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MULTI INDEX MONTE CARLO: WHEN SPARSITY MEETS SAMPLING

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Abstract. We propose and analyze a novel Multi Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with random coefficients. The MIMC method is both a stochastic version of the combination technique introduced by Zenger, Griebel and collaborators and an extension of the Multilevel Monte Carlo (MLMC) method first described by Heinrich and Giles. Inspired by Giles's seminal work, instead of using first-order differences as in MLMC, we use in MIMC high-order mixed differences to reduce the variance of the hierarchical differences dramatically. This in turn yields new and improved complexity results, which are natural generalizations of Giles's MLMC analysis, and which increase the domain of problem parameters for which we achieve the optimal convergence, $\mathcal{O}(\mathrm{TOL}^{-2})$.

Moreover, we motivate the systematic construction of optimal sets of indices for MIMC based on properly defined profits that in turn depend on the average cost per sample and the corresponding weak error and variance. Under standard assumptions on the convergence rates of the weak error, variance and work per sample, the optimal index set turns out to be of Total Degree (TD) type. In some cases, using optimal index sets, MIMC achieves a better rate for the computational complexity than does the corresponding rate when using Full Tensor sets. We also show the asymptotic normality of the statistical error in the resulting MIMC estimator and justify in this way our error estimate, which allows both the required accuracy and the confidence in our computational results to be prescribed. Finally, we include numerical experiments involving a partial differential equation posed in three spatial dimensions and with random coefficients to substantiate the analysis and illustrate the corresponding computational savings of MIMC.

Keywords: Multilevel Monte Carlo, Monte Carlo, Partial Differential Equations with random data, Stochastic Differential Equations, Weak Approximation, Sparse Approximation, Combination technique

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1. Introduction

The main concept of Multilevel Monte Carlo (MLMC) Sampling was first introduced for applications in parametric integration by Heinrich [20, 21]. Later, for weak approximation of stochastic differential equations (SDEs) in mathematical finance, Kebaier [24] used a two-level Monte Carlo technique, effectively using a coarse numerical approximation as a control variate to a fine one, thus reducing the variance and the required number of samples on the fine grid. In a seminal work, Giles [12] extended this idea to multiple levels and gave it its familiar name: Multilevel Monte Carlo. Giles introduced a hierarchy of discretizations with geometrically decreasing grid sizes and optimized the number of samples on each level of the hierarchy. This resulted in a reduction in the computational burden from $\mathcal{O}\left(\mathrm{TOL}^{-3}\right)$ of the standard Euler-Maruyama Monte Carlo method with accuracy TOL to $\mathcal{O}\left(\log\left(\mathrm{TOL}\right)^2\mathrm{TOL}^{-2}\right)$, assuming that the work to generate a single realization on the finest level is $\mathcal{O}\left(\mathrm{TOL}^{-1}\right)$. More recently, [14] reduced this computational complexity to $\mathcal{O}\left(\mathrm{TOL}^{-2}\right)$ by using antithetic control variates with MLMC in multi-dimensional SDEs with smooth and piecewise smooth payoffs. The MLMC method has also been extended and applied in a wide variety of applications, including jump diffusions [33] and Partial Differential Equations (PDEs) with random coefficients [4, 8, 9, 13, 31, 10, 17]. The goal in these applications is to compute a scalar quantity of interest that is a functional of the solution of a PDE with random coefficients. In [31, Theorem 2.5], it has been proved that there is an optimal complexity rate similar to the previously mentioned one, but that depends on the dimensionality of the problem, the relation between the rate of variance convergence of the discretization method of the PDE and the work complexity associated with generating a single sample of the quantity of interest. In fact, in certain cases, the computational complexity can achieve the optimal rate, namely $\mathcal{O}\left(\mathrm{TOL}^{-2}\right)$.

More recently, sparse approximation techniques [6] have been coupled with MLMC in other works. In [26], the MLMC sampler was combined with a sparse tensor approximation method to estimate high-order moments of the finite volume approximate solution of a hyperbolic conservation law that has random initial data. Moreover, in [18, 32], new techniques were developed using sparse-grid stochastic collocation methods instead of Monte Carlo sampling in a multilevel setting that resembles that of MLMC.

