

Efficient implementations of the Multivariate Decomposition Method for Approximating Infinite-Variate Integrals

Alexander D. Gilbert Frances Y. Kuo Dirk Nuyens
Grzegorz W. Wasilkowski

May 10, 2019

Abstract

In this paper we focus on efficient implementations of the Multivariate Decomposition Method (MDM) for approximating integrals of ∞ -variate functions. Such ∞ -variate integrals occur for example as expectations in uncertainty quantification. Starting with the anchored decomposition $f = \sum_{\mathbf{u} \subset \mathbb{N}} f_{\mathbf{u}}$, where the sum is over all finite subsets of \mathbb{N} and each $f_{\mathbf{u}}$ depends only on the variables x_j with $j \in \mathbf{u}$, our MDM algorithm approximates the integral of f by first truncating the sum to some ‘active set’ and then approximating the integral of the remaining functions $f_{\mathbf{u}}$ term-by-term using Smolyak or (randomized) quasi-Monte Carlo (QMC) quadratures. The anchored decomposition allows us to compute $f_{\mathbf{u}}$ explicitly by function evaluations of f . Given the specification of the active set and theoretically derived parameters of the quadrature rules, we exploit structures in both the formula for computing $f_{\mathbf{u}}$ and the quadrature rules to develop computationally efficient strategies to implement the MDM in various scenarios. In particular, we avoid repeated function evaluations at the same point. We provide numerical results for a test function to demonstrate the effectiveness of the algorithm.

1 Introduction

The *Multivariate Decomposition Method* (MDM) is an algorithm for approximating the integral of an ∞ -variate function f defined on some domain $D^{\mathbb{N}}$ with $D \subseteq \mathbb{R}$, and this paper presents the first results on the implementation of the MDM. The general idea of the MDM, see [4, 7, 13, 16, 17] (as well as [9, 12] under the name of *Changing Dimension Algorithm*), goes as follows. Assume that f admits a decomposition

$$f(\mathbf{x}) = \sum_{\mathbf{u} \subset \mathbb{N}} f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}), \quad (1)$$

where the sum is taken over all finite subsets of

$$\mathbb{N} := \{1, 2, 3, \dots\},$$

and where each function $f_{\mathbf{u}}$ depends only on the variables in $\mathbf{x}_{\mathbf{u}} = (x_j)_{j \in \mathbf{u}}$. With ρ a given probability density function on D and $\rho_{\mathbf{u}}(\mathbf{x}) := \prod_{j \in \mathbf{u}} \rho(x_j)$, we define the integral of f by

$$\mathcal{I}(f) := \sum_{\mathbf{u} \subset \mathbb{N}} I_{\mathbf{u}}(f_{\mathbf{u}}), \quad \text{with} \quad I_{\mathbf{u}}(f_{\mathbf{u}}) := \int_{D^{|\mathbf{u}|}} f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \rho_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) d\mathbf{x}_{\mathbf{u}}, \quad (2)$$

and let $I_{\emptyset}(f_{\emptyset}) := f_{\emptyset}$. The MDM algorithm for approximating the integral is

$$\mathcal{A}(f) := \sum_{\mathbf{u} \in \mathcal{U}} A_{\mathbf{u}}(f_{\mathbf{u}}), \quad (3)$$

where \mathcal{U} is the ‘‘active set’’; for $\mathbf{u} \neq \emptyset$, each $A_{\mathbf{u}}$ is a $|\mathbf{u}|$ -dimensional quadrature rule, and $A_{\emptyset}(f_{\emptyset}) := f_{\emptyset}$.

The error of the MDM algorithm satisfies the trivial bound

$$|\mathcal{I}(f) - \mathcal{A}(f)| \leq \sum_{\mathbf{u} \notin \mathcal{U}} |I_{\mathbf{u}}(f_{\mathbf{u}})| + \sum_{\mathbf{u} \in \mathcal{U}} |I_{\mathbf{u}}(f_{\mathbf{u}}) - A_{\mathbf{u}}(f_{\mathbf{u}})|. \quad (4)$$

Given $\varepsilon > 0$, the strategy is to first choose an active set \mathcal{U} such that the first sum in (4) is at most $\varepsilon/2$, and then specify the quadrature rules such that the second sum in (4) is also at most $\varepsilon/2$, giving a total error of at most ε . It is known that the sets $\mathbf{u} \in \mathcal{U}$ have cardinalities increasing very slowly with decreasing ε ,

$$\max_{\mathbf{u} \in \mathcal{U}(\varepsilon)} |\mathbf{u}| = O\left(\frac{\ln(1/\varepsilon)}{\ln(\ln(1/\varepsilon))}\right) \quad \text{as } \varepsilon \rightarrow 0,$$

see, e.g., [4, 12].

We would need to impose additional conditions on the class of functions to ensure that the sum (1) is absolutely convergent, the integral (2) is well defined, and the quadrature rules in (3) converge appropriately to the corresponding integrals. The precise details will depend on the mathematical setting within which we choose to analyze the problem. We will outline some variants below, but this is not the focus of the present paper.

The main focus of this paper is on the implementation of the MDM algorithm, which involves the two following steps. The first step is to construct the active set given an abstract definition of \mathcal{U} from the theory. Then in the second step, supposing we are given an active set and the choice of quadrature rules $A_{\mathbf{u}}$, we develop computationally efficient strategies to evaluate (3) in certain scenarios by exploiting specific structures in the MDM algorithm and the quadrature rules of choice. Specifically,

- we assume a *product and order dependent* (POD) structure in the definition of the active set \mathcal{U} ;
- we utilize the *anchored decomposition* of functions; and
- we consider *quasi-Monte Carlo methods* and *Smolyak’s methods* as two alternatives for the quadrature rules $A_{\mathbf{u}}$.

In Section 2 we explain the structure of our active set \mathcal{U} and provide an efficient strategy to construct it. Once the active set \mathcal{U} has been constructed, we need to evaluate the quadrature rules $A_{\mathbf{u}}(f_{\mathbf{u}})$ for each $\mathbf{u} \in \mathcal{U}$; this is formulated in Section 3. In this paper we use the anchored decomposition [10] of f so that the terms $f_{\mathbf{u}}$ can be computed explicitly via

$$f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) = \sum_{\mathbf{v} \subseteq \mathbf{u}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} f(\mathbf{x}_{\mathbf{v}}; \mathbf{0}), \quad (5)$$

where $f(\mathbf{x}_{\mathbf{v}}; \mathbf{0})$ indicates that we evaluate the function at $f(\mathbf{t})$ with components $t_j = x_j$ for $j \in \mathbf{v}$ and $t_j = 0$ for $j \notin \mathbf{v}$. Throughout this paper, by a “naive” implementation of the MDM algorithm, we mean an implementation which computes the sum in (3) term by term, with each $f_{\mathbf{u}}$ evaluated using (5).

We consider only linear algorithms $A_{\mathbf{u}}$ as the quadrature rules and our MDM algorithm can therefore be expressed as

$$\mathcal{A}(f) = \sum_{\mathbf{u} \in \mathcal{U}} \sum_{\mathbf{v} \subseteq \mathbf{u}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0})). \quad (6)$$

Notice inside the double sum in (6) that we would be applying a $|\mathbf{u}|$ -dimensional quadrature rule to a function which depends only on a subset $\mathbf{v} \subseteq \mathbf{u}$ of the variables. Moreover, the same evaluations of f could be repeated for different combinations of \mathbf{u} and \mathbf{v} , while in practice the cost of evaluating f could be quite expensive. We will exploit structures in the quadrature rules to save on repeated evaluations in (6).

In Section 3.1 we first consider *Smolyak quadrature* to be used as the quadrature rules $A_{\mathbf{u}}$ (see, e.g., [3, 15]). Then in Section 3.2 we consider instead an *extensible quasi-Monte Carlo (QMC) sequence* to be used for the quadrature rules (see, e.g., [1, 2]). In both sections we explain how to regroup the terms by making use of the recursive structure and how to store some intermediate calculations for the specific quadrature rules to evaluate (6) efficiently.

Section 4 considers two different approaches to implement the Smolyak quadratures: the direct method and the combination technique. In Section 5 we consider a *randomized quasi-Monte Carlo* sequence for the quadrature rules. This enables us to obtain an unbiased result and a practical estimate of the quadrature error for the MDM algorithm.

Each variant of our MDM algorithm involves three stages, as outlined in the pseudocodes; a summary is given as follows:

Pseudocodes 1 + 2A + 3A	Smolyak MDM – direct implementation
Pseudocodes 1 + 2A' + 3A'	Smolyak MDM – combination technique
Pseudocodes 1 + 2B + 3B	Extensible QMC MDM
Pseudocodes 1 + 2B + 3B'	Extensible randomized QMC MDM

In Section 6 we derive a computable expression for estimating an infinite series that may appear in the definition of the active set, which is another novel and significant contribution of this paper. Finally in Section 7 we combine all ingredients and follow the mathematical setting of [7] to construct the active set and choose the quadrature

rules. We then apply the MDM algorithm to an example integrand that mimics the characteristics of the integrands arising from some parametrized PDE problems (see, e.g., [8]).

2 Constructing the active set

Letting $w(\mathbf{u})$ be a measure of the “significance” of the subset \mathbf{u} , we assume that the mathematical analysis yields the definition of an active set of the general form

$$\mathcal{U} := \{\mathbf{u} \subset \mathbb{N} : w(\mathbf{u}) > T\}, \quad (7)$$

where $T > 0$ is a “threshold” parameter that depends on the overall error demand $\varepsilon > 0$ and possibly on all of $w(\mathbf{u})$. For example, $w(\mathbf{u})$ can be related to the weight parameters from a weighted function space setting (as in [16, 17, 13, 4]), or it can be related to the bounds on the norm of $f_{\mathbf{u}}$ (as in [7]).

In this section we will treat T and $w(\mathbf{u})$ as input parameters (ignoring the mathematical details of where they come from), and focus on the efficient implementation of the active set given these parameters. Then in Section 6 we will consider a special form of T (arising from analysis) which requires numerical estimation of an infinite series.

We assume $w(\emptyset) > T$ so that we always have $\emptyset \in \mathcal{U}$. Furthermore, we assume specifically for $\mathbf{u} \neq \emptyset$ that $w(\mathbf{u})$ takes the *product and order dependent* (POD) form (a structure that first appeared in [8]):

$$w(\mathbf{u}) := \Omega_{|\mathbf{u}|} \prod_{j \in \mathbf{u}} \omega_j, \quad (8)$$

where $\omega_1 \geq \omega_2 \geq \dots$ is a non-increasing sequence of nonnegative real numbers controlling the “product aspect”, and $\Omega_1, \Omega_2, \dots$ is a second sequence of nonnegative real numbers controlling the “order dependent aspect”, with the restriction on Ω_ℓ that its growth is controlled by ω_ℓ , i.e., $\Omega_{\ell+1}\omega_{\ell+1} \leq \Omega_\ell$ for all $\ell \in \mathbb{N}$. This assumption is satisfied in all practical cases that we are aware of. Further, in the theoretical framework for the MDM (see, e.g., [7]), a sufficient condition for the infinite-dimensional integral to be well-defined is for the parameters $w(\mathbf{u})$ to be summable, $\sum_{\mathbf{u} \subset \mathbb{N}} w(\mathbf{u}) < \infty$, which will not hold unless the condition $\Omega_{\ell+1}\omega_{\ell+1} \leq \Omega_\ell$ holds (at least asymptotically in ℓ).

With the active set defined by (7) and (8), we make a couple of obvious remarks:

1. If $\mathbf{v} \in \mathcal{U}$ then $\mathbf{u} \in \mathcal{U}$ for all sets \mathbf{u} satisfying $w(\mathbf{u}) \geq w(\mathbf{v})$.
2. If $\mathbf{u} \notin \mathcal{U}$ then $\mathbf{v} \notin \mathcal{U}$ for all sets \mathbf{v} satisfying $w(\mathbf{u}) \geq w(\mathbf{v})$.

We identify any finite set $\mathbf{u} \subset \mathbb{N}$ with a vector containing the elements of \mathbf{u} in increasing order, i.e., if $|\mathbf{u}| = \ell$ then

$$\mathbf{u} := (u_1, u_2, \dots, u_\ell), \quad u_1 < u_2 < \dots < u_\ell.$$

Then, due to our assumed POD structure in (8), we note that

3. $w(\mathbf{u}) \geq w(\mathbf{v})$ if $|\mathbf{u}| = |\mathbf{v}|$ and $u_i \leq v_i$ for all $i = 1, \dots, \ell$.
4. $w(\{1, \dots, \ell\}) \geq w(\{1, \dots, \ell + 1\})$ for all $\ell \in \mathbb{N}$.
5. For any $\mathbf{u} \in \mathcal{U}$, a subset of \mathbf{u} need *not* be included in \mathcal{U} .

Note that if the opposite of Item 5 were true, i.e., every subset of $\mathbf{u} \in \mathcal{U}$ also belongs to \mathcal{U} , then the set \mathcal{U} is said to be “downward closed” in some papers; we do not impose this condition.

Combining the above, we deduce the following simple lemma.

