the variances and square of means indeed matter.

2.3. Comparison of different choices of anchor points. In this subsection, we will show how to choose the anchor points using different criteria in order to reduce the ANOVA integration and truncation errors.

Example 2.9 (Example 2.2 revisited). Consider the Genz function G_5 [8]

$$G_5 = \otimes_{i=1}^N \exp(-c_i |x_i - w_i|) =: \otimes_{i=1}^N f^{(k)}(x_k),$$

$N = 10$; c_i and w_i are exactly the same as in Example 2.2.

Here $\mathbf{c}^1$ is the centered point in $[0, 1]$, i.e., $\mathbf{c}^1 = (\frac{1}{2}, \frac{1}{2}, \dots, \frac{1}{2})$, and $\mathbf{c}^2$ is chosen such that $f^{(k)}(c_k^2) = \frac{1}{2}(\min_{x_k \in [0, 1]} f^{(k)}(x_k) + \max_{x_k \in [0, 1]} f^{(k)}(x_k))$. Note that this point in each dimension will give minimized weights in the L^∞ -norm. Also, $\mathbf{c}^3$ is the anchor point such that $f^{(k)}(c_k^3) = \tau_k = \int_0^1 f^{(k)}(x) dx$, which will lead to the standard ANOVA expansion. The anchor point $\mathbf{c}^4$ is determined by $f^{(k)}(c_k^4) = Q^m(f_k) = \sum_{i=1}^m f^{(k)}(x_i^{(k)}) \omega_i^{(k)}$, where $(x_i^{(k)}, \omega_i^{(k)})_{i=1}^m$ come from Gauss–Legendre quadrature with $m = 3$; $\mathbf{c}^5$ is the anchor point minimizing the weights $\frac{\|f^{(k)} - f^{(k)}(c_k)\|_{L^2}}{|f^{(k)}(c_k)|}$.

First, consider multidimensional integration by comparing the relative integration error $\epsilon_{\nu, \mathbf{c}^k}(G_5) = \frac{|I(\mathcal{I}_{N, \nu} G_5) - I(G_5)|}{|I(G_5)|}$ ($k = 1, 2, 4, 5$). In Table 2.5, we note that the point $\mathbf{c}^4$, which is the “numerical analog” of $\mathbf{c}^3$, gives the best convergence rates for numerical integration using the anchored ANOVA expansion. This is expected since the weights in that case are especially designed for integration.

Next, let us consider the L^2 -norm, which concerns the integration of the square of functions. In Table 2.6 and Figure 2.3, we compare the truncation errors $\varepsilon_{\nu, \mathbf{c}^k}(G_5) = \|G_5 - \mathcal{I}_{N, \nu} G_5\|_{L^2}$, where $\mathcal{I}_{N, \nu} G_5$ is the truncated anchored ANOVA using $\mathbf{c}^k$, $k = 1, \dots, 5$.

It is interesting to compare the truncation error in the L^2 -norm and also the integration error, e.g., for the points $\mathbf{c}^1$ and $\mathbf{c}^2$. From Tables 2.5 and 2.6, the error associated with $\mathbf{c}^2$ is always smaller than that associated with $\mathbf{c}^1$. This can be explained

TABLE 2.6
Truncation errors $\|G_5 - \mathcal{I}_{N,\nu}(G_5)\|_{L^2}$ using different anchor points.

ν	$\varepsilon_{\nu, \mathbf{c}^1}(G_5)$	$\varepsilon_{\nu, \mathbf{c}^2}(G_5)$	$\varepsilon_{\nu, \mathbf{c}^3}(G_5)$	$\varepsilon_{\nu, \mathbf{c}^4}(G_5)$	$\varepsilon_{\nu, \mathbf{c}^5}(G_5)$
0	2.7232 e-2	9.3491 e-3	8.4888 e-3	8.4893 e-3	9.2035 e-3
1	1.9309 e-3	3.1582 e-4	2.6157 e-4	2.6161 e-4	2.9707 e-4
2	6.0135 e-5	5.3350 e-6	4.0803 e-6	4.0810 e-6	4.7440 e-6
3	9.4136 e-7	5.0200 e-8	3.6252 e-8	3.6259 e-8	4.2518 e-8
4	7.8926 e-9	2.7706 e-10	1.9402 e-10	1.9407 e-10	2.2720 e-10

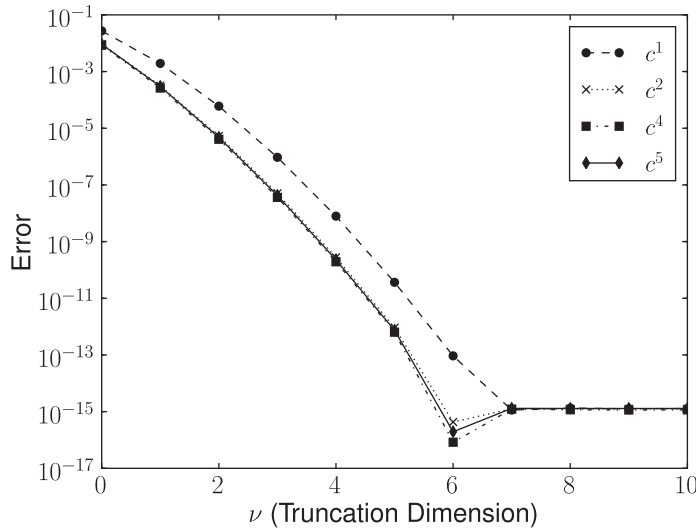


FIG. 2.3. Truncation error $\|G_5 - \mathcal{I}_{N,\nu}G_5\|_{L^2}$ versus truncation dimension ν for different anchor points: $N = 10$.