Lemma 1. *Assume that the active set \mathcal{U} is defined by (7) and (8).*

- (“Superposition dimension”) *Let σ^* be the largest possible value of ℓ for which $(1, 2, \dots, \ell) \in \mathcal{U}$, i.e., $w(\{1, 2, \dots, \ell\}) > T$. Then for all $\mathbf{u} \in \mathcal{U}$ we have $|\mathbf{u}| \leq \sigma^*$.*
- (“Truncation dimension for sets of order ℓ ”) *For any $\ell = 1, \dots, \sigma^*$, let τ_ℓ be the largest possible value of $j \geq \ell$ for which $(1, 2, \dots, \ell - 1, j) \in \mathcal{U}$, That is, $w(\{1, 2, \dots, \ell - 1, j\}) > T$. Then for all $\mathbf{u} \in \mathcal{U}$ with $|\mathbf{u}| = \ell$, we have $u_\ell \leq \tau_\ell$; and consequently, $i \leq u_i \leq \tau_\ell - \ell + i$ for all $1 \leq i \leq \ell$.*
- (“Truncation dimension”) *Let τ^* be the largest possible value of j for which $j \in \mathbf{u} \in \mathcal{U}$, i.e., $\tau^* = \max_{\mathbf{u} \in \mathcal{U}} \max_{j \in \mathbf{u}} j$. Then $\tau^* = \max_{1 \leq \ell \leq \sigma^*} \tau_\ell$.*

Proof. For the first point, suppose on the contrary that $\mathbf{u} = (u_1, \dots, u_{\sigma^*+1}) \in \mathcal{U}$. Then letting $\mathbf{v} := (1, \dots, \sigma^* + 1)$ we have $w(\mathbf{v}) \geq w(\mathbf{u}) > T$, which indicates that $\mathbf{v} \in \mathcal{U}$, contradicting the definition of σ^* .

To demonstrate the second point, suppose on the contrary that $\mathbf{u} = (u_1, \dots, u_\ell) \in \mathcal{U}$ with $u_\ell > \tau_\ell$. Then we have $\mathbf{v} = (1, \dots, \ell - 1, u_\ell)$ with $w(\mathbf{v}) \geq w(\mathbf{u}) > T$, which indicates that $\mathbf{v} \in \mathcal{U}$, but this contradicts the definition of τ_ℓ . The bound on u_i then follows easily.

The third point is straightforward. \square

We construct the active set as outlined in Pseudocode 1. The algorithm adds the qualifying sets to the collection in the order of increasing cardinality. For each $\ell \geq 1$, starting from the set $(1, 2, \dots, \ell)$, the algorithm incrementally generates and checks sets to be added to the collection. The algorithm terminates when it reaches a value of ℓ for which $(1, 2, \dots, \ell) \notin \mathcal{U}$, i.e., $w(\{1, 2, \dots, \ell\}) \leq T$.

The assumptions on the structure of $w(\mathbf{u})$ and properties 1–5 above ensure that this stopping criteria is valid, and hence that Pseudocode 1 does indeed construct the active set (7). In particular, property 3 implies $w(\mathbf{u}) \leq w(\{1, 2, \dots, \ell\})$ for all sets with $|\mathbf{u}| = \ell$, and then Property 4 implies $w(\mathbf{u}) \leq w(\{1, 2, \dots, \ell\})$ for all sets with $|\mathbf{u}| \geq \ell$. Thus, if $\{1, 2, \dots, \ell\} \notin \mathcal{U}$ then no set with cardinality ℓ or higher is in \mathcal{U} .

We recommend storing the active set \mathcal{U} as an array of hash tables, with one table for each cardinality, since in the next section we will have to iterate over all subsets $\mathbf{v} \subseteq \mathbf{u} \in \mathcal{U}$ and be able to update a table stored with each such \mathbf{v} .

Pseudocode 1 (Constructing the active set)

```
1: Add  $\emptyset$  to  $\mathcal{U}$ 
2: for  $\ell$  from 1 to  $\ell_{\text{threshold}}$  do ▷  $\ell_{\text{threshold}}$  is a computational threshold
3:    $\mathbf{u} \leftarrow (1, 2, \dots, \ell)$ 
4:    $i \leftarrow \ell$  ▷  $i$  is the index for the next increment
5:   loop
6:     if  $w(\mathbf{u}) > T$  then
7:        $i \leftarrow \ell$ 
8:       Add  $\mathbf{u}$  to  $\mathcal{U}$  ▷ add  $\mathbf{u}$  to the active set
9:     else
10:       $i \leftarrow i - 1$ 
11:    end if
12:    break the inner loop if  $i = 0$  ▷ move to next cardinality
13:    for  $j$  from  $i$  to  $\ell$  do ▷ increment  $\mathbf{u}$  from  $u_i$ 
14:       $u_j \leftarrow u_i + j - i + 1$ 
15:    end for
16:  end loop
17:  break the outer loop if no sets of size  $\ell$  found ▷ terminate
18: end for
```

Remark 1. *The paper [4] provides an efficient algorithm to construct the optimal active set $\mathcal{U}^{\text{opt}}(\varepsilon)$, i.e., an active set that has the smallest cardinality among all active sets $\mathcal{U}(\varepsilon)$ with the same error demand ε . The construction principle is based on sorting so is quite different to Pseudocode 1, and it works only for parameters of product form. Once the active set is constructed, the remaining steps for implementing the MDM algorithm will be the same as we discuss below.*

3 Formulating the MDM algorithm

In this section we outline how to formulate the MDM algorithm (6) in a way that is specific to the quadrature rules used, so that the implementation can be as efficient as possible. We do this by exploiting the structure in the anchored decomposition (5), and also in the quadrature rules, which will be Smolyak's methods (also known as sparse grid methods) and quasi-Monte Carlo rules.

In each case we treat the parameters of the quadrature rules (i.e., the number of quadrature points or levels) as input, and focus on the efficient implementation of the MDM given these parameters. Specific choices of parameters for a test integrand following the theoretical analysis in [7] are given in Section 7.

Recall from (6) that the MDM algorithm using the anchored decomposition is given by

$$\mathcal{A}(f) = \sum_{\mathbf{u} \in \mathcal{U}} \sum_{\mathbf{v} \subseteq \mathbf{u}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0})).$$

Clearly there will be subsets \mathbf{v} that will occur many times over, so implementing the MDM in this way could be severely inefficient, because it would evaluate the same functions $f(\cdot; \mathbf{v}; \mathbf{0})$ at the same quadrature points over and over again. The goal of this section is to detail how to implement the quadrature approximations in such a way that each function $f(\cdot; \mathbf{v}; \mathbf{0})$ is evaluated at each quadrature point *once only*.

The first step is to introduce the *extended active set*:

$$\mathcal{U}_{\text{ext}} := \{\mathbf{v} \subset \mathbb{N} : \mathbf{v} \subseteq \mathbf{u} \text{ for } \mathbf{u} \in \mathcal{U}\},$$

that is, it includes all subsets of the sets in the active set. Then we can swap the sums above to give

$$\begin{aligned} \mathcal{A}(f) &= \sum_{\mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq \mathbf{v}}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0})) \\ &= c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq \mathbf{v}}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0})), \end{aligned} \quad (9)$$

where we separated out the $\mathbf{v} = \emptyset$ terms, with

$$c_{\emptyset} := \sum_{\mathbf{u} \in \mathcal{U}} (-1)^{|\mathbf{u}|}.$$

After constructing the active set \mathcal{U} , we go through it again to construct the extended active set \mathcal{U}_{ext} , and at the same time store information regarding the superset structure of each element in \mathcal{U}_{ext} . We would like to store just enough details so that for each $\mathbf{v} \in \mathcal{U}_{\text{ext}}$ we can compute the approximation $\sum_{\mathbf{u} \in \mathcal{U} : \mathbf{u} \supseteq \mathbf{v}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0}))$ without the need to access the supersets of \mathbf{v} . Specific details on how this is done will depend on the quadrature rule used.

3.1 Quadrature rules based on Smolyak's method

For a nonempty set $\mathbf{u} \subset \mathbb{N}$ and integer $m \geq 1$, Smolyak's method (see, e.g., [3, 15, 18]) applied to a function $g_{\mathbf{u}}$ of the variables $\mathbf{x}_{\mathbf{u}}$ takes the form

$$Q_{\mathbf{u}, m}(g_{\mathbf{u}}) := \sum_{\substack{\mathbf{i}_{\mathbf{u}} \in \mathbb{N}^{|\mathbf{u}|} \\ |\mathbf{i}_{\mathbf{u}}| \leq |\mathbf{u}| + m - 1}} \bigotimes_{j \in \mathbf{u}} (U_{i_j} - U_{i_j - 1})(g_{\mathbf{u}}), \quad (10)$$

where $|\mathbf{i}_{\mathbf{u}}| := \sum_{j \in \mathbf{u}} i_j$, $m \geq 1$, and $\{U_i\}_{i \geq 1}$ is a sequence of one-dimensional quadrature rules, not necessarily nested, with $U_0 := 0$ denoting the zero algorithm. Furthermore we assume that constant functions are integrated exactly, so that $U_i(1) = 1$ for $i \geq 1$.

For a nonempty subset $\mathbf{v} \subseteq \mathbf{u}$, suppose now that the function $g_{\mathbf{v}}$ depends only on the

variables \mathbf{x}_v . Then we have

$$\begin{aligned}
Q_{\mathbf{u},m}(g_v) &= \sum_{\substack{\mathbf{i}_u \in \mathbb{N}^{|\mathbf{u}|} \\ |\mathbf{i}_u| \leq |\mathbf{u}|+m-1}} \left(\bigotimes_{j \in v} (U_{i_j} - U_{i_{j-1}})(g_v) \right) \left(\bigotimes_{j \in \mathbf{u} \setminus v} (U_{i_j} - U_{i_{j-1}})(1) \right) \\
&= \sum_{\substack{\mathbf{i}_u \in \mathbb{N}^{|\mathbf{u}|} \\ |\mathbf{i}_u| \leq |\mathbf{u}|+m-1, \mathbf{i}_{u \setminus v} = \mathbf{1}}} \bigotimes_{j \in v} (U_{i_j} - U_{i_{j-1}})(g_v) \\
&= \sum_{\substack{\mathbf{i}_v \in \mathbb{N}^{|\mathbf{v}|} \\ |\mathbf{i}_v| \leq |\mathbf{v}|+m-1}} \bigotimes_{j \in v} (U_{i_j} - U_{i_{j-1}})(g_v) = Q_{v,m}(g_v). \tag{11}
\end{aligned}$$

In the second equality above we used the assumption that the one-dimensional quadrature rules integrate the constant functions exactly and thus $(U_{i_j} - U_{i_{j-1}})(1)$ is 1 if $i_j = 1$ and is 0 otherwise. The above derivation (11) indicates how a Smolyak quadrature rule is projected down when it is applied to a lower dimensional function. This property is important in our efficient evaluation of (9).

In (9) we take

$$A_{\mathbf{u}} \equiv Q_{\mathbf{u},m_{\mathbf{u}}},$$

where the level $m_{\mathbf{u}}$ determines the number of quadrature points $n_{\mathbf{u}}$ used by $Q_{\mathbf{u},m_{\mathbf{u}}}$. The exact relationship between $m_{\mathbf{u}}$ and $n_{\mathbf{u}}$ will depend on the choice of the one-dimensional quadrature rules $\{U_i\}$.

Here we treat the levels $m_{\mathbf{u}}$, hence also the number of points $n_{\mathbf{u}}$, as input parameters to our MDM algorithm. Then we define the maximum level to occur as

$$m_{\max} := \max\{m_{\mathbf{u}} : \emptyset \neq \mathbf{u} \in \mathcal{U}\}.$$

For Smolyak grids based on one-dimensional rules $\{U_i\}$ that each use $\mathcal{O}(2^i)$ points (e.g., trapezoidal rules) the value of $m_{\mathbf{u}}$ is roughly the logarithm of $n_{\mathbf{u}}$ (see, e.g., [3]). Hence in practice we observe that m_{\max} is relatively small, e.g., $m_{\max} \approx 25$.

Using (11) we can rewrite (9) as follows (note the change from $Q_{\mathbf{u},m_{\mathbf{u}}}$ to $Q_{v,m_{\mathbf{u}}}$):

$$\begin{aligned}
\mathcal{A}^S(f) &= c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq v \in \mathcal{U}_{\text{ext}}} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq v}} (-1)^{|\mathbf{u}|-|v|} Q_{\mathbf{u},m_{\mathbf{u}}}(f(\cdot; \mathbf{v}; \mathbf{0})) \\
&= c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq v \in \mathcal{U}_{\text{ext}}} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq v}} (-1)^{|\mathbf{u}|-|v|} Q_{v,m_{\mathbf{u}}}(f(\cdot; \mathbf{v}; \mathbf{0})) \\
&= c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq v \in \mathcal{U}_{\text{ext}}} \sum_{\substack{m=1 \\ c(v,m) \neq 0}}^{m_{\max}} c(v,m) Q_{v,m}(f(\cdot; \mathbf{v}; \mathbf{0})), \tag{12}
\end{aligned}$$

where for $v \neq \emptyset$ and $m = 1, \dots, m_{\max}$ we define

$$c(v,m) := \sum_{\substack{\mathbf{u} \in \mathcal{U}, \mathbf{u} \supseteq v \\ m_{\mathbf{u}} = m}} (-1)^{|\mathbf{u}|-|v|}. \tag{13}$$

Pseudocode 2A (Constructing the extended active set for Smolyak)

```
1: Initialize  $\mathcal{U}_{\text{ext}} \leftarrow \mathcal{U}$  ▷ start from the active set
2: Initialize  $c_\emptyset \leftarrow 1$  ▷ for  $\mathbf{u} = \emptyset$ 
3: for  $\emptyset \neq \mathbf{u} \in \mathcal{U}$  with  $|\mathbf{u}|$  from 1 to  $\sigma^*$  do ▷ traverse in increasing cardinality
4:   Calculate  $m_{\mathbf{u}}$  ▷ formula for  $m_{\mathbf{u}}$  is given from theory
5:   Update  $c_\emptyset \leftarrow c_\emptyset + (-1)^{|\mathbf{u}|}$ 
6:   Initialize  $c(\mathbf{u}, m) \leftarrow 0$  for  $m$  from 1 to  $m_{\text{max}}$ 
7:   for  $\emptyset \neq \mathbf{v} \subseteq \mathbf{u}$  do ▷ generate nonempty subsets
8:     if  $\mathbf{v} \notin \mathcal{U}_{\text{ext}}$  then ▷ look up and add missing subset
9:       Add  $\mathbf{v}$  to  $\mathcal{U}_{\text{ext}}$ 
10:      Initialize  $c(\mathbf{v}, m) \leftarrow 0$  for  $m$  from 1 to  $m_{\text{max}}$ 
11:    end if
12:    Update  $c(\mathbf{v}, m_{\mathbf{u}}) \leftarrow c(\mathbf{v}, m_{\mathbf{u}}) + (-1)^{|\mathbf{u}|-|\mathbf{v}|}$  ▷ update relevant entry
13:  end for
14: end for
```

Pseudocode 3A (Implementing the Smolyak MDM)

```
1: Initialize  $\mathcal{A}^{\text{S}}(f) \leftarrow c_\emptyset \times f(\mathbf{0})$ 
2: for  $\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}$  do
3:   for  $m$  from 1 to  $m_{\text{max}}$  do
4:     if  $c(\mathbf{v}, m) \neq 0$  then
5:       Calculate  $Q_{\mathbf{v},m}(f(\cdot; \mathbf{v}; \mathbf{0}))$  using (20)–(21) or (22)–(23)
6:       Update  $\mathcal{A}^{\text{S}}(f) \leftarrow \mathcal{A}^{\text{S}}(f) + c(\mathbf{v}, m) \times Q_{\mathbf{v},m}(f(\cdot; \mathbf{v}; \mathbf{0}))$ 
7:     end if
8:   end for
9: end for
10: return  $\mathcal{A}^{\text{S}}(f)$ 
```

The values of $c(\mathbf{v}, m)$ can be computed and stored while we construct the extended active set \mathcal{U}_{ext} as follows. We work through the sets in the active set in order of increasing cardinality. For each nonempty set $\mathbf{u} \in \mathcal{U}$ with required level $m_{\mathbf{u}}$, we generate all nonempty subsets $\mathbf{v} \subseteq \mathbf{u}$, add the missing subsets to \mathcal{U}_{ext} , and update $c(\mathbf{v}, m_{\mathbf{u}})$ as we go. This procedure is given in Pseudocode 2A.

This formulation (12)–(13) allows us to compute the $Q_{\mathbf{v},m}(f(\cdot; \mathbf{v}; \mathbf{0}))$ for different supersets \mathbf{u} with the same value of $m_{\mathbf{u}}$ only once. If the Smolyak MDM algorithm is implemented in this way then there is no need to access the superset structure. Obviously, if $c(\mathbf{v}, m) = 0$ then we do not perform the quadrature approximation.

Note that in practice calculating the number of Smolyak levels $m_{\mathbf{u}}$ (or the number of QMC points in the next subsection) normally requires knowledge of the entire active set \mathcal{U} , see, e.g., [7, Section 4.3], hence we compute them when constructing \mathcal{U}_{ext} .

Note also that we do not need a separate data structure for \mathcal{U}_{ext} : we can simply extend \mathcal{U} to \mathcal{U}_{ext} since Step 9 in Pseudocode 2A only adds subsets with lower cardinalities and

would not interfere with Step 3 since we iterate in increasing cardinality. As we explained in the previous section, we store the active set \mathcal{U} , and by extension the extended active set \mathcal{U}_{ext} , as an array of hash tables to easily retrieve the $c(\mathbf{v}, \cdot)$ table for each \mathbf{v} .

A direct implementation of the MDM algorithm with Smolyak quadratures is given in Pseudocode 3A. The different formulas (20)–(21) or (22)–(23) for implementing the Smolyak quadrature, which depend on whether we have a non-nested or nested rule, will be discussed in Section 4.

3.2 Quadrature rules based on quasi-Monte Carlo methods

Here we assume for simplicity that $D = [0, 1]$ and $\rho \equiv 1$. A d -dimensional *quasi-Monte Carlo* (QMC) rule with n points $\mathbf{t}^{(i)} = (t_1^{(i)}, t_2^{(i)}, \dots, t_d^{(i)})$, $i = 0, \dots, n-1$, approximates the integral of a function g by the equal-weight average

$$\int_{[0,1]^d} g(\mathbf{x}) \, d\mathbf{x} \approx \frac{1}{n} \sum_{i=0}^{n-1} g(\mathbf{t}^{(i)}). \quad (14)$$

For more details on QMC methods we refer to [11, 14] and [2].

In (3) each $A_{\mathbf{u}}$ could be a different $|\mathbf{u}|$ -dimensional QMC rule with $n_{\mathbf{u}}$ points, but in that case we would not be able to reuse any function evaluation. Instead, we consider here an “*extensible quasi-Monte Carlo sequence*”. By “extensible” we mean that we can take just the initial dimensions of the initial points in the sequence. By “quasi-Monte Carlo” we mean that a quadrature rule based on the first n points of this sequence has equal quadrature weights $1/n$. We choose to use a QMC rule with σ^* dimensions instead of τ^* , since τ^* can be really large (e.g., 30000) while σ^* is rather small (e.g., 15), and QMC rules with fewer dimensions are of better quality.

Then for any nonempty set $\mathbf{u} \in \mathcal{U}$ and nonempty subset $\mathbf{v} \subseteq \mathbf{u}$ we have

$$A_{\mathbf{u}}(f(\cdot_{\mathbf{v}}; \mathbf{0})) = \frac{1}{n_{\mathbf{u}}} \sum_{i=0}^{n_{\mathbf{u}}-1} f\left(\mathbf{t}_{\mathbf{u}|\mathbf{v} \rightarrow \mathbf{v}}^{(i)}; \mathbf{0}\right), \quad (15)$$

where, loosely speaking, $\mathbf{t}_{\mathbf{u}|\mathbf{v} \rightarrow \mathbf{v}}^{(i)}$ indicates that we map the quadrature point $\mathbf{t}^{(i)}$ to the variables $\mathbf{x}_{\mathbf{u}}$ and then to $\mathbf{x}_{\mathbf{v}}$, which is *not* the same as mapping $\mathbf{t}^{(i)}$ directly to $\mathbf{x}_{\mathbf{v}}$. More explicitly, recalling that \mathbf{u} has ordered elements, $\mathbf{t}_{\mathbf{u}|\mathbf{v} \rightarrow \mathbf{v}}^{(i)}$ denotes that we take the first $|\mathbf{u}|$ -dimensions of $\mathbf{t}^{(i)}$ and apply them to the variables in $\mathbf{x}_{\mathbf{u}}$, then retain only those components in $\mathbf{x}_{\mathbf{v}}$. The function f is then evaluated by anchoring all other components outside of \mathbf{v} to zero. Thus the algorithm (9) in this case is given by

$$\mathcal{A}^{\mathbf{Q}}(f) = c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq \mathbf{v}}} (-1)^{|\mathbf{u}|-|\mathbf{v}|} \left(\frac{1}{n_{\mathbf{u}}} \sum_{i=0}^{n_{\mathbf{u}}-1} f\left(\mathbf{t}_{\mathbf{u}|\mathbf{v} \rightarrow \mathbf{v}}^{(i)}; \mathbf{0}\right) \right). \quad (16)$$

For example, take $\mathbf{u} = (1, 5, 7)$ and $\mathbf{v} = (1, 7)$. We get $\mathbf{u}|\mathbf{v} = (1, 3)$ since the set \mathbf{v} originates from the position $\mathbf{w} = (1, 3)$ of its superset \mathbf{u} . We assign the quadrature point

$(t_1^{(i)}, t_2^{(i)}, t_3^{(i)})$ to the variables (x_1, x_5, x_7) . Then the point $(t_1^{(i)}, t_3^{(i)})$ is assigned to the variables (x_1, x_7) , and hence we evaluate $f(t_1^{(i)}, 0, 0, 0, 0, 0, t_3^{(i)}, 0, \dots)$.

Note that the same set $\mathbf{v} = (1, 7)$ can originate from the position $\mathbf{w} = (1, 3)$ of different supersets \mathbf{u} : for example, $\mathbf{u} = (1, 6, 7)$, $\mathbf{u} = (1, 4, 7, 13)$, and many others. We can make use of this repetition to save on computational cost.

Let $\mathcal{M}(\mathbf{v})$ denote the set of all different positions that a nonempty set \mathbf{v} can originate from for all its supersets in the active set:

$$\mathcal{M}(\mathbf{v}) := \{\mathbf{w} \subseteq \{1, \dots, \sigma^*\} : \mathbf{w} \equiv \mathbf{u}|\mathbf{v} \text{ for some } \mathbf{u} \in \mathcal{U} \text{ with } \mathbf{u} \supseteq \mathbf{v}\}.$$

For simplicity and for convenience, we assume further that $n_{\mathbf{u}} = 2^{m_{\mathbf{u}}}$, with $0 \leq m_{\mathbf{u}} \leq m_{\max}$ (e.g., with $m_{\max} \approx 25$). This allows us to rewrite each QMC approximation as a sum of blocks of points (recall that the QMC points are extensible)

$$\frac{1}{2^{m_{\mathbf{u}}}} \sum_{i=0}^{2^{m_{\mathbf{u}}}-1} f(\mathbf{t}_{\mathbf{u}|\mathbf{v} \rightarrow \mathbf{v}}^{(i)}; \mathbf{0}) = \frac{1}{2^{m_{\mathbf{u}}}} \sum_{m=0}^{m_{\mathbf{u}}} \sum_{i=\lfloor 2^{m-1} \rfloor}^{2^m-1} f(\mathbf{t}_{\mathbf{u}|\mathbf{v} \rightarrow \mathbf{v}}^{(i)}; \mathbf{0}),$$

where the floor function is used specifically to take care of the $m = 0$ case. Substituting this into (16) and introducing a sum over $\mathcal{M}(\mathbf{v})$, we have

$$\mathcal{A}^{\text{Q}}(f) = c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\mathbf{w} \in \mathcal{M}(\mathbf{v})} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq \mathbf{v} \\ \mathbf{u}|\mathbf{v} \equiv \mathbf{w}}} (-1)^{|\mathbf{u}|-|\mathbf{v}|} \frac{1}{2^{m_{\mathbf{u}}}} \sum_{m=0}^{m_{\mathbf{u}}} \sum_{i=\lfloor 2^{m-1} \rfloor}^{2^m-1} f(\mathbf{t}_{\mathbf{w} \rightarrow \mathbf{v}}^{(i)}; \mathbf{0}),$$

where in the third sum we have added the restriction that $\mathbf{u}|\mathbf{v}$ is equivalent to the position \mathbf{w} . Collecting the sums

$$S_{\mathbf{v}, \mathbf{w}, m}(f) := \sum_{i=\lfloor 2^{m-1} \rfloor}^{2^m-1} f(\mathbf{t}_{\mathbf{w} \rightarrow \mathbf{v}}^{(i)}; \mathbf{0}), \quad (17)$$

we can then rewrite the QMC MDM (16) as

$$\mathcal{A}^{\text{Q}}(f) = c_{\emptyset} f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\mathbf{w} \in \mathcal{M}(\mathbf{v})} \sum_{\substack{m=0 \\ c(\mathbf{v}, \mathbf{w}, m) \neq 0}}^{m_{\max}} c(\mathbf{v}, \mathbf{w}, m) \frac{S_{\mathbf{v}, \mathbf{w}, m}(f)}{2^{m_{\max}}}, \quad (18)$$

where for a nonempty set \mathbf{v} , a position $\mathbf{w} \in \mathcal{M}(\mathbf{v})$, and $m = 0, \dots, m_{\max}$ we define

$$c(\mathbf{v}, \mathbf{w}, m) := \sum_{\substack{\mathbf{u} \in \mathcal{U}, \mathbf{u} \supseteq \mathbf{v} \\ \mathbf{u}|\mathbf{v} \equiv \mathbf{w}, m_{\mathbf{u}} \geq m}} (-1)^{|\mathbf{u}|-|\mathbf{v}|} 2^{m_{\max}-m_{\mathbf{u}}}. \quad (19)$$