TABLE 2.7
Comparison between weights with respect to different measures using anchor points $\mathbf{c}^1$ and $\mathbf{c}^2$.

i	$\gamma_i^{int}(\mathbf{c}^1)$	$\gamma_i^{int}(\mathbf{c}^2)$	$\gamma_i^{L^2}(\mathbf{c}^1)$	$\gamma_i^{L^2}(\mathbf{c}^2)$
1	6.1592 e-2	2.1521 e-2	2.1142 e-2	1.9858 e-2
2	9.3640 e-5	9.7456 e-3	2.2804 e-2	2.3099 e-2
3	8.6163 e-2	1.0477 e-2	1.2845 e-2	6.4699 e-3
4	7.0501 e-2	1.0342 e-2	8.8571 e-3	4.5330 e-3
5	1.5179 e-2	1.6346 e-2	6.2548 e-3	6.4742 e-3
6	2.3611 e-2	1.4545 e-2	3.7274 e-3	3.5203 e-3
7	5.4349 e-2	1.0850 e-3	4.0766 e-3	1.2060 e-3
8	5.5157 e-3	9.5996 e-3	2.2984 e-3	2.3895 e-3
9	2.0810 e-4	3.2642 e-3	1.9996 e-3	2.0156 e-3
10	3.0928 e-2	6.7473 e-4	1.3142 e-3	3.7199 e-4

by the smaller weights, as shown in Table 2.7, leading to better error behavior. Here $\gamma_i^{int}(\mathbf{c}^k)$ is the i th weight associated with integration using the points $\mathbf{c}^k$ and $\gamma_i^{L^2}(\mathbf{c}^k)$ the i th weight associated with the L^2 -norm using the points $\mathbf{c}^k$. For more examples, see section 5.

3. Error estimates of anchored ANOVA for continuous functions. In this section we derive an estimate for the truncation error of anchored ANOVA expansion in the Korobov space, $K_\gamma^r([0, 1])$, a special type of Sobolev–Hilbert spaces.

We first consider the one-dimensional case and assume that r is an integer. This space is equipped with the inner product

$$\langle f, g \rangle_{K_\gamma^r([0,1])} = f(c)g(c) + \gamma^{-1} \left(\sum_{k=1}^{r-1} \partial_x^k f(c) \partial_x^k g(c) + \int_0^1 \partial_x^r f \partial_x^r g(x) dx \right).$$

Correspondingly, the norm of f in the Korobov space is $\|f\|_{K_\gamma^r([0,1])} = \langle f, f \rangle_{K_\gamma^r([0,1])}^{\frac{1}{2}}$. When $r > \frac{1}{2}$ is not an integer, the corresponding space can be well defined through the Hilbert space interpolation theory; see Adams [1].

Denote $K_\gamma^r([0,1]) \times K_\gamma^r([0,1]) \cdots \times K_\gamma^r([0,1])$ (N times) by $K_\gamma^r([0,1])^{\otimes N}$. Then $K_\gamma^r([0,1])^{\otimes N}$ is a Hilbert space with the inner product

$$\langle f, g \rangle_{K_\gamma^r([0,1])^{\otimes N}} = \prod_{k=1}^N \langle f^{(k)}, g^{(k)} \rangle_{K_\gamma^r([0,1])}$$

for $f = \otimes_{k=1}^N f^{(k)}$, $g = \otimes_{k=1}^N g^{(k)}$ with $f^{(k)}, g^{(k)} \in K_\gamma^r([0,1])$; that is $K_\gamma^r([0,1])^{\otimes N}$ is the completion of linear combinations of tensor product functions. Here we are especially concerned with tensor product functions $f = \otimes_{k=1}^N f^{(k)} \in K_\gamma^r([0,1])^{\otimes N}$, whose norms are $\|f\|_{K_\gamma^r([0,1])^{\otimes N}} = \prod_{k=1}^N \|f^{(k)}\|_{K_\gamma^r([0,1])}$. Specifically, in the domain of interest for anchored ANOVA, the weighted Korobov space can be decomposed as [9]

$$K_\gamma^r([0,1]) = \text{span}\{1\} \oplus K_{\gamma,0}^r([0,1]),$$

where $K_{\gamma,0}^r([0,1]) = \{f \in K_\gamma^r([0,1]) | f(c) = 0\}$.

In the following, we will discuss the approximation error in the L^2 -norm for tensor product functions in the weighted Korobov spaces. We split the estimate into two parts: $\|f - \mathcal{I}_{N,\nu,\mu} f\|_{L^2([0,1]^N)} \leq \|f - \mathcal{I}_{N,\nu} f\|_{L^2([0,1]^N)} + \|\mathcal{I}_{N,\nu} f - \mathcal{I}_{N,\nu,\mu} f\|_{L^2([0,1]^N)}$. We call the first and second terms in the right-hand side *truncation error* and *interpolation error*, respectively. Here $\mathcal{I}_{N,\nu,\mu} f = \sum_{\substack{S \subseteq \{1,2,\dots,N\} \\ |S| \leq \nu}} \mathfrak{I}_{S,\nu,\mu} f_S$, where $\mathfrak{I}_{S,\nu,\mu}$ is the $|S|$ -dimensional finite element interpolation operator with μ th order polynomial in each interval of each dimension with $\mathfrak{I}_{S,\nu,\mu} f_S \in L^\infty([0,1]^S)$.

3.1. Truncation error.

THEOREM 3.1. *Suppose that the tensor product function f belongs to $K_\gamma^r([0,1])^{\otimes N}$. Then the truncation error of the anchored ANOVA expansion can be bounded as*

$$\|f - \mathcal{I}_{N,\nu} f\|_{L^2([0,1]^N)} \leq (C_1 \gamma 2^{-2r})^{\frac{\nu+1}{2}} \sum_{\substack{S \subseteq \{1,2,\dots,N\} \\ |S| \geq \nu+1}} (C_1 \gamma 2^{-2r})^{\frac{|S|-\nu-1}{2}} \|f_S\|_{K_\gamma^r([0,1])^{\otimes |S|}},$$

where the constant C_1 is from Lemma 3.2.

We need the following lemma to prove this theorem. See the appendix for the proof of the lemma.