Pseudocode 2B (Constructing the extended active set for QMC)

```
1: Initialize  $\mathcal{U}_{\text{ext}} \leftarrow \mathcal{U}$  ▷ start from the active set
2: Initialize  $c_\emptyset \leftarrow 1$  ▷ for  $\mathbf{u} = \emptyset$ 
3: for  $\emptyset \neq \mathbf{u} \in \mathcal{U}$  with  $|\mathbf{u}|$  from 1 to  $\sigma^*$  do ▷ traverse in increasing cardinality
4:   Calculate  $m_{\mathbf{u}}$  ▷ formula for  $m_{\mathbf{u}}$  is given from theory
5:   Update  $c_\emptyset \leftarrow c_\emptyset + (-1)^{|\mathbf{u}|}$ 
6:   Initialize  $\mathcal{M}(\mathbf{u}) \leftarrow \emptyset$ 
7:   for  $\emptyset \neq \mathbf{v} \subseteq \mathbf{u}$  do ▷ generate nonempty subsets
8:     if  $\mathbf{v} \notin \mathcal{U}_{\text{ext}}$  then ▷ look up and add missing subset
9:       Add  $\mathbf{v}$  to  $\mathcal{U}_{\text{ext}}$ 
10:      Initialize  $\mathcal{M}(\mathbf{v}) \leftarrow \emptyset$ 
11:     end if
12:     Set  $\mathbf{w} \leftarrow \mathbf{u} \setminus \mathbf{v}$  ▷ identify the position where  $\mathbf{v}$  originates from  $\mathbf{u}$ 
13:     if  $\mathbf{w} \notin \mathcal{M}(\mathbf{v})$  then ▷ look up and add missing position
14:       Add  $\mathbf{w}$  to  $\mathcal{M}(\mathbf{v})$ 
15:       Initialize  $c(\mathbf{v}, \mathbf{w}, m) \leftarrow 0$  for  $m$  from 1 to  $m_{\text{max}}$ 
16:     end if
17:     for  $m$  from 0 to  $m_{\mathbf{u}}$  do ▷ update relevant entries
18:       Update  $c(\mathbf{v}, \mathbf{w}, m) \leftarrow c(\mathbf{v}, \mathbf{w}, m) + (-1)^{|\mathbf{u}|-|\mathbf{v}|} \times 2^{m_{\text{max}}-m_{\mathbf{u}}}$ 
19:     end for
20:   end for
21: end for
```

Pseudocode 3B (Implementing the QMC MDM)

```
1: Initialize  $\mathcal{A}^{\text{Q}}(f) \leftarrow c_\emptyset \times f(\mathbf{0})$ 
2: for  $\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}$  do
3:   for  $\mathbf{w} \in \mathcal{M}(\mathbf{v})$  do
4:     for  $m$  from 0 to  $m_{\text{max}}$  do
5:       if  $c(\mathbf{v}, \mathbf{w}, m) \neq 0$  then
6:         Calculate  $S_{\mathbf{v}, \mathbf{w}, m}(f)$  using (17)
7:         Update  $\mathcal{A}^{\text{Q}}(f) \leftarrow \mathcal{A}^{\text{Q}}(f) + c(\mathbf{v}, \mathbf{w}, m) \times S_{\mathbf{v}, \mathbf{w}, m}(f) / 2^{m_{\text{max}}}$ 
8:       end if
9:     end for
10:   end for
11: end for
12: return  $\mathcal{A}^{\text{Q}}(f)$ 
```

Note that we have chosen to multiply and divide by $2^{m_{\text{max}}}$ to ensure that each $c(\mathbf{v}, \mathbf{w}, m)$ is integer valued.

We can compute and store a list of positions $\mathcal{M}(\mathbf{v})$ and the values $c(\mathbf{v}, \mathbf{w}, m)$ when we construct the extended active set \mathcal{U}_{ext} by extending the active set \mathcal{U} , in a similar way to the Smolyak case in the previous subsection. This is presented in Pseudocode 2B.

The new algorithm is more complicated due to the need to store the positions $\mathcal{M}(\mathbf{v})$.

The MDM implementation using the formulation (17)–(19) does not require access to any subsets or supersets. For each nonempty $\mathbf{v} \subseteq \mathcal{U}_{\text{ext}}$ and each position $\mathbf{w} \in \mathcal{M}(\mathbf{v})$ and for the different m , with $c(\mathbf{v}, \mathbf{w}, m) \neq 0$, the sums $S_{\mathbf{v}, \mathbf{w}, m}(f)$ are over disjoint sets of QMC points. In this way we will only evaluate each function $f(\cdot_{\mathbf{w} \rightarrow \mathbf{v}}; \mathbf{0})$ at each quadrature point once. An implementation of the MDM algorithm with QMC quadratures is given in Pseudocode 3B.

4 Two implementations of Smolyak MDM

Here we compare two approaches to implement Smolyak quadrature in the context of MDM: the direct implementation and the combination technique.

4.1 Direct Smolyak implementation

From a practical point of view, it is more useful to write Smolyak’s method as an explicit weighted quadrature rule as opposed to the tensor product form (10), see, e.g., [3]. We summarize this formulation below.

For each one-dimensional rule U_i , let n_i denote the number of quadrature points, $(w_{i,k})_{k=0}^{n_i-1}$ the quadrature weights, and $(t_{i,k})_{k=0}^{n_i-1}$ the quadrature nodes. Here for simplicity of notation we present the formula for a d -dimensional rule, with $d \geq 1$, which would need to be mapped to the set \mathbf{v} appropriately. To this end we write $Q_{d,m} = Q_{\{1,2,\dots,d\},m}$. The formula depends on whether the quadrature rules are nested, i.e., whether U_i includes all the quadrature points from U_{i-1} .

Non-nested case For non-nested one-dimensional rules, Smolyak’s method can be written explicitly as

$$Q_{d,m}(g) = \sum_{\substack{\mathbf{i} \in \mathbb{N}^d \\ d \leq |\mathbf{i}| \leq d+m-1}} \sum_{k_1=0}^{n_{(i_1)}-1} \cdots \sum_{k_d=0}^{n_{(i_d)}-1} w_{\mathbf{i},\mathbf{k}} g(\mathbf{t}_{\mathbf{i},\mathbf{k}}), \quad (20)$$

where the quadrature point $\mathbf{t}_{\mathbf{i},\mathbf{k}} \in D^d$ has coordinates $(\mathbf{t}_{\mathbf{i},\mathbf{k}})_j = t_{i_j, k_j}$ for $j = 1, 2, \dots, d$ and

$$w_{\mathbf{i},\mathbf{k}} = \sum_{\substack{\mathbf{p} \in \{0,1\}^d \\ d \leq |\mathbf{i}+\mathbf{p}| \leq d+m-1}} \prod_{j=1}^d ((-1)^{p_j} w_{i_j, k_j}). \quad (21)$$

Nested case When the U_i are nested, we assume that the quadrature points and weights are ordered such that at level i the new points occur at the end of the point set, from index n_{i-1} onwards. That is, for all $i \in \mathbb{N}$ we have $t_{i,k} = t_{i+1,k}$ for $k = 0, 1, \dots, n_i-1$.

Then, to ensure that the function is only evaluated at each node once, (10) can be rewritten as

$$Q_{d,m}(g) = \sum_{\substack{\mathbf{i} \in \mathbb{N}^d \\ d \leq |\mathbf{i}| \leq d+m-1}} \sum_{k_1=n_{(i_1-1)}}^{n_{(i_1)}-1} \cdots \sum_{k_d=n_{(i_d-1)}}^{n_{(i_d)}-1} w_{\mathbf{i},\mathbf{k}} g(\mathbf{t}_{\mathbf{i},\mathbf{k}}), \quad (22)$$

with weights

$$w_{\mathbf{i},\mathbf{k}} = \sum_{\substack{\mathbf{q} \in \mathbb{N}^d, \mathbf{q} \geq \mathbf{i} \\ d \leq |\mathbf{q}| \leq d+m-1}} \prod_{j=1}^d (w_{q_j, k_j} - w_{q_j-1, k_j}), \quad (23)$$

where we set $w_{0,k} \equiv 0$ for all $k \geq 0$ and $w_{q,k} \equiv 0$ when $k \geq n_q$. In particular, when $q_j = i_j$ in (23) the weight that is subtracted is 0, that is, $w_{q_j-1, k_j} = w_{i_j-1, k_j} = 0$, since in (22) $k_j \geq n_{i_j-1}$.

4.2 Smolyak quadrature via the combination technique

The combination technique (it combines different straightforward tensor product rules, hence the name) provides an alternative formulation to (10) as follows, see, e.g., [5, 18],

$$\begin{aligned} Q_{d,m}(g) &= \sum_{\substack{\mathbf{i} \in \mathbb{N}^d \\ \max(m,d) \leq |\mathbf{i}| \leq d+m-1}} (-1)^{d+m-1-|\mathbf{i}|} \binom{d-1}{|\mathbf{i}|-m} \left(\bigotimes_{j=1}^d U_{i_j} \right)(g) \\ &= \sum_{r=\max(m-d+1,1)}^m (-1)^{m-r} \binom{d-1}{d+r-1-m} \sum_{\substack{\mathbf{i} \in \mathbb{N}^d \\ |\mathbf{i}|=d+r-1}} \left(\bigotimes_{j=1}^d U_{i_j} \right)(g) \\ &= \sum_{r=\max(m-d+1,1)}^m (-1)^{m-r} \binom{d-1}{m-r} \sum_{\substack{\mathbf{i} \in \mathbb{N}^d \\ |\mathbf{i}|=d+r-1}} \left(\bigotimes_{j=1}^d U_{i_j} \right)(g), \end{aligned} \quad (24)$$

where we have simplified using the symmetry of the binomial coefficient: $\binom{n}{k} = \binom{n}{n-k}$. We adopt the usual convention that $\binom{0}{0} := 1$.

Using (24), we can now rewrite the MDM algorithm from the second equality in (12)

as

$$\begin{aligned}
\mathcal{A}^C(f) &= c_\emptyset f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{\mathbf{u} \in \mathcal{U} \\ \mathbf{u} \supseteq \mathbf{v}}} (-1)^{|\mathbf{u}| - |\mathbf{v}|} \\
&\quad \times \sum_{m=\max(m_{\mathbf{u}} - |\mathbf{v}| + 1, 1)}^{m_{\mathbf{u}}} (-1)^{m_{\mathbf{u}} - m} \binom{|\mathbf{v}| - 1}{m_{\mathbf{u}} - m} \sum_{\substack{\mathbf{i}_{\mathbf{v}} \in \mathbb{N}^{|\mathbf{v}|} \\ |\mathbf{i}_{\mathbf{v}}| = |\mathbf{v}| + m - 1}} \left(\bigotimes_{j \in \mathbf{v}} U_{i_j} \right) (f(\cdot; \mathbf{v}; \mathbf{0})) \\
&= c_\emptyset f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{m=1 \\ \tilde{c}(\mathbf{v}, m) \neq 0}}^{m_{\text{max}}} \tilde{c}(\mathbf{v}, m) \tilde{Q}_{\mathbf{v}, m}(f(\cdot; \mathbf{v}; \mathbf{0})), \tag{25}
\end{aligned}$$

where for a nonempty set \mathbf{v} and $m = 1, \dots, m_{\text{max}}$ we define

$$\tilde{Q}_{\mathbf{v}, m}(g_{\mathbf{v}}) := \sum_{\substack{\mathbf{i}_{\mathbf{v}} \in \mathbb{N}^{|\mathbf{v}|} \\ |\mathbf{i}_{\mathbf{v}}| = |\mathbf{v}| + m - 1}} \left(\bigotimes_{j \in \mathbf{v}} U_{i_j} \right) (g_{\mathbf{v}}), \tag{26}$$

and

$$\tilde{c}(\mathbf{v}, m) := \sum_{\substack{\mathbf{u} \in \mathcal{U}, \mathbf{u} \supseteq \mathbf{v} \\ m_{\mathbf{u}} - |\mathbf{v}| + 1 \leq m \leq m_{\mathbf{u}}}} (-1)^{|\mathbf{u}| - |\mathbf{v}| + m_{\mathbf{u}} - m} \binom{|\mathbf{v}| - 1}{m_{\mathbf{u}} - m}. \tag{27}$$

The formulation (25)–(27) is very similar to the formulation (12)–(13), and the computation of the values $\tilde{c}(\mathbf{v}, m)$ can also be done while constructing the extended active set. This is shown in Pseudocode 2A', which works in a similar way to Pseudocode 2A. The key change is that Step 12 of Pseudocode 2A is replaced by Steps 12–14 of Pseudocode 2A'.

The quantity $\tilde{Q}_{\mathbf{v}, m}(g_{\mathbf{v}})$ is a straightforward tensor product quadrature rule

$$\tilde{Q}_{d, m}(g) := \sum_{\substack{\mathbf{i} \in \mathbb{N}^d \\ |\mathbf{i}| = d + m - 1}} \sum_{k_1=0}^{n_{(i_1)} - 1} \cdots \sum_{k_d=0}^{n_{(i_d)} - 1} w_{\mathbf{i}, \mathbf{k}} g(\mathbf{t}_{\mathbf{i}, \mathbf{k}}), \tag{28}$$

with $w_{\mathbf{i}, \mathbf{k}} = \prod_{j=1}^d w_{i_j, k_j}$ and $(\mathbf{t}_{\mathbf{i}, \mathbf{k}})_j = t_{i_j, k_j}$ for $j = 1, \dots, d$. So the implementation of the Smolyak MDM algorithm using the combination technique can be obtained analogously by modifying Pseudocode 3A, shown in Pseudocode 3A'. The essential changes are in Steps 5 and 6.

Pseudocode 2A' (The extended active set for Smolyak with combination technique)

```

1: Initialize  $\mathcal{U}_{\text{ext}} \leftarrow \mathcal{U}$  ▷ start from the active set
2: Initialize  $c_\emptyset \leftarrow 1$  ▷ for  $\mathbf{u} = \emptyset$ 
3: for  $\emptyset \neq \mathbf{u} \in \mathcal{U}$  with  $|\mathbf{u}|$  from 1 to  $\sigma^*$  do ▷ traverse in increasing cardinality
4:   Calculate  $m_{\mathbf{u}}$  ▷ formula for  $m_{\mathbf{u}}$  is given from theory
5:   Update  $c_\emptyset \leftarrow c_\emptyset + (-1)^{|\mathbf{u}|}$ 
6:   Initialize  $\tilde{c}(\mathbf{u}, m) \leftarrow 0$  for  $m$  from 1 to  $m_{\text{max}}$ 
7:   for  $\emptyset \neq \mathbf{v} \subseteq \mathbf{u}$  do ▷ generate nonempty subsets
8:     if  $\mathbf{v} \notin \mathcal{U}_{\text{ext}}$  then ▷ look up and add missing subset
9:       Add  $\mathbf{v}$  to  $\mathcal{U}_{\text{ext}}$ 
10:      Initialize  $\tilde{c}(\mathbf{v}, m) \leftarrow 0$  for  $m$  from 1 to  $m_{\text{max}}$ 
11:     end if
12:     for  $m$  from  $m_{\mathbf{u}} - |\mathbf{v}| + 1$  to  $m_{\mathbf{u}}$  do ▷ update relevant entries
13:       Update  $\tilde{c}(\mathbf{v}, m) \leftarrow \tilde{c}(\mathbf{v}, m) + (-1)^{|\mathbf{u}|-|\mathbf{v}|+m_{\mathbf{u}}-m} \binom{|\mathbf{v}|-1}{m_{\mathbf{u}}-m}$ 
14:     end for
15:   end for
16: end for

```

Pseudocode 3A' (Implementing the Smolyak MDM with combination technique)

```

1: Initialize  $\mathcal{A}^{\text{C}}(f) \leftarrow c_\emptyset \times f(\mathbf{0})$ 
2: for  $\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}$  do
3:   for  $m$  from 1 to  $m_{\text{max}}$  do
4:     if  $\tilde{c}(\mathbf{v}, m) \neq 0$  then
5:       Calculate  $\tilde{Q}_{\mathbf{v},m}(f(\cdot; \mathbf{v}; \mathbf{0}))$  using (28)
6:       Update  $\mathcal{A}^{\text{C}}(f) \leftarrow \mathcal{A}^{\text{C}}(f) + \tilde{c}(\mathbf{v}, m) \times \tilde{Q}_{\mathbf{v},m}(f(\cdot; \mathbf{v}; \mathbf{0}))$ 
7:     end if
8:   end for
9: end for
10: return  $\mathcal{A}^{\text{C}}(f)$ 

```

4.3 Direct Smolyak vs combination technique

Here we compare the computational cost between the direct Smolyak implementation \mathcal{A}^{S} given by (12)–(13) and the combination technique implementation \mathcal{A}^{C} given by (25)–(27). Throughout, we will use the notation $\text{cost}(\cdot)$ to denote the whole cost, $\#(\cdot)$ to denote the number of function evaluations, and $\$(|\mathbf{v}|)$ to denote the cost of evaluating the original integrand f at some anchored point $(\mathbf{x}_{\mathbf{v}}; \mathbf{0})$.

The cost of the direct Smolyak implementation is

$$\text{cost}(\mathcal{A}^S) = \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{m=1 \\ c(\mathbf{v}, m) \neq 0}}^{m_{\text{max}}} \text{cost}\left(Q_{\mathbf{v}, m}(f(\cdot; \mathbf{v}; \mathbf{0}))\right).$$

Similarly for the combination technique the cost is

$$\text{cost}(\mathcal{A}^C) = \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\substack{m=1 \\ \tilde{c}(\mathbf{v}, m) \neq 0}}^{m_{\text{max}}} \text{cost}\left(\tilde{Q}_{\mathbf{v}, m}(f(\cdot; \mathbf{v}; \mathbf{0}))\right).$$

We expect that $\tilde{c}(\mathbf{v}, m)$ will be nonzero more often than $c(\mathbf{v}, m)$ would be nonzero, so that the combination technique approach needs to compute more quadrature approximations. We need to account for both the cost to construct the quadrature weights and the cost of function evaluations.

In terms of the number of function evaluations, we have for the direct Smolyak implementation

$$\#(Q_{d, m}) = \begin{cases} \sum_{|\mathbf{i}| \leq d+m-1} \prod_{j=1}^d n_{i_j} & \text{if non-nested,} \\ \sum_{|\mathbf{i}| \leq d+m-1} \prod_{j=1}^d (n_{i_j} - n_{i_{j-1}}) & \text{if nested.} \end{cases} \quad (29)$$

For the combination technique, we have

$$\begin{aligned} \#(\tilde{Q}_{d, m}) &= \sum_{|\mathbf{i}|=d+m-1} \prod_{j=1}^d n_{i_j} \\ &= \sum_{|\mathbf{i}|=d+m-1} \prod_{j=1}^d \left(\sum_{p_j=1}^{i_j} n_{p_j} - n_{p_j-1} \right) \\ &= \sum_{|\mathbf{i}|=d+m-1} \sum_{\mathbf{p} \in \mathbb{N}^d, \mathbf{p} \leq \mathbf{i}} \prod_{j=1}^d (n_{p_j} - n_{p_j-1}) \\ &= \sum_{|\mathbf{p}| \leq d+m-1} \binom{2d+m-|\mathbf{p}|-2}{d-1} \prod_{j=1}^d (n_{p_j} - n_{p_j-1}). \end{aligned}$$

So $\#(Q_{d, m}^{\text{nested}}) \leq \#(\tilde{Q}_{d, m}) \leq \#(Q_{d, m}^{\text{non-nested}})$.

For the direct Smolyak implementation we note that (20) (or (22) in the nested case) using the weights (21) (respectively (23)) is simply a grouping of all of the quadrature points, but the total collection of one-dimensional weights that need to be evaluated is the same as in (10); so the cost of computing the weights is $\sum_{|\mathbf{i}| \leq d+m-1} d \prod_{j=1}^d (n_{i_j} + n_{i_{j-1}})$. On the other hand, the cost of computing the weights in (26) is clearly $\sum_{|\mathbf{i}|=|\mathbf{v}|+m-1} |\mathbf{v}| \prod_{j \in \mathbf{v}} n_{i_j}$.

Thus for the direct Smolyak implementation we have

$$\text{cost}(Q_{\mathbf{v}, m}) = \begin{cases} \sum_{|\mathbf{i}| \leq |\mathbf{v}|+m-1} \left(|\mathbf{v}| \prod_{j \in \mathbf{v}} (n_{i_j} + n_{i_{j-1}}) + \$(|\mathbf{v}|) \prod_{j \in \mathbf{v}} n_{i_j} \right) & \text{if non-nested,} \\ \sum_{|\mathbf{i}| \leq |\mathbf{v}|+m-1} \left(|\mathbf{v}| \prod_{j \in \mathbf{v}} (n_{i_j} + n_{i_{j-1}}) + \$(|\mathbf{v}|) \prod_{j \in \mathbf{v}} (n_{i_j} - n_{i_{j-1}}) \right) & \text{if nested,} \end{cases}$$

and for the combination technique

$$\text{cost}(\tilde{Q}_{\mathbf{v},m}) = \sum_{|\mathbf{i}|=|\mathbf{v}|+m-1} \left(|\mathbf{v}| \prod_{j \in \mathbf{v}} n_{i_j} + \$(|\mathbf{v}|) \prod_{j \in \mathbf{v}} n_{i_j} \right).$$

To summarize, the combination technique implementation is likely to require more quadrature approximations than the direct method (more nonzero $\tilde{c}(\mathbf{v}, m)$ than $c(\mathbf{v}, m)$), and it uses more function evaluations than the direct method in the nested case, but the cost of computing the weights is cheaper. It is not immediately clear which method would be the overall winner.

5 MDM with randomized QMC

A randomly shifted version of the QMC approximation (14) takes the form (see, e.g., [2])

$$\frac{1}{n} \sum_{i=0}^{n-1} g \left(\left\{ \mathbf{t}^{(i)} + \mathbf{\Delta} \right\} \right),$$

where $\mathbf{\Delta} \in [0, 1)^d$ is the random shift with independent and uniformly distributed components $\Delta_j \in [0, 1)$ for $j = 1, \dots, d$, and the braces around a vector indicate that we take the fractional part of each component in the vector. The advantage of a randomly shifted QMC method is that it provides an unbiased estimate of the integral, and moreover, one can obtain a practical error estimate by using a number of independent random shifts.

In this section we outline how to implement randomized QMC (RQMC) versions of the QMC MDM from Section 3.2 by random shifting. One approach that comes to mind is to use a completely different set of independent shifts for each $A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0}))$ in (15). But with this approach none of the function evaluations can be reused. Another approach would be to use the same set of independent shifts for those $A_{\mathbf{u}}(f(\cdot; \mathbf{v}; \mathbf{0}))$ with the same cardinality $|\mathbf{u}|$, in a similar way to how the QMC method is applied to the MDM. But this approach also conflicts with our strategy to reuse function values based on the position where a subset \mathbf{v} originates from \mathbf{u} . Furthermore, it is unclear in this case how to obtain a valid error estimate of the overall MDM algorithm because of the dependence between many shifts. So, instead of these two approaches, we will describe a third approach which allows for a valid error estimate and the reuse of function values as in the case of the non-randomized QMC MDM.

Instead, our approach is to randomize the MDM algorithm itself, by treating it as an algorithm that acts on a function of τ^* variables, and then independently shifting each of the τ^* variables (recall from Lemma 1 that τ^* is the truncation dimension, i.e., the largest index of the variables that appear in the active set). We generate r independent random shifts $\mathbf{\Delta}^{(1)}, \dots, \mathbf{\Delta}^{(r)} \in [0, 1)^{\tau^*}$, and we take

$$\mathcal{A}^R(f) = \frac{1}{r} \sum_{q=1}^r \mathcal{A}_q(f), \tag{30}$$

where each $\mathcal{A}_q(f)$ is a shifted QMC MDM algorithm analogous to (17)–(19),

$$\mathcal{A}_q(f) := c_\emptyset f(\mathbf{0}) + \sum_{\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}} \sum_{\mathbf{w} \in \mathcal{M}(\mathbf{v})} \sum_{\substack{m=0 \\ c(\mathbf{v}, \mathbf{w}, m) \neq 0}}^{m_{\text{max}}} c(\mathbf{v}, \mathbf{w}, m) \frac{\tilde{S}_{\mathbf{v}, \mathbf{w}, m}^{(q)}(f)}{2^{m_{\text{max}}}}, \quad (31)$$

but now with function values shifted by $\Delta^{(q)}$ in

$$\tilde{S}_{\mathbf{v}, \mathbf{w}, m}^{(q)}(f) := \sum_{i=\lfloor 2^{m-1} \rfloor}^{2^m-1} f\left(\left\{\mathbf{t}_{\mathbf{w} \rightarrow \mathbf{v}}^{(i)} + \Delta_{\mathbf{v}}^{(q)}\right\}; \mathbf{0}\right). \quad (32)$$

In this way, for each independent shift $\Delta^{(q)}$ we can perform the MDM approximation $\mathcal{A}_q(f)$ using the reformulation described in Section 3.2. Note that the reuse of function values is only possible inside the approximation for a single shift, reuse across different shifts will never be possible because the shifted approximations must be independent. As such, the cost of our RQMC MDM using r shifts is r times the cost of the deterministic QMC MDM from Section 3.2.