LEMMA 3.2. *There exists a complete orthonormal basis $\{\psi_i\}_{i=2}^\infty$ in $K_{1,0}^r([0,1])$ such that $(\psi_i, \psi_j)_{L^2([0,1])} = \lambda_i \delta_{ij}$ and $\{1, \psi_2, \psi_3, \dots\}$ forms a complete orthogonal basis in $L^2([0,1])$, where $\lambda_2 \geq \lambda_3 \geq \dots \geq 0$ and $\lambda_i \leq C_1 i^{-2r}$, C_1 decreases with r for all i .*

Proof of Theorem 3.1. We first prove that for any function f in $K_{\gamma,0}^r([0,1])$, it holds that

$$(3.1) \quad \|f\|_{L^2([0,1])} \leq (C_1 \gamma)^{\frac{1}{2}} 2^{-r} \|f\|_{K_\gamma^r([0,1])}.$$

By Lemma 3.2, for $f \in K_{\gamma,0}^r([0,1])$, we have $f = \sum_{i=2}^{\infty} f_i \psi_i$ and

$$\begin{aligned} \|f\|_{L^2([0,1])}^2 &= \left\| \sum_{i=2}^{\infty} f_i \psi_i \right\|_{L^2([0,1])}^2 = \sum_{i=2}^{\infty} f_i^2 \|\psi_i\|_{L^2([0,1])}^2 = \sum_{i=2}^{\infty} f_i^2 \lambda_i \\ &= \gamma \sum_{i=2}^{\infty} f_i^2 \gamma^{-1} \lambda_i \leq C_1 \gamma 2^{-2r} \sum_{i=2}^{\infty} f_i^2 \gamma^{-1} \leq C_1 \gamma 2^{-2r} \|f\|_{K_{\gamma}^r([0,1])}^2. \end{aligned}$$

Noting that $\|f_S\|_{L^2([0,1]^S)} \leq (\gamma^{|S|} (C_1 2^{-2r})^{|S|})^{\frac{1}{2}} \|f_S\|_{K_{\gamma}^r([0,1])^{\otimes |S|}}$, a tensor product version of (3.1), we have

$$\begin{aligned} \|f - \mathcal{I}_{N,\nu} f\|_{(L^2([0,1])^N)} &\leq \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \geq \nu+1}} \|f_S\|_{L^2([0,1]^{|S|})} \\ &\leq \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \geq \nu+1}} (\gamma^{|S|} (C_1 2^{-2r})^{|S|})^{\frac{1}{2}} \|f_S\|_{K_{\gamma}^r([0,1])^{\otimes |S|}} \\ &\leq (C_1 \gamma 2^{-2r})^{\frac{\nu+1}{2}} \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \geq \nu+1}} (C_1 \gamma 2^{-2r})^{\frac{|S|-\nu-1}{2}} \|f_S\|_{K_{\gamma}^r([0,1])^{\otimes |S|}}. \end{aligned}$$

Therefore, we may expect the truncation error to decrease when ν goes to N if $C_1 \gamma 2^{-2r} < 1$ and the summation in the last inequality is bounded.

Remark 3.3. The weight γ in the Korobov space can be defined as $\frac{\|f^{(k)}\|_{K_{\gamma}^r([0,1])}^2}{|f^{(k)}(c_k)|^2} -$

1. The role of the weight γ is to lift the norm of the derivative of $f^{(k)}$ to the level of $f^{(k)}(c_k)$.

3.2. Interpolation error. Here we consider the interpolation operator $\mathcal{I}_{N,\nu,\mu}$ as an approximation to $\mathcal{I}_{N,\nu}$: $\mathcal{I}_{N,\nu,\mu} f = \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \leq \nu}} \mathcal{J}_{S,\nu,\mu} f_S$, where

$$\mathcal{J}_{S,\nu,\mu} f_S = \otimes_{k \in S} (\mathbb{I}_{\mu}^h f^{(k)} - f^{(k)}(c_k)) \prod_{k \notin S} f^{(k)}(c_k), \quad f_S = \otimes_{k \in S} (f^{(k)} - f^{(k)}(c_k)),$$

$\mathbb{I}_{\mu}^h$ is the Lagrange interpolation operator such that $\mathbb{I}_{\mu}^h f^{(k)}(y)|_{y=y_m^j} = f^{(k)}(y_m^j)$, $y_m^j = jh + h\frac{1+x_m}{2}$, $j = 0, 1, \dots, J-1$ ($Jh = 1$), and $m = 0, 1, \dots, \mu$. Here $x_m \in [-1, 1]$ ($0 \leq m \leq \mu$) are Gauss–Jacobi or Gauss–Jacobi–Radau or Gauss–Jacobi–Lobatto quadrature points and the indices associated with the Jacobi polynomial are $(1-x)^{\alpha}(1+x)^{\beta}$ with $(\alpha, \beta) \in (-1, 0] \times (-1, 0]$. Here we may drop the continuity condition as in [7, 21] in the context of probabilistic collocation and stochastic Galerkin methods.

THEOREM 3.4. *If a tensor product function f lies in $K_{\gamma}^r([0,1])^{\otimes N}$, $r > \frac{1}{2}$, then the interpolation error of the truncated anchored ANOVA expansion can be estimated as*

$$\|\mathcal{I}_{N,\nu} f - \mathcal{I}_{N,\nu,\mu} f\|_{L^2([0,1]^N)} \leq C_2 \nu^{\frac{1}{2}} 2^{-k} h^k \mu^{-r} \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \leq \nu}} \gamma^{\frac{|S|}{2}} \|f_S\|_{K_{\gamma}^r([0,1])^{\otimes |S|}},$$

where $k = \min(r, \mu + 1)$ and the constant C_2 depends solely on r .

Proof. First recall that if ψ belongs to the standard Hilbert space $H^r([0, 1])$, where $r > \frac{1}{2}$, we have

$$(3.2) \quad \|\psi - \mathbb{I}_\mu^1 \psi\|_{L^2([0, 1])} \leq C_2 h^k 2^{-k} \mu^{-r} \|\partial_x^r \psi\|_{L^2([0, 1])},$$

where $\mathbb{I}_\mu^1 = \mathbb{I}_\mu^h|_{h=1}$, $k = \min(r, \mu + 1)$, $r > \frac{1}{2}$, and C_2 depends only on r . See Ma [12] and Li [11] for proofs.