Pseudocode 3B' (Implementing the RQMC MDM)

```

1: Initialize  $\mathcal{A}^{\text{R}}(f) \leftarrow 0$ 
2: Initialize  $E \leftarrow 0$ 
3: for  $q$  from 1 to  $r$  do ▷ compute MDM for each shift
4:   Generate  $\Delta^{(q)}$  independently and uniformly from  $[0, 1)^{\tau^*}$ 
5:   Initialize  $\mathcal{A}_q(f) \leftarrow c_\emptyset \times f(\mathbf{0})$ 
6:   for  $\emptyset \neq \mathbf{v} \in \mathcal{U}_{\text{ext}}$  do
7:     for  $\mathbf{w} \in \mathcal{M}(\mathbf{v})$  do
8:       for  $m$  from 0 to  $m_{\text{max}}$  do
9:         if  $c(\mathbf{v}, \mathbf{w}, m) \neq 0$  then
10:          Calculate  $\tilde{S}_{\mathbf{v}, \mathbf{w}, m}^{(q)}(f)$  using (32)
11:          Update  $\mathcal{A}_q(f) \leftarrow \mathcal{A}_q(f) + c(\mathbf{v}, \mathbf{w}, m) \times \tilde{S}_{\mathbf{v}, \mathbf{w}, m}^{(q)}(f)/2^{m_{\text{max}}}$ 
12:        end if
13:      end for
14:    end for
15:  end for
16:  Update  $\mathcal{A}^{\text{R}}(f) \leftarrow \mathcal{A}^{\text{R}}(f) + \mathcal{A}_q(f)$  ▷ sum up from different shifts
17:  Update  $E \leftarrow E + (\mathcal{A}_q(f))^2$  ▷ estimate error from different shifts
18: end for
19: Compute  $\mathcal{A}^{\text{R}}(f) \leftarrow \mathcal{A}^{\text{R}}(f)/r$  ▷ final MDM approximation
20: Compute  $E \leftarrow \sqrt{[E - r \times (\mathcal{A}^{\text{R}}(f))^2]/[r(r-1)]}$  ▷ final error estimate
21: return  $\mathcal{A}^{\text{R}}(f)$  and  $E$ 

```

Since $\mathcal{A}_1(f), \dots, \mathcal{A}_r(f)$ are independent random variables each with the same mean $\sum_{\mathbf{u} \in \mathcal{U}} I_{\mathbf{u}}(f_{\mathbf{u}})$, their average $\mathcal{A}^{\text{R}}(f)$ also has the same mean. Moreover, the variance of $\mathcal{A}^{\text{R}}(f)$ is $1/r$ times the variance of each $\mathcal{A}_q(f)$. The quadrature component of the root-mean-square error, i.e., $\sqrt{\mathbb{E} |\sum_{\mathbf{u} \in \mathcal{U}} I_{\mathbf{u}}(f_{\mathbf{u}}) - \mathcal{A}^{\text{R}}(f)|^2}$, can be estimated from these r sample values by

$$\sqrt{\frac{1}{r(r-1)} \sum_{q=1}^r (\mathcal{A}^{\text{R}}(f) - \mathcal{A}_q(f))^2} = \sqrt{\frac{1}{r(r-1)} \left(\sum_{q=1}^r (\mathcal{A}_q(f))^2 - r (\mathcal{A}^{\text{R}}(f))^2 \right)}.$$

The computation of $\mathcal{M}(\mathbf{v})$ and $c(\mathbf{v}, \mathbf{w}, m)$ is exactly the same as in Pseudocode 2B. We only need to replace Pseudocode 3B by Pseudocode 3B', where we include also the error estimation.

Note that due to linearity in (30)–(31), we can also interpret $\mathcal{A}^{\text{R}}(f)$ as one MDM algorithm where each of the quadrature approximations $\mathcal{A}_{\mathbf{u}}$ is obtained by the average of r randomly shifted QMC rules. In this case we can also estimate the root-mean-square error corresponding to each \mathbf{u} . However, note that the shifts between different sets \mathbf{u} are correlated and an estimate for the total variance cannot be obtained by simply summing up the individual variance estimates.

6 Computing the tolerance T

Under the theoretical setting of the paper [7], the threshold parameter T to construct an active set (7) takes the form (see Formula (26) of [7])

$$T = \left(\frac{\varepsilon/2}{\sum_{\mathbf{u} \in \mathbb{N}} [w(\mathbf{u})]^{1/\alpha}} \right)^{\alpha/(\alpha-1)}, \quad (33)$$

where $\varepsilon > 0$ is a given error tolerance parameter, while $\alpha > 1$ is a free parameter with the constraint that $\sum_{\mathbf{u} \in \mathbb{N}} [w(\mathbf{u})]^{1/\alpha} < \infty$. Since the active set constructed by Pseudocode 1 is uniquely defined by T and $w(\mathbf{u})$, computing the tolerance is another important step in implementing the MDM. In this section we outline how to estimate T by presenting novel estimates on the sum in (33).

In a practical implementation, we need to estimate the infinite sum in the denominator *from above*, to yield an underestimate of T , so that the required theoretical error tolerance ε is guaranteed, at the expense of enlarging the active set. Understandably, we should aim for a tight estimate of the infinite sum to avoid making the active set too large and thus the algorithm too expensive. Similarly, the free parameter α should be chosen so as to make the threshold parameter T as large as possible.

Here we derive upper bounds on the infinite sum by assuming further structure in $w(\mathbf{u})$, namely, that the POD form of $w(\mathbf{u})$, see (8), is further parametrized for $\ell \geq 0$ and $j \geq 1$ by

$$\Omega_{\ell} = c_1(\ell!)^{b_1} \quad \text{and} \quad \omega_j = c_2 j^{-b_2}, \quad (34)$$

with $b_1 \geq 0$, $b_2 > 1$, $b_2 > b_1$, and $c_1, c_2 > 0$. Thus

$$\sum_{\mathbf{u} \subset \mathbb{N}} [w(\mathbf{u})]^{1/\alpha} = \sum_{\ell=0}^{\infty} \sum_{|\mathbf{u}|=\ell} \left(c_1 (\ell!)^{b_1} \prod_{j \in \mathbf{u}} (c_2 j^{-b_2}) \right)^{1/\alpha} = c_1^{1/\alpha} \sum_{\ell=0}^{\infty} (\ell!)^a c_2^\ell \sum_{|\mathbf{u}|=\ell} \prod_{j \in \mathbf{u}} j^{-b}, \quad (35)$$

with

$$a = \frac{b_1}{\alpha}, \quad b = \frac{b_2}{\alpha}, \quad \text{and} \quad c = c_2^{1/\alpha}. \quad (36)$$

We know from [7, Lemma 10] that the infinite sum in (35) is finite if $b > 1$ and $b > a$. In turn this means that the free parameter $\alpha > 1$ in (33) should satisfy $\alpha < b_2$.

In the next two lemmas we obtain an upper bound on the infinite sum in (35) for somewhat general parameters a, b, c , without taking into account the constraints in how they relate to each other or how they relate to α . After the two lemmas we will discuss when and how the lemmas can be applied in our case.

Lemma 2. *For any $b > 1$ and $\ell \geq 1$ we have*

$$\sum_{|\mathbf{u}|=\ell} \prod_{j \in \mathbf{u}} j^{-b} \leq \frac{z^{\ell-1}}{(\ell-1)!} \left(1 + \frac{z}{\ell} \right), \quad z := \frac{(2/3)^{b-1}}{b-1}. \quad (37)$$

Proof. By identifying \mathbf{u} with the vector $(j_1, j_2, \dots, j_\ell)$ with ordered elements $j_1 < j_2 < \dots < j_\ell$, we see that

$$\sum_{|\mathbf{u}|=\ell} \prod_{j \in \mathbf{u}} j^{-b} = \sum_{j_1=1}^{\infty} j_1^{-b} \sum_{j_2=j_1+1}^{\infty} j_2^{-b} \dots \sum_{j_{\ell-1}=j_{\ell-2}+1}^{\infty} j_{\ell-1}^{-b} \sum_{j_\ell=j_{\ell-1}+1}^{\infty} j_\ell^{-b}. \quad (38)$$

For any $k \in \mathbb{N}$ and $p > 1$ we have

$$\sum_{j=k+1}^{\infty} j^{-p} \leq \int_{k+1/2}^{\infty} x^{-p} dx = \frac{(k+1/2)^{-(p-1)}}{p-1} < \frac{k^{-(p-1)}}{p-1},$$

which holds since the mid-point rule underestimates this integral. Therefore, the very last sum in (38) is bounded by

$$\int_{j_{\ell-1}+1/2}^{\infty} x^{-b} dx = \frac{(j_{\ell-1}+1/2)^{-(b-1)}}{b-1} < \frac{j_{\ell-1}^{-(b-1)}}{b-1},$$

and in turn the last two sums in (38) are bounded by

$$\frac{1}{b-1} \int_{j_{\ell-2}+1/2}^{\infty} x^{-(2b-1)} dx = \frac{(j_{\ell-2}+1/2)^{-2(b-1)}}{2(b-1)^2} < \frac{j_{\ell-2}^{-2(b-1)}}{2(b-1)^2}.$$

Similarly, the last $\ell-1$ sums are bounded by

$$\frac{(j_1+1/2)^{-(\ell-1)(b-1)}}{(\ell-1)! (b-1)^{\ell-1}}.$$

The sum with respect to j_1 has to be treated differently since we do not want to integrate over $[1/2, \infty)$. For that purpose, we treat differently $j_1 = 1$ and $j_1 \geq 2$, to obtain

$$\begin{aligned} \sum_{|u|=\ell} \prod_{j \in u} j^{-b} &\leq \frac{1}{(\ell-1)!(b-1)^{\ell-1}} \sum_{j_1=1}^{\infty} j_1^{-b} (j_1 + 1/2)^{-(\ell-1)(b-1)} \\ &< \frac{(2/3)^{(\ell-1)(b-1)}}{(\ell-1)!(b-1)^{\ell-1}} + \frac{1}{(\ell-1)!(b-1)^{\ell-1}} \sum_{j_1=2}^{\infty} j_1^{-\ell b + (\ell-1)}. \end{aligned}$$

Applying the integration estimate again to the sum over $j_1 \geq 2$, we get that

$$\frac{1}{(\ell-1)!(b-1)^{\ell-1}} \sum_{j_1=2}^{\infty} j_1^{-\ell b + (\ell-1)} \leq \frac{1}{\ell!(b-1)^\ell} \left(\frac{2}{3}\right)^{\ell(b-1)}.$$

Combining the last two steps yields the estimate in (37). \square

Lemma 3. For every $a \in (0, 1)$, $b > 1$, $c > 0$, $s \in \mathbb{N}$ and $t \in (0, 1)$, we have

$$\sum_{\ell=0}^{\infty} (\ell!)^a c^\ell \sum_{|u|=\ell} \prod_{j \in u} j^{-b} \leq 1 + \sum_{\ell=1}^s (\ell!)^a c^\ell \frac{z^{\ell-1}}{(\ell-1)!} \left(1 + \frac{z}{\ell}\right) + E_{s,t},$$

with $z := (2/3)^{b-1}/(b-1)$ as in (37), and

$$\begin{aligned} E_{s,t} &:= c \left(1 + \frac{z}{s+1}\right) \left[\frac{t^{s/a}}{1-t^{1/a}} \left(s + \frac{1}{1-t^{1/a}}\right) \right]^a \\ &\quad \times \left[\exp\left(\left(\frac{cz}{t}\right)^{1/(1-a)}\right) \min\left(1, \left(\frac{cz}{t}\right)^{s/(1-a)}\right) \frac{1}{s!} \right]^{1-a}. \end{aligned} \quad (39)$$

Proof. The result is obtained by applying Lemma 2 and then estimating the tail sum from $\ell = s+1$ by $E_{s,t}$. Indeed, we have

$$\begin{aligned} &\sum_{\ell=s+1}^{\infty} (\ell!)^a c^\ell \frac{z^{\ell-1}}{(\ell-1)!} \left(1 + \frac{z}{\ell}\right) \\ &\leq c \left(1 + \frac{z}{s+1}\right) \sum_{\ell=s+1}^{\infty} \ell^a t^{\ell-1} \left(\frac{cz}{t}\right)^{\ell-1} \frac{1}{[(\ell-1)!]^{1-a}} \\ &\leq c \left(1 + \frac{z}{s+1}\right) \left[\sum_{\ell=s+1}^{\infty} \ell t^{(\ell-1)/a} \right]^a \left[\sum_{\ell=s+1}^{\infty} \frac{1}{(\ell-1)!} \left(\frac{cz}{t}\right)^{(\ell-1)/(1-a)} \right]^{1-a}, \end{aligned}$$

where the last step follows from Hölder's inequality with the conjugate pair $1/a$ and $1/(1-a)$.

Consider the equality

$$\sum_{\ell=s+1}^{\infty} \ell x^{\ell-1} = \frac{d}{dx} \left(\frac{x^{s+1}}{1-x} \right) = \frac{x^s}{1-x} \left(s + \frac{1}{1-x} \right),$$

which after substituting in $x = t^{1/a}$ yields the third factor in (39).

We also have

$$\sum_{\ell=s+1}^{\infty} \frac{y^{(\ell-1)/(1-a)}}{(\ell-1)!} = \frac{y^{s/(1-a)}}{s!} \sum_{\ell=0}^{s-1} \frac{y^{\ell/(1-a)}}{\ell!} \leq \exp(y^{1/(1-a)}) \min\left(1, \frac{y^{s/(1-a)}}{s!}\right),$$

with last inequality due to Taylor's theorem. Substituting $y = cz/t$ yields the fourth factor in (39). \square

The following corollary summarizes the upper bound on the sum. It introduces two new free parameters: $s \in \mathbb{N}$ and $t \in (0, 1)$.

Corollary 1. *Let $w(\mathbf{u})$ have product and order dependent components satisfying (34) with $b_2 > 0$, also let $\alpha \geq 1$ and $\alpha \in (b_1, b_2)$. Then for every $s \in \mathbb{N}$ and every $t \in (0, 1)$ we have*

$$\sum_{\mathbf{u} \in \mathbb{N}} [w(\mathbf{u})]^{1/\alpha} \leq c_1^{1/\alpha} \left(1 + \sum_{\ell=1}^s (\ell!)^a c^\ell \frac{z^{\ell-1}}{(\ell-1)!} \left(1 + \frac{z}{\ell} \right) + E_{s,t} \right), \quad (40)$$

where a, b, c are specified in (36), and z and $E_{s,t}$ are as defined in Lemma 3.

Note that when $\alpha = 1$ the upper bound (40) on the sum is valid, even though in this case the tolerance T in (33) is undefined.