By (3.2), for fixed S , we have

$$\|f_S - \mathfrak{I}_{S, \nu, \mu} f_S\|_{L^2([0, 1]^{|S|})} \leq C_2 \sum_{n \in S} h^k 2^{-k} \mu^{-r_n} \|\partial_{x_n}^{r_n} f_S\|_{L^2([0, 1]^{|S|})},$$

where $r_n = r$ is the regularity index of f_S as a function of x_n . Thus, taking $\gamma_n = \gamma$ gives

$$(3.3) \quad \|f_S - \mathfrak{I}_{S, \nu, \mu} f_S\|_{L^2([0, 1]^{|S|})} \leq C_2 |S|^{\frac{1}{2}} (\gamma^{\frac{|S|}{2}} h^k 2^{-k} \mu^{-r}) \|f_S\|_{K_\gamma^r([0, 1])^{\otimes |S|}}.$$

Here we have utilized the inequality of $(a_1 + a_2 + \cdots + a_n) \leq n^{\frac{1}{2}}(a_1^2 + a_2^2 + \cdots + a_n^2)^{\frac{1}{2}}$ for real numbers.

Following (3.3), we then have

$$\begin{aligned} \|\mathcal{I}_{N, \nu} f - \mathcal{I}_{N, \nu, \mu} f\|_{L^2([0, 1]^N)} &\leq \sum_{\substack{S \subseteq \{1, 2, \dots, N\} \\ 1 \leq |S| \leq \nu}} \|f_S - \mathfrak{I}_{S, \nu, \mu} f_S\|_{L^2([0, 1]^{|S|})} \\ &\leq \sum_{\substack{\emptyset \neq S \subseteq \{1, \dots, N\} \\ |S| \leq \nu}} C_2 |S|^{\frac{1}{2}} h^k 2^{-k} \mu^{-r} \gamma^{\frac{|S|}{2}} \|f_S\|_{K_\gamma^r([0, 1])^{\otimes |S|}} \\ &\leq C_2 \nu^{\frac{1}{2}} h^k 2^{-k} \mu^{-r} \sum_{\substack{\emptyset \neq S \subseteq \{1, \dots, N\} \\ |S| \leq \nu}} \gamma^{\frac{|S|}{2}} \|f_S\|_{K_\gamma^r([0, 1])^{\otimes |S|}}. \end{aligned}$$

This ends the proof. $\square$

Remark 3.5. Taking $h = 1$ in Theorem 3.4 gives the following estimate:

$$\|\mathcal{I}_{N, \nu} f - \mathcal{I}_{N, \nu, \mu} f\|_{L^2([0, 1]^N)} \leq C \nu^{\frac{1}{2}} 2^{-k} \mu^{-r} \sum_{\substack{\emptyset \neq S \subseteq \{1, \dots, N\} \\ |S| \leq \nu}} \gamma^{\frac{|S|}{2}} \|f_S\|_{K_\gamma^r([0, 1])^{\otimes |S|}}.$$

It is worth mentioning that the factor in front of μ^{-r} can be very large if N is large. Also large ν can lead to large values of the summation since there are $\sum_{k=1}^{\nu} \binom{N}{k} \approx \nu \binom{N}{\frac{N}{2}}$ terms even if $\nu < \frac{N}{2}$. And again, if the weights are not small, then the norm of f_S can be very large; the norms can be small and grow relatively slowly with ν when the weights are much smaller than 1.

Remark 3.6. Section 5 of [23] gives an example of functions in Korobov spaces in applications. The function is of a tensor product, $f(\mathbf{x}) = \otimes_{k=1}^N \exp(a_k \Phi^{-1}(x_k))$, where $a_k = O(N^{-\frac{1}{2}})$, $k = 1, 2, \dots, N$, and $\Phi^{-1}(x)$ is the inverse of $\Phi(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^x \exp(-\frac{t^2}{2}) dt$. It can be readily checked that

$$\gamma_k = \frac{\lambda_k^2}{\tau_k^2} = \frac{\exp(a_k^2)(\exp(a_k^2) - 1)}{(\exp(\frac{1}{2}a_k^2))^2} = \exp(a_k^2) - 1, \quad k = 1, 2, \dots, N,$$

and according to (2.7), $D_s = O(1)$. This implies that the problem is of *low effective dimension*. These weights decay fast, thus contributing to the fast convergence rate in the approximation.

Remark 3.7 (multielement interpolation error for piecewise continuous functions). For piecewise continuous functions, the interpolation error can be bounded as

$$\|\mathcal{I}_{N,\nu}f - \mathcal{I}_{N,\nu,\mu}f\|_{L^2([0,1]^N)} \leq C\nu^{\frac{1}{2}} \left(\frac{h}{2}\right)^{\mu+1} \mu^{-r} \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \leq \nu}} \gamma^{\frac{|S|}{2}} \|f_S\|_{K_\gamma^r([0,1]^{\otimes |S|})},$$

where h is the length of one edge in an element, ν the truncation dimension, and μ the polynomial order and the constant C depends only on r .

4. Error estimates of (Lebesgue) ANOVA for continuous functions.

The results for the standard ANOVA with the Lebesgue measure are very similar to the results for the anchored ANOVA. We present them here without any proofs as the proofs are similar to those in section 3. Here we will adopt another weighted Korobov space $H_\gamma^r([0,1])$. For an integer r , the space is equipped with the inner product

$$\langle f, g \rangle_{H_\gamma^r([0,1])} = I(f)I(g) + \gamma^{-1} \left(\sum_{k=1}^{r-1} I(\partial_x^k f)I(\partial_x^k g) + I(\partial_x^r f \partial_x^r g) \right)$$

and the norm $\|f\|_{H_\gamma^r([0,1])} = \sqrt{\langle f, f \rangle_{H_\gamma^r([0,1])}}$. Again using the Hilbert space interpolation [1], such a space with noninteger r can be defined. The product space $H_\gamma^r([0,1])^{\otimes N} := H_\gamma^r([0,1]) \times \dots \times H_\gamma^r([0,1])$ (N times) is defined in the same way of defining $K_\gamma^r([0,1])^{\otimes N}$ in section 3.

THEOREM 4.1 (truncation error). *Assume that the tensor product function f belongs to $H_\gamma^r([0,1])^{\otimes N}$. Then the truncation error of the standard ANOVA expansion can be bounded as*

$$\|f - \mathcal{I}_{N,\nu}f\|_{L^2([0,1]^N)} \leq (C\gamma 2^{-2r})^{\frac{\nu+1}{2}} \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \geq \nu+1}} (C\gamma 2^{-2r})^{\frac{|S|-\nu-1}{2}} \|f_S\|_{H_\gamma^r([0,1]^{\otimes |S|})},$$

where the constant C is decreasing with r .

The proof of this theorem is similar to that of Theorem 3.1. One first finds a complete orthogonal basis both in $L^2([0,1]) \cap \{f : I(f) = 0\}$ and $H_1^r([0,1]) \cap \{f : I(f) = 0\}$ by investigating the eigenvalue problem of the Rayleigh quotient $\frac{\|f\|_{L^2([0,1])}^2}{\|f\|_{H_1^r([0,1])}^2}$ (see the appendix for the definition of the eigenvalue problem) and following the proof of Theorem 3.1. The following theorem can be proved in the same fashion as Theorem 3.4.

THEOREM 4.2 (interpolation error). *Assume that the tensor product function f lies in $H_\gamma^r([0,1])^{\otimes N}$, where $r > \frac{1}{2}$. Then the interpolation error of the standard ANOVA expansion can be bounded as*

$$\|\mathcal{I}_{N,\nu}f - \mathcal{I}_{N,\nu,\mu}f\|_{L^2([0,1]^N)} \leq C\nu^{\frac{1}{2}} 2^{-k} h^k \mu^{-r} \sum_{\substack{S \subset \{1,2,\dots,N\} \\ |S| \leq \nu}} \gamma^{\frac{|S|}{2}} \|f_S\|_{H_\gamma^r([0,1]^{\otimes |S|})},$$

where $k = \min(r, \mu + 1)$, $\mathcal{I}_{N,\nu,\mu}f$ is defined as in section 3.2, and the constant C depends solely on r .

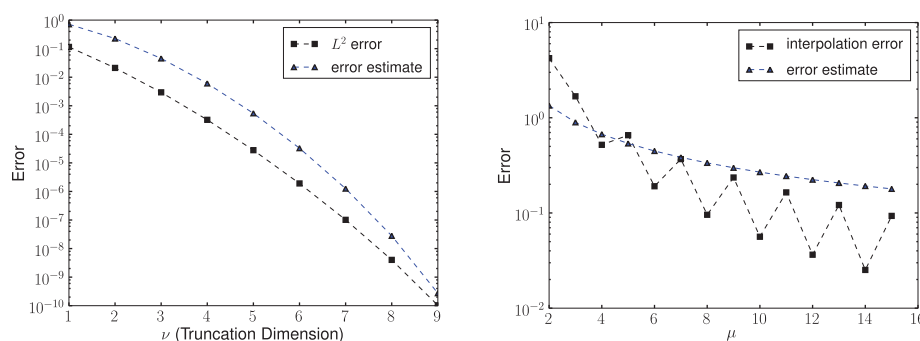


FIG. 5.1. Truncation and interpolation error in L^2 : comparison of numerical results against error estimates from Theorems 4.1 and 4.2. Left: truncation error; right: interpolation error.

TABLE 5.1
Relative integration errors for G_4 using different anchor points: $N = 10$.

ν	$\epsilon_{\nu, \mathbf{c}^1}(G_4)$	$\epsilon_{\nu, \mathbf{c}^2}(G_4)$	$\epsilon_{\nu, \mathbf{c}^4}(G_4)$	$\epsilon_{\nu, \mathbf{c}^5}(G_4)$
0	2.8111 e-2	3.1577 e-2	6.9005 e-6	5.4637 e-2
1	5.5920 e-3	1.0985 e-2	3.9702 e-10	1.8717 e-2
2	6.3516 e-4	2.4652 e-3	1.4093 e-14	3.5770 e-3
3	4.6657 e-5	3.7620 e-4	2.7825 e-15	4.3819 e-4
4	2.3331 e-6	4.0082 e-5	9.6520 e-15	3.6379 e-5
5	8.0681 e-8	2.9961 e-6	3.6533 e-14	2.0833 e-6
6	1.9081 e-9	1.5455 e-7	3.4521 e-14	8.1459 e-8

5. Numerical results. Here we provide numerical results, which verify the aforementioned theorems and show the effectiveness of the anchored ANOVA expansion and its dependence on different anchor points.

5.1. Verification of the error estimates. We compute the truncation error in the standard ANOVA expansion of the Sobol's function $f(\mathbf{x}) = \otimes_{k=1}^N \frac{|4x_k - 2| + a_k}{1 + a_k}$, where we compute the error for $a_k = 1$, k , and k^2 with $N = 10$. In Figure 5.1 we show numerical results for $a_k = k$ and $N = 10$ along with the error estimates that demonstrate good agreement. For $a_k = 1$ and k^2 , we have similar trends for the decay of error, and in particular we observe that larger a_k (hence, smaller weights) will lead to faster error decay.

Compared to Figure 2.1, there is no sudden drop in Figure 5.1 (left) since the weights $\gamma_k^A = \frac{1}{3(1+k)^2}$ are basically larger than those of G_5 in Example 2.2 and decay slowly; this points to the importance of higher-order terms in the standard ANOVA expansion. In Figure 5.1 (right), we note that small μ may not admit good approximations of the ANOVA terms.

5.2. Genz function G_4 [8]. Consider a 10-dimensional Genz function $G_4 = \exp(-\sum_{i=1}^{10} x_i^2)$, where the relative integration error and the truncation error are considered. In this case, only second-order terms are required for obtaining small integration error in Table 5.1. For the truncation error, shown in Table 5.2, more terms are required to reach a level of 10^{-3} , and the convergence is rather slow. Note that for this example, the sparse grid method of Smolyak [17] does not work well either.

5.3. Genz function G_5 [8]. Here we address the errors in different norms using different anchor points. Recall that $\mathbf{c}^1$ is the centered point and $\mathbf{c}^2, \mathbf{c}^4$, and $\mathbf{c}^5$ are

TABLE 5.2

Truncation error $\|G_4 - \mathcal{I}_{N,\nu}(G_4)\|_{L^2}$ versus truncation dimension ν using different anchor points: $N = 10$.