Remark 2. *If $b_1 = 0$ so that $w(\mathbf{u})$ is of product form, then $a = 0$ in (36) and the sum can be bounded above using the same method as in [4, equation (7)], namely, for every $s \in \mathbb{N}$,*

$$\sum_{\mathbf{u} \in \mathbb{N}} [w(\mathbf{u})]^{1/\alpha} \leq c_1^{1/\alpha} \exp\left(\frac{c}{(b-1)(s+\frac{1}{2})^{b-1}}\right) \prod_{j=1}^s (1 + cj^{-b}),$$

where b, c are as given in (36). In this case the size of the active set will be smaller than the general case because with $b_1 = 0$ each $w(\mathbf{u})$ is smaller so the exact value of the sum $\sum_{\mathbf{u} \in \mathbb{N}} [w(\mathbf{u})]^{1/\alpha}$ is smaller, and moreover our upper bound on the sum is tighter.

Note that the threshold parameter in the construction of optimal and quasi-optimal active sets in [4] (see Remark 1) also requires a good upper bound on the sum with $\alpha = 1$.

7 Numerical experiments

Until now we have ignored any theoretical details of the MDM and focussed purely on the implementation given the arbitrary input parameters ε , $\{\omega(\mathbf{u})\}_{|\mathbf{u}| < \infty}$, T and $\{m_{\mathbf{u}}\}_{\mathbf{u} \in \mathcal{U}}$. Below we give some brief details on how to specify these parameter values for a particular test integrand following the setting of [7]. We compare between QMC MDM and Smolyak MDM, as well as demonstrate the speedup of our efficient implementations over the naive implementations.

7.1 Test integrand

We consider the integrand $f : [-\frac{1}{2}, \frac{1}{2}]^{\mathbb{N}} \rightarrow \mathbb{R}$ given by

$$f(\mathbf{x}) = \frac{1}{1 + \sum_{j \geq 1} x_j / j^\beta}, \quad (41)$$

with different parameters $\beta > 1$. This integrand with $\beta = 2$ has previously been considered in, e.g., [7, Example 5]. Although we do not know the exact value of the integral, we are able to calculate a good approximation as a reference value and use this reference value to calculate the total error of our MDM algorithms. This integrand is considered a prototype function for some PDE applications, see e.g., [8].

In the theoretical setting of [7], it is assumed that each decomposition function $f_{\mathbf{u}}$ belongs to some normed space $F_{\mathbf{u}}$, and that bounds on the norms are known, i.e., $\|f_{\mathbf{u}}\|_{F_{\mathbf{u}}} \leq B_{\mathbf{u}}$ for all $\mathbf{u} \neq \emptyset$.

In the particular case of the anchored decomposition combined with the anchored norm over the shifted unit cube $[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}$, we have

$$\begin{aligned} \|f_{\mathbf{u}}\|_{F_{\mathbf{u}}} &= \left(\int_{[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}} \left(\frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{x}_{\mathbf{u}}} f_{\mathbf{u}}(\mathbf{x}_{\mathbf{u}}) \right)^2 d\mathbf{x}_{\mathbf{u}} \right)^{1/2} \\ &= \left(\int_{[-\frac{1}{2}, \frac{1}{2}]^{|\mathbf{u}|}} \left(\frac{\partial^{|\mathbf{u}|}}{\partial \mathbf{x}_{\mathbf{u}}} f(\mathbf{x}_{\mathbf{u}}; \mathbf{0}) \right)^2 d\mathbf{x}_{\mathbf{u}} \right)^{1/2}, \end{aligned} \quad (42)$$

and the induced operator norm of $I_{\mathbf{u}}$ in $F_{\mathbf{u}}$ is given by $\|I_{\mathbf{u}}\| = 12^{-|\mathbf{u}|/2} =: C_{\mathbf{u}}$ (see [7, Subsection 5.3]). Moreover, for the integrand (41) this norm is bounded by (see [7, Subsection 5.4] for derivation of the case $\beta = 2$)

$$\|f_{\mathbf{u}}\|_{F_{\mathbf{u}}} \leq \left(1 - \frac{1}{2}\zeta(\beta)\right)^{-(|\mathbf{u}|+1)} |\mathbf{u}|! \prod_{j \in \mathbf{u}} j^{-\beta} =: B_{\mathbf{u}},$$

where $\zeta(x) = \sum_{k=1}^{\infty} k^{-x}$ for $x > 1$ is the Riemann zeta function.

7.2 Active set construction

We continue under the assumption that $f_{\mathbf{u}}$ is in the Hilbert space whose norm is given by (42).

Following [7, Formula (26)], the above description leads to an active set (7) with $w(\mathbf{u}) := C_{\mathbf{u}} B_{\mathbf{u}}$, which is in POD form (34) with

$$c_1 = \frac{1}{1 - \frac{1}{2}\zeta(\beta)}, \quad c_2 = \frac{c_1}{\sqrt{12}}, \quad b_1 = 1, \quad b_2 = \beta,$$

and where the tolerance T is given by (33). We estimate T by the upper bound (40), which we compute by fixing $s = 1000$, $t = 0.5$, and then maximizing the estimated tolerance for α over 100 equispaced points in $(1, \beta)$.

Table 1 presents details on the active set for the parameter values $\beta = 4, 3, 2.5$ and $\varepsilon = 10^{-1}, 10^{-2}, 10^{-3}$. The rows are labelled as follows: ε is the error request, T is the computed tolerance for the active set, σ^* is the superposition dimension, τ^* is the maximum truncation dimension, and the last ten rows display the number of sets of each size in the active set.

We see that although there are many sets to consider in MDM, even in the hardest case with $\beta = 2.5$ and $\varepsilon = 10^{-2}$ we only ever deal with integrals up to 10 dimensions, with the highest coordinate considered being 24724.

Below we will restrict ourselves to the case $\beta = 3$, with error request down to $\varepsilon = 10^{-6}$.

Actually, the above approach from [7] for prescribing the parameters $w(\mathbf{u})$ and T overestimates the truncation error for our test integrand and makes the active set much larger than necessary. A tighter truncation error estimate can be done for this test integrand using a Taylor series argument (see e.g., [7, Remark 13]) and this should yield better input parameters $w(\mathbf{u})$ and T to our efficient MDM algorithms. Analysis on the best strategy to prescribe the active set parameters for any given practical integrand falls outside the scope of this paper.

	$\beta = 4$			$\beta = 3$			$\beta = 2.5$	
ε	1e-1	1e-2	1e-3	1e-1	1e-2	1e-3	1e-1	1e-2
T	1.4e-4	2.8e-6	6.4e-8	4.0e-6	3.6e-8	3.8e-10	1.5e-8	4.9e-11
σ^*	3	4	5	5	6	7	8	10
τ^*	10	28	72	86	418	1907	2528	24724
size 1	9	26	68	76	370	1686	2019	19750
2	12	48	159	195	1285	7327	10077	126882
3	5	28	132	202	1828	13117	21996	354377
4	0	4	36	80	1234	11907	26258	559155
5	0	0	1	10	361	5578	17874	536133
6	0	0	0	0	32	1145	6513	313623
7	0	0	0	0	0	69	1088	106877
8	0	0	0	0	0	0	47	18582
9	0	0	0	0	0	0	0	1210
10	0	0	0	0	0	0	0	8

Table 1: Results from the active set construction for various β and ε .

7.3 QMC MDM

For the randomized QMC MDM we use an extensible rank-1 lattice rule with generating vector

$$\mathbf{z} = (1, 756581, 694385, 178383, 437131, 945527, 62405, 1079809, \\ 991997, 750785, 187845, 1666795, 491701, 1092667, \\ 1279469, 817683, 1946073, 1946073, 1530387, 686611, \dots),$$

with $n = 2^m$ points for any $m = 0, \dots, 25$. It is constructed by a component-by-component (CBC) algorithm as outlined in [1], but the search criterion was appropriately modified to match the norm (42). Also, we apply the tent-transform (see [6]) $x \mapsto 1 - |2x - 1|$ to each component of the shifted quadrature points in $[0, 1]$, and then translate it to $[-\frac{1}{2}, \frac{1}{2}]$.

Following [7], we assume that the quadrature error for each decomposition term f_u to be bounded by $G_{u,q} (n_u + 1)^{-q} \|f_u\|_{F_u}$ with appropriate constants $G_{u,q}$ and q ; a Lagrange optimization argument then results in choosing the number of points $n_u \geq h_u$, with

$$h_u = \left(\frac{2}{\varepsilon} \sum_{\mathbf{v} \in \mathcal{U}} \mathcal{L}(|\mathbf{v}|)^{q/(q+1)} (G_{\mathbf{v},q} B_{\mathbf{v}})^{1/(q+1)} \right)^{1/q} \left(\frac{G_{u,q} B_u}{\mathcal{L}(|\mathbf{u}|)} \right)^{1/(q+1)}, \quad (43)$$

where $\mathcal{L}(|\mathbf{u}|)$ is the cost of evaluating the decomposition term f_u .

Although the above formula for h_u is precisely [7, Formula (28)], how we specify the other parameters here will deviate from [7]. Based on (5) we set $\mathcal{L}(|\mathbf{u}|) = \max(2^{|\mathbf{u}|} |\mathbf{u}|, 1)$. The constant $G_{u,q}$ arising from the theoretical error bound is far too large, so we set instead $G_{u,q} = 1$ after some experiments (see below). In the theoretical setting with the norm (42) involving mixed first order derivatives, we expect only up to first order convergence, leading to the choice $q = 1$. However, it is known from [6] that randomly-shifted and then tent-transformed lattice rules can achieve nearly second order convergence if the integrand has mixed second order derivatives; thus we take instead $q = 2$ (see justification by experiments below) without formally switching the setting. Finally we set $n_u = 2^{m_u}$ with $m_u = \max(\lceil \log_2(h_u) \rceil, 0)$.

In Figure 1 on the left we plot the error request ε against the estimated standard error obtained using 16 random shifts. This gives an idea of the quadrature error alone. By taking $q = 2$ instead of $q = 1$, we see that the error request ε and the estimated standard error are in agreement up to a constant factor. It is possible to tune this constant factor by changing the value of $G_{u,q}$ (it should be at least as large as $\|I_u\| = 12^{-|\mathbf{u}|/2}$ and indeed the theoretical bound yields $G_{u,q} = g^{|\mathbf{u}|}$ with some $g > 1$), but taking $G_{u,q} = 1$ appears to give reasonable results in practice (if it is too big then the quadrature rules will do too much work, while if it is too small they will underperform).

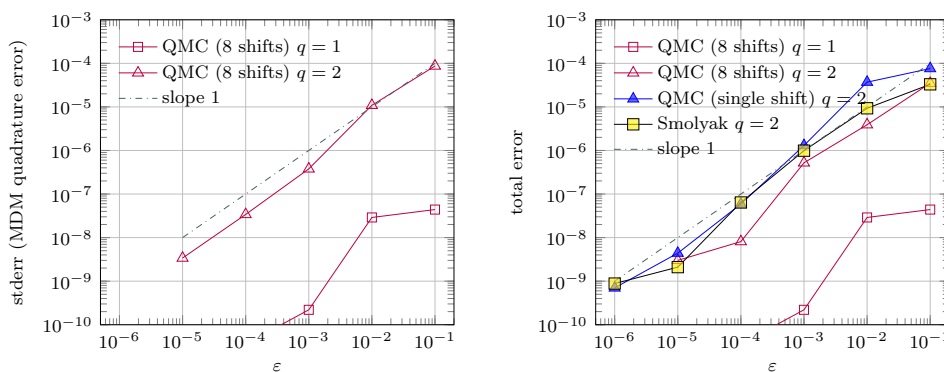


Figure 1: Error request ε against estimated standard error (left) and total error (right).

In Figure 1 on the right we plot the error request ε against the estimated total error (combining both the truncation error and the quadrature error) by comparing the results with a reference solution obtained using a higher precision QMC quadrature rule. The reference solution was computed using 2^{22} QMC points and 16 shifts in quad precision in 600 dimensions and resulted in a standard error of 8×10^{-13} . A similar computation in 800 dimensions with 2^{20} QMC points agreed up to 10 digits. The two graphs in Figure 1 show the same trend, indicating that the truncation error is no worse than the quadrature error.

7.4 Smolyak MDM

For the Smolyak MDM we will use the composite trapezoidal rule as the one-dimensional rules. These rules are nested. We set $U_0 := 0$ to be the zero algorithm, and following [3, Section 3] we take the first one-dimensional quadrature rule U_1 to be the single (mid-)point rule, i.e., $n_1 := 1$ with point $t_{1,0} := 0$ and weight $w_{1,0} := 1$. This extra level ensures that the number of points does not grow too quickly. Then for each $i \geq 2$ we take the one-dimensional quadrature rule U_i to be the composite trapezoidal rule in $[-\frac{1}{2}, \frac{1}{2}]$ with $n_i := 2^{i-1} + 1$ points at multiples of $1/2^{i-1}$, with the weights being $1/2^{i-1}$ for the interior points and $1/2^i$ at the two end points $\pm 1/2$.