ν	$\varepsilon_{\nu, \mathbf{c}^1}(G_4)$	$\varepsilon_{\nu, \mathbf{c}^2}(G_4)$	$\varepsilon_{\nu, \mathbf{c}^3}(G_4)$	$\varepsilon_{\nu, \mathbf{c}^4}(G_4)$	$\varepsilon_{\nu, \mathbf{c}^5}(G_4)$
0	6.1149 e-2	6.2818 e-2	5.4305 e-2	5.4305 e-2	7.7034 e-2
1	3.6243 e-2	3.9884 e-2	2.8965 e-2	2.8965 e-2	5.3008 e-2
2	1.6569 e-2	1.9881 e-2	1.2297 e-2	1.2297 e-2	2.6415 e-2
3	6.0440 e-3	7.9242 e-3	4.2887 e-3	4.2887 e-3	1.0098 e-2
4	1.7925 e-3	2.5497 e-3	1.2472 e-3	1.2472 e-3	3.0503 e-3
5	4.3473 e-4	6.6163 e-4	3.0346 e-4	3.0346 e-4	7.3564 e-4
6	8.5654 e-5	1.3662 e-4	6.1292 e-5	6.1292 e-5	1.4083 e-4
7	1.3402 e-5	2.1745 e-5	1.0045 e-5	1.0045 e-5	2.0877 e-5
8	1.5799 e-6	2.4900 e-6	1.2688 e-6	1.2688 e-6	2.2590 e-6
9	1.2184 e-7	1.7163 e-7	1.0819 e-7	1.0754 e-7	1.5257 e-7

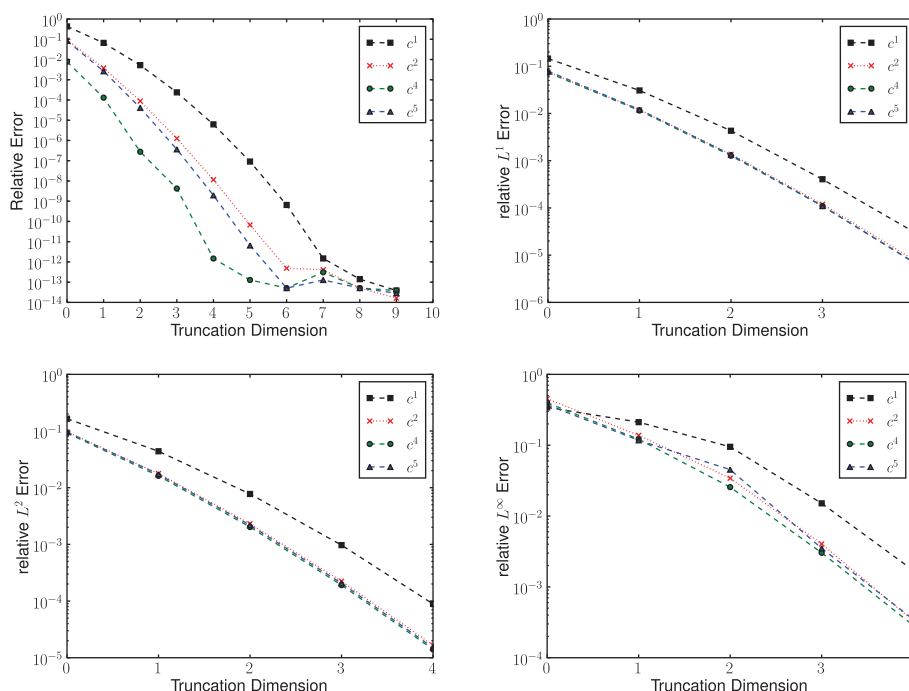


FIG. 5.2. Testing Genz function G_5 using different anchor points in different measure. Top left: relative integration error; top right: relative error in the L^1 -norm; lower left: relative error in the L^2 -norm; lower right: relative error in the L^∞ -norm.

defined exactly as in Example 2.9. For these four different choices of anchor points, we test two cases: (i) relative error of numerical integration using the anchored ANOVA expansion and (ii) approximation error using the anchored ANOVA expansion in different norms; see Figure 5.2. In both cases $\mathbf{c}^4$ gives the best approximation followed by $\mathbf{c}^5$. Observe that for this example $\mathbf{c}^4$ among the four anchor points gives the best approximation to the function with respect to the L^1 -, L^2 -, and L^∞ -norms although the theorems in section 2 imply that different measures will lead to different “optimal” points.

We have also verified numerically that the numerical integration error is bounded by the approximation error with respect to L^1 - and L^∞ -norms as shown in Figure 5.3.

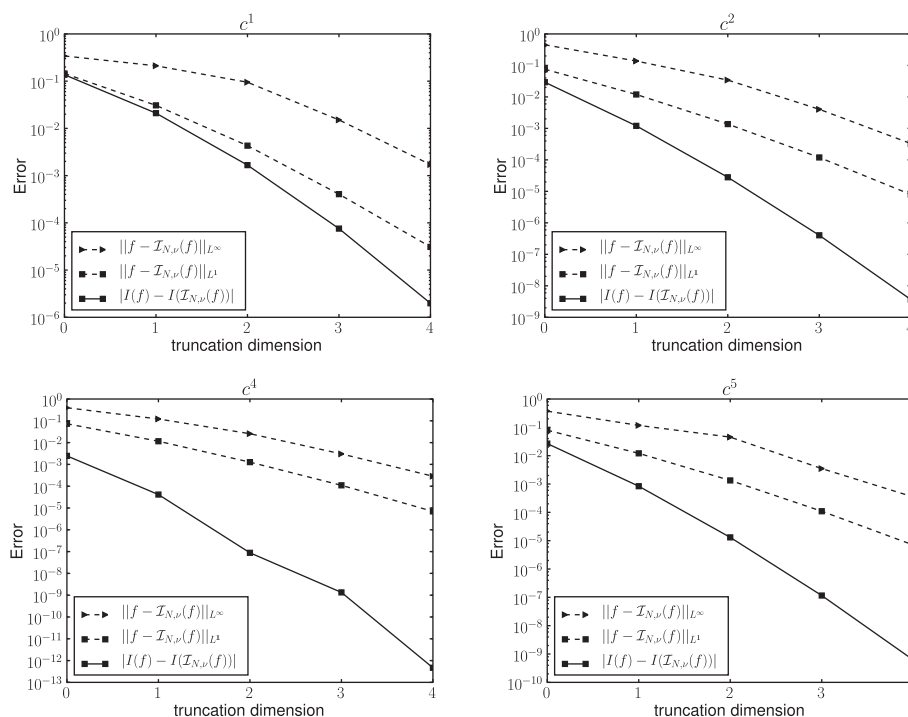


FIG. 5.3. Verification of the relationships between errors in different measures.

For different choices of anchor points, the integration error is bounded by the approximation error between the function and its anchored ANOVA truncation with respect to the L^1 -norm that is bounded by the approximation error with respect to the L^∞ -norm. In addition to the above tests, we have also investigated the errors of the Genz functions G_2 [8] with the same c_i and w_i as in Example 2.2; similar results were obtained (not shown here for brevity).

6. Summary. We considered the truncation of the ANOVA expansion for high dimensional tensor-product functions. We have defined different sets of weights that reflect the importance of each dimension. Based on these weights, we find that only those functions with small weights (smaller than 1) can admit low effective dimension in the standard ANOVA expansion. High regularity of a function would not necessarily lead to a smaller truncation error; instead only the functions with smaller weights have smaller truncation error.

For the anchored ANOVA expansion, we proposed new anchor points, which minimize the weights in different norms to improve the truncation error. The optimality of different sets of anchor points is examined through numerical examples in measure of the relative integration error and the truncation error. For the L^2 -truncation error, it seems that the choice of anchor points should be such that the target function at the point has a value close to its mean. Numerical tests show the superiority of the anchor point c^4 , which minimizes the weights with respect to numerical integration, compared to other anchor points.

We also derived rigorous error estimates for the truncated ANOVA expansion, as well as estimates for representing the terms in truncated ANOVA expansion with

multielement methods. These estimates show that the truncated ANOVA expansion converges in terms of the weights and smoothness; the multielement method converges to the truncated ANOVA expansion and thus it converges fast to the ANOVA expansion if the weights are small.

7. Appendix: Detailed proofs.

7.1. Proof of Theorem 2.5. By the anchored ANOVA expansion and the triangle inequality, we have

$$\begin{aligned} \frac{\|f - \mathcal{I}_{N,\bar{\nu}} f\|_{L^\infty}}{\|f\|_{L^\infty}} &= \frac{\|f - \mathcal{I}_{N,\bar{\nu}} f\|_{L^\infty}}{\prod_{k=1}^N |f^{(k)}(c_k)|} \frac{\prod_{k=1}^N |f^{(k)}(c_k)|}{\|f\|_{L^\infty}} \\ &\leq \frac{\sum_{m=\bar{\nu}+1}^N \sum_{|S|=m} \prod_{k \in S} \|f^{(k)} - f^{(k)}(c_k)\|_{L^\infty}}{\prod_{k=1}^N |f^{(k)}(c_k)|} \frac{\prod_{k=1}^N |f^{(k)}(c_k)|}{\|f\|_{L^\infty}} \\ &\leq \sum_{m=\bar{\nu}+1}^N \sum_{|S|=m} \prod_{k \in S} \gamma_k^\infty \left(\prod_{k=1}^N \frac{|f^{(k)}(c_k)|}{\|f^{(k)}\|_{L^\infty}} \right), \end{aligned}$$

where we used the definition of weights (2.9). Then the assumption with the above inequality yields the desired error estimate. The following will complete the proof of how to minimize the weights.

Suppose that $f^{(k)}(x_k)$ does not change sign over the interval $[0, 1]$. Without loss of generality, let $f^{(k)}(x_k) > 0$. Denote the maximum and the minimum of $f^{(k)}(x_k)$ by M_k and m_k , respectively, and assume that $f^{(k)}(c_k) = \alpha_k M_k + (1 - \alpha_k)m_k$, where $\alpha_k \in [0, 1]$. Then $\|f^{(k)} - f^{(k)}(c_k)\|_{L^\infty} = (M_k - m_k) \max(1 - \alpha_k, \alpha_k)$, and the weight

$$\gamma_k^\infty = \frac{\|f^{(k)} - f^{(k)}(c_k)\|_{L^\infty}}{|f^{(k)}(c_k)|} = \frac{(M_k - m_k) \max(1 - \alpha_k, \alpha_k)}{\alpha_k M_k + (1 - \alpha_k)m_k}.$$

Note that the minimum of the function $g(\alpha_k) = \frac{(1-m_k) \max(1-\alpha_k, \alpha_k)}{\alpha_k + (1-\alpha_k)m_k}$ can be attained only at $\alpha_k = \frac{1}{2}$, where $\alpha_k \in [0, 1]$, $m_k = \frac{m_k}{M_k} \in (0, 1)$. This ends the proof.

We note that

$$\begin{aligned} \left(\prod_{k=1}^N (1 + \gamma_k) - 1 \right) \prod_{k=1}^N \frac{|f^{(k)}(c_k)|}{\|f^{(k)}\|_{L^\infty}} &= \prod_{k=1}^N (\max(2\alpha_k, 1)(1 - m_k) + m_k) \\ &\quad - \prod_{k=1}^N (\alpha_k(1 - m_k) + m_k) \end{aligned}$$

attains its minimum at $(\frac{1}{2}, \frac{1}{2}, \dots, \frac{1}{2})$. Since smaller weights lead to smaller $1 - p_{\bar{\nu}}$, we have then a tighter error estimate (2.10).

7.2. Proof of Theorem 2.7. The inequality (2.12) can be readily obtained as in the proof of Theorem 2.5.

For simplicity, we denote $\alpha_k = \frac{f^{(k)}(c_k)}{\|f^{(k)}\|_{L^2}}$. To minimize the weights (2.11), α_k has to be $\frac{\|f^{(k)}\|_{L^2}}{\tau_k}$, since the quadratic function of $\frac{1}{\alpha_k}$,

$$(\gamma_k^{L^2})^2 = \left\| \frac{f^{(k)}}{f^{(k)}(c_k)} - 1 \right\|_{L^2}^2 = \frac{1}{\alpha_k^2} - 2 \frac{1}{\alpha_k} \frac{\tau_k}{\|f^{(k)}\|_{L^2}} + 1,$$

attains its minimum at $\alpha_k = \frac{\|f^{(k)}\|_{L^2}}{\tau_k}$ for $k = 1, 2, \dots, N$.