To ensure that we iterate the points in a nested fashion, we label the points in the order of $0, \pm 1/2, \pm 1/4, \pm 1/8, \pm 3/8, \dots$ and so on. Explicitly, for $i \geq 2$ we can write

$$t_{i,k} := \begin{cases} k/2^p - 1/2 & \text{if } k \text{ is odd, and } p \text{ is such that } 2^{p-1} < k < 2^p, \\ -t_{i,k-1} & \text{if } k \text{ is even,} \end{cases}$$

with the corresponding weights

$$w_{i,k} := \begin{cases} 1/2^i & \text{if } k = 1, 2, \\ 1/2^{i-1} & \text{if } k = 0, 3, 4, \dots, n_i - 1. \end{cases}$$

We choose the approximation levels m_u of our quadrature rules in the direct Smolyak MDM implementation to be such that the number of function evaluations, see (29) with nested points, is at least h_u given by the formula (43), with the same definitions of $\mathcal{L}(|u|) = \max(2^{|u|}|u|, 1)$, $G_{u,q} = 1$ and $q = 2$. The justification for taking $q = 2$ here is that composite trapezoidal rules are known to give second order convergence for sufficiently smooth integrands in one dimension, and this convergence is transferred, modulo log-factors, to the Smolyak rule for multivariate integrands with sufficient smoothness, see e.g., [3]. We use the same values of m_u for the combination technique variant even though the actual numbers of function evaluations are higher.

In particular, our chosen values of m_u mean that the naive implementations of Smolyak MDM and QMC MDM would use roughly the same number of function evaluations for each f_u . However, the actual number of function evaluations for our efficient implementations would be lower and hence achieve the savings we aim for; see the timings in the next subsection.

In Figure 1 on the right we also plot the error request ε against the estimated total error of the direct Smolyak MDM implementation compared with the same reference solution as for QMC MDM. We see that all results are comparable.

7.5 Timing results

In Table 2 we present results on the run-time of our efficient MDM implementations compared with the naive implementations for error request ε from 10^{-1} down to 10^{-6} . We include results for QMC MDM with a single random shift, direct Smolyak MDM, and Smolyak MDM based on combination technique (CT-Smolyak). We report the total error with respect to the same reference solution in each case, as well as the run-time in seconds. The QMC results can vary between runs depending on the random shift. All calculations were done in x86 long double precision on a single node of the UNSW Katana cluster with an Intel Xeon X5675 3.07GHz CPU.

The values of t_{act} in the first column are the time in seconds used to construct the active set (Pseudocode 1), while the values of t_{ext} are the average time used to construct the extended active set and compute the three sets of coefficients (13), (27), (19) (Pseudocode 2A, 2A', 2B).

We clearly see increasing speedup of the efficient implementations over the naive ones as ε decreases. The reformulation of the MDM algorithm into this efficient formulation is the main result of this paper.

We see more speedup in the case of Smolyak MDM compared with QMC MDM. This is as expected, because for QMC MDM there is extra work in managing the different positions that a nonempty set can originate from as a subset of another set in the active set: we need to cope with a more complicated data structure for (19) compared with (13) or (27), and we need more function evaluations. Additionally, we expect the QMC algorithms to be much more efficient when the truncation dimension goes up (i.e., when ε goes down), since the sizes of the Smolyak grids based on trapezoidal rules then increase faster than the powers of 2 of the QMC algorithms.

If we compare the direct Smolyak MDM with the combination technique Smolyak MDM then we notice that for our efficient reformulation the two methods have very similar running times, with a very minor advantage for the direct method, but with the naive formulation the direct method is the clear winner. Note that we can see the effect of rounding errors in the calculations for $\varepsilon = 10^{-5}$ and 10^{-6} , since the total errors should remain the same between the naive and efficient implementations of the same algorithm, while the direct Smolyak and combination technique should also have the same total errors.

In Figure 2 we plot the total error against time for the results in Table 2 to demonstrate the speedup of the efficient implementations. For each pair of efficient and naive results, we expect the data points to be at the same horizontal level (same total error) but with bigger and bigger gaps in time (the speedup factor increases) as the errors go down.

$\beta = 3$, reference value = 1.1011984577041

ε	method	efficient		naive		speedup
		total error	time (s)	total error	time (s)	
1e-01 $t_{\text{act}} = 0.000768$ $t_{\text{ext}} = 0.00339$	QMC	7.57e-05	0.0017576	7.57e-05	0.0032837	1.9
	Smolyak	3.26e-05	0.0047466	3.26e-05	0.0063622	1.3
	CT-Smolyak	3.26e-05	0.0042816	3.26e-05	0.0088774	2.1
1e-02 $t_{\text{act}} = 0.00899$ $t_{\text{ext}} = 0.049$	QMC	3.66e-05	0.062643	3.66e-05	0.067456	1.1
	Smolyak	9.34e-06	0.074826	9.34e-06	0.12321	1.6
	CT-Smolyak	9.34e-06	0.073692	9.34e-06	0.19568	2.7
1e-03 $t_{\text{act}} = 0.0401$ $t_{\text{ext}} = 0.339$	QMC	1.26e-06	0.4301	1.26e-06	1.1336	2.6
	Smolyak	9.92e-07	0.49712	9.92e-07	1.9859	4.0
	CT-Smolyak	9.92e-07	0.48502	9.92e-07	3.4984	7.2
1e-04 $t_{\text{act}} = 0.34$ $t_{\text{ext}} = 4.08$	QMC	5.90e-08	4.8547	5.90e-08	15.766	3.2
	Smolyak	6.39e-08	5.5186	6.39e-08	27.89	5.1
	CT-Smolyak	6.39e-08	5.5692	6.39e-08	53.191	9.6
1e-05 $t_{\text{act}} = 2.79$ $t_{\text{ext}} = 41.7$	QMC	4.41e-09	47.64	4.51e-09	188.61	4.0
	Smolyak	2.13e-09	54.331	2.12e-09	346.79	6.4
	CT-Smolyak	2.11e-09	56.083	2.12e-09	734.87	13.1
1e-06 $t_{\text{act}} = 20.2$ $t_{\text{ext}} = 435$	QMC	7.01e-10	442.8	4.31e-10	2163.1	4.9
	Smolyak	8.76e-10	504.78	1.14e-09	4093.9	8.1
	CT-Smolyak	2.08e-09	535.74	1.14e-09	9255.4	17.3

Table 2: Timing comparisons between efficient and naive MDM implementations. t_{act} is the time to construct \mathcal{U} and t_{ext} is the average time to construct \mathcal{U}_{ext} for the 3 reformulations.

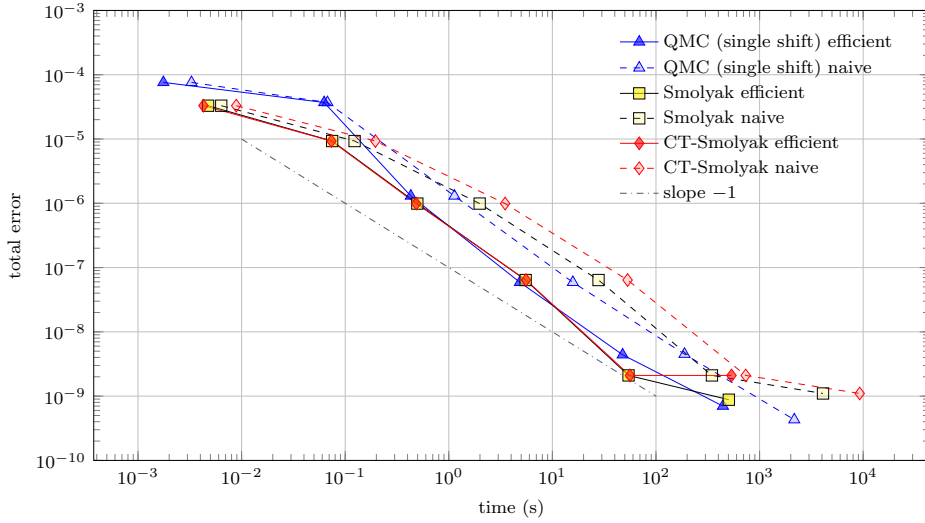


Figure 2: Estimated total error against time.

8 Conclusion

The MDM is a powerful algorithm for approximating integrals of ∞ -variate functions, but care must be taken to ensure the implementation is efficient. In this paper we have

provided details and explicit pseudocodes explaining how to efficiently run all components of the algorithm: from constructing the active set to running the MDM for both randomized QMC rules and Smolyak quadrature rules. By reformulating the MDM we are able to save cost by reducing the amount of repeated function evaluations incurred because of the recursive structure of the anchored decomposition. We applied the MDM to an example integrand that possesses similar properties to those that arise in recent PDE problems with random coefficients. The numerical results clearly support the cost savings of the efficient reformulations.

Acknowledgements

We gratefully acknowledge the financial support from the Australian Research Council (FT130100655 and DP150101770), the KU Leuven research fund (OT:3E130287 and C3:3E150478), the Taiwanese National Center for Theoretical Sciences (NCTS) – Mathematics Division, and the Statistical and Applied Mathematical Sciences Institute (SAMSI) 2017 Year-long Program on Quasi-Monte Carlo and High-Dimensional Sampling Methods for Applied Mathematics.

References

- [1] R. COOLS, F. Y. KUO AND D. NUYENS, *Constructing embedded lattice rules for multivariate integration*, SIAM J. Sci. Comp., 28 (2006), pp. 2162–2188.
- [2] J. DICK, F. Y. KUO AND I. H. SLOAN, *High-dimensional integration: The quasi-Monte Carlo way*, Acta Numerica, 22 (2013), pp. 133–288.
- [3] T. GERSTNER AND M. GRIEBEL, *Numerical integration using sparse grids*, Numer. Alg., 18 (1998), pp. 209–232.
- [4] A. D. GILBERT AND G. W. WASILKOWSKI, *Small superposition dimension and active set construction for multivariate integration under modest error demand*, J. Complexity, 42 (2017), pp. 94–109.
- [5] M. GRIEBEL, M. SCHNEIDER AND C. ZENGER, *A combination technique for the solution of sparse grid problems*, in Iterative Methods in Linear Algebra, R. Bequwens, P. de Groen (eds.), Elsevier, North Holland, (1992), pp. 263–281.
- [6] F. J. HICKERNELL, *Obtaining $O(n^{-2+\epsilon})$ convergence for lattice quadrature rules*, in Monte Carlo and Quasi-Monte Carlo Methods 2000, K. T. Fang, F. J. Hickernell, H. Niederreiter (eds.), Springer, Berlin-Heidelberg, (2002), pp. 274–289.
- [7] F. Y. KUO, D. NUYENS, L. PLASKOTA, I. H. SLOAN AND G. W. WASILKOWSKI, *Infinite-dimensional integration and the multivariate decomposition method*, J. Comput. Appl. Math., 326 (2017), pp. 217–234.
- [8] F. Y. KUO, CH. SCHWAB AND I. H. SLOAN, *Quasi-Monte Carlo finite element methods for a class of partial differential equations with random coefficients*, SIAM J. Numer. Anal., 50 (2012), pp. 3351–3374.

- [9] F. Y. KUO, I. H. SLOAN, G. W. WASILKOWSKI AND H. WOŹNIAKOWSKI, *Liberating the dimension*, J. Complexity, 26 (2010), pp. 422–454.
- [10] F. Y. KUO, I. H. SLOAN, G. W. WASILKOWSKI AND H. WOŹNIAKOWSKI, *On decompositions of multivariate functions*, Math. Comp., 79 (2010), 953–966.
- [11] H. NIEDERREITER, *Random Number Generation and Quasi-Monte Carlo Methods*, SIAM, Philadelphia, 1992.
- [12] L. PLASKOTA AND G. W. WASILKOWSKI, *Tractability of infinite-dimensional integration in the worst case and randomized settings*, J. Complexity, 27 (2011), pp. 505–518.
- [13] L. PLASKOTA AND G. W. WASILKOWSKI, *Efficient algorithms for multivariate and ∞ -variate integration with exponential weight*, Numer. Alg., 67 (2014), pp. 385–403.
- [14] I. H. SLOAN AND S. JOE, *Lattice Methods for Multiple Integration*, Oxford University Press, Oxford, 1994.
- [15] S. A. SMOLYAK, *Quadrature and interpolation formulas for tensor products of certain classes of functions*, Dokl. Acad. Nauk. SSSR, 4 (1963), pp. 240–243.
- [16] G. W. WASILKOWSKI, *On tractability of linear tensor product problems for ∞ -variate classes of functions*, J. Complexity, 29 (2013), pp. 351–369.
- [17] G. W. WASILKOWSKI, *Tractability of approximation of ∞ -variate functions with bounded mixed partial derivatives*, J. Complexity, 30 (2014), pp. 325–346.
- [18] G. W. WASILKOWSKI AND H. WOŹNIAKOWSKI, *Explicit cost bounds of algorithms for multivariate tensor product problems*, J. Complexity, 11 (1995), pp. 1–56.

Authors' addresses

Alexander D. Gilbert
 School of Mathematics and Statistics, The University of New South Wales
 Sydney, NSW 2052, Australia
 adgilbert91@gmail.com

Dirk Nuyens
 Department of Computer Science, KU Leuven
 Celestijnenlaan 200A, 3001 Heverlee, Belgium
 dirk.nuyens@cs.kuleuven.be

Frances Y. Kuo
 School of Mathematics and Statistics, The University of New South Wales
 Sydney, NSW 2052, Australia
 f.kuo@unsw.edu.au

Grzegorz W. Wasilkowski
 Department of Computer Science, University of Kentucky
 301 David Marksbury Building, Lexington, KY 40506, USA
 greg@cs.uky.edu