7.3. Proof of Lemma 3.2. Here we adopt the methodology in [26] to prove the lemma. We will prove the lemma when r is an integer. When r is not an integer, we may apply the Hilbert space interpolation theory for $K_1^r([0, 1])$.

Define the eigenvalues of the Rayleigh quotient $R_K(f) = \frac{\|f\|_{L^2([0,1])}^2}{\|f\|_{K_1^r([0,1])}^2}$ for $f \in K_1^r([0, 1])$ as follows: for $n \geq 2$,

$$\lambda_n = \inf_{\langle f, \psi_i \rangle_{K_1^r([0,1])} = 0, \quad 1 \leq i \leq n-1} \sup_{\|f\|_{K_1^r([0,1])}^2 = 1} \|f\|_{L^2([0,1])}^2$$

with $\lambda_1 = \inf_{f \in K_1^r([0,1])} \sup_{\|f\|_{K_1^r([0,1])}^2 = 1} \|f\|_{L^2([0,1])}^2$. Let ψ_i be the corresponding eigenfunctions to λ_i with $\|\psi_i\|_{K_1^r([0,1])} = 1$.

First, this eigenvalue problem is well defined (see [26, p. 45]) as $\langle f, f \rangle_{K_1^r([0,1])}$ is positive definite and $R_K(f)$ is bounded from above. In fact, for $f \in K_1^r([0, 1])$ $R_K(f) \leq C_l^{-1} \frac{\|f\|_{L^2([0,1])}^2}{\|f\|_{H^r([0,1])}^2} \leq C_l^{-1}$ according to the fact that there exist positive constants C_l and C_u independent of r and f such that

$$(7.1) \quad C_l \|f\|_{H^r([0,1])}^2 \leq \|f\|_{K_1^r([0,1])}^2 \leq C_u \|f\|_{H^r([0,1])}^2.$$

Here the Hilbert space $H^r([0, 1])$ has the norm $\|f\|_{H^r([0,1])} = (\sum_{k=0}^r I((\partial_x^k f)^2))^{\frac{1}{2}}$. We will prove this fact shortly.

Second, $\|f\|_{L^2([0,1])}^2$ is completely continuous with respect to $\|f\|_{K_1^r([0,1])}^2$ by definition (see [26, p. 50]). This can be seen from the following. By the Poincaré–Friedrich inequality [26], for any $\epsilon > 0$, there exists a finite set of linear functionals $l_1, l_2, \dots, l_k$ such that for f with $f(c) = 0$, $l_i(f) = 0$, $i = 1, \dots, k$ implies that $\int_0^1 f^2 dx \leq \epsilon \int_0^1 (\partial_x f)^2 dx$ and hence that, by (7.1),

$$\int_0^1 f^2 dx \leq \epsilon \int_0^1 (\partial_x f)^2 dx \leq \epsilon \|f\|_{H^r([0,1])}^2 \leq C_l^{-1} \epsilon \|f\|_{K_1^r([0,1])}^2.$$

Since the two forms $(\cdot, \cdot)_{L^2([0,1])}$ and $(\cdot, \cdot)_{K_1^r([0,1])}$ are positive definite, according to Theorem 3.1, in [26, p. 52], the eigenfunctions corresponding to the eigenvalues of the Rayleigh quotient $R_K(f)$ actually form a complete orthogonal basis not only in $L^2([0, 1])$ but in $K_1^r([0, 1])$.

By (7.1) and the second monotonicity principle (Theorem 8.1 in [26, p. 62]), $\lambda_n \in [C_u^{-1}\beta_n, C_l^{-1}\beta_n]$, where β_n are eigenvalues of the Rayleigh quotient $\frac{\|f\|_{L^2([0,1])}^2}{\|f\|_{H^r([0,1])}^2}$. Note that the β_n are of order n^{-2r} . Actually, a complete orthogonal basis both in $L^2([0, 1])$ and $H^r([0, 1])$ is $\{\cos(n\pi x)\}_{n=0}^\infty$. Thus $\beta_n = (n\pi)^{-2r}$ and $\lambda_n \leq C_1 n^{-2r}$, where C_1 decreases with r .

At last, it can be readily checked that the first eigenvalue $\lambda_1 = 1$ and the corresponding eigenfunction is the constant 1. Recall that $K_1^r([0, 1])$ can be decomposed as $\text{span}\{1\} \oplus K_{1,0}^r([0, 1])$. We then reach the conclusion if (7.1) is true.

Now we verify (7.1). By the Sobolev embedding inequality, we have $\|f\|_{L^\infty} \leq C_s \|f\|_{H^1([0,1])}$. Since $|g(c)| \leq \|g\|_{L^\infty}$ for any $g \in K_1^r([0, 1])$, this leads to

$$\sum_{i=1}^{r-1} [\partial_x^i f(c)]^2 + \int_0^1 [\partial_x^r f(x)]^2 dx \leq \frac{1}{2} C_s^2 \int_0^1 (\partial_x f)^2 dx + \left(\frac{1}{2} C_s^2 + 1\right) \sum_{k=2}^r \int_0^1 (\partial_x^k f)^2 dx.$$

This proves that $\|f\|_{K_1^r([0,1])}^2 \leq C_u \|f\|_{H^r([0,1])}^2$, where $C_u = C_s^2 + 1$. The inequality $C_l \|f\|_{H^r([0,1])}^2 \leq \|f\|_{K_1^r([0,1])}^2$ can be seen from the basic inequality, for any $c \in [0, 1]$, $\int_0^1 f^2(x) dx \leq 2f^2(c) + \frac{2}{3} \int_0^1 [\partial_x f(x)]^2 dx$. Applying repeatedly this inequality for $\partial_x^k f$ ($k = 1, \dots, r$) and summing them up, we have with $C_l = \frac{1}{6}$,

$$\|f\|_{H^r([0,1])}^2 = \int_0^1 f^2(x) dx + \sum_{k=1}^{r-1} \int_0^1 [\partial_x^k f(x)]^2 dx \leq C_l^{-1} \|f\|_{K_1^r([0,1])}^2.$$

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