In the present work, we follow a different approach by introducing a stochastic version of a sparse combination technique [34, 16, 7, 5, 6, 19] in the construction of a new *Monte Carlo* sampler, which we refer to as Multi Index Monte Carlo (MIMC). MIMC can be seen as a generalization of the standard Multilevel Monte Carlo Sampling method. This generalization departs from the notion of one-dimensional levels and first-order differences and instead uses multidimensional levels and high-order mixed differences to reduce the variance of the resulting estimator and its corresponding computational work drastically. The goal of MIMC is to achieve the optimal complexity of the Monte Carlo sampler, $\mathcal{O}\left(\mathrm{TOL}^{-2}\right)$, in a larger class of problems and to provide better convergence rates in other classes. The main results of our work are summarized in Theorems 2.1 and 2.2. These theorems contain the optimal work estimates of MIMC when using Full Tensor index sets and Total Degree index sets, respectively. We show that the rate of computational complexity of MIMC when using Total Degree index sets is, in some cases, better than the corresponding rate when using Full Tensor sets. In fact, we show that in some cases, the rate when using optimal index sets is independent of the dimensionality of the underlying problem.

In the next section, we start by motivating the class of problems we consider and we introduce some notation that is used throughout this work. Section 2 introduces MIMC and lists the necessary assumptions. Section 2.1 presents the computational complexity of a full-tensor index set, and Section 2.2 motivates an optimal total degree index set and shows the computational complexity of MIMC when using this index set. Next, Section 3 presents the numerical experiments to substantiate the derived results. Section 4 summarizes the work in the conclusions and outlines future work. Finally, Appendix A contains a proof of the asymptotic normality of the MIMC estimator.

1.1. **Problem Setting.** Let $S = \Psi(u)$ denote a real-valued functional applied to the unique solution, u, of an underlying stochastic model. We assume that Ψ is a smooth functional with respect to u. Here, smoothness is characterized by S satisfying **Assumptions 1-2** as presented in the next section. Our goal is to approximate the expected value of S, $\mathrm{E}[S]$, to a given accuracy TOL and a given confidence level. We assume that individual outcomes of the underlying solution, u, and the evaluation of the functional, S, are approximated by a discretization-based numerical scheme characterized by a multidimensional discretization parameter, $\boldsymbol{h}$. For instance, for a multidimensional PDE, the vector $\boldsymbol{h}$ could represent the space discretization parameter in each direction separately, while for a time dependent PDE, the vector $\boldsymbol{h}$ could collect the space and time discretization parameters. The value of the vector, $\boldsymbol{h}$, will govern the weak error and variance of the approximation of S as we will see below. To motivate this setting, we now give one example and identify the corresponding numerical discretizations, the discretization parameter, $\boldsymbol{h}$, and the corresponding rates of approximation.

Example 1. *Let $(\Omega, \mathcal{F}, P)$ be a complete probability space and $\mathcal{D} = \prod_{i=1}^{d} [0, D_i]$ for $D_i \in \mathbb{R}_+$ be a hypercube domain in $\mathbb{R}^d$. The solution $u : \mathcal{D} \times \Omega \to \mathbb{R}$ here solves almost surely (a.s.) the following equation:*

$$\begin{aligned} -\nabla \cdot (a(\boldsymbol{x};\omega)\nabla u(\boldsymbol{x};\omega)) &= f(\boldsymbol{x};\omega) \qquad \text{for } \boldsymbol{x} \in \mathcal{D}, \\ u(\boldsymbol{x};\omega) &= 0 \qquad\qquad \text{for } \boldsymbol{x} \in \partial\mathcal{D}. \end{aligned} \tag{1}$$

This example is common in engineering applications like heat conduction and groundwater flow. Here, the value of the diffusion coefficient and the forcing are represented by random fields, yielding a random solution and a functional to be approximated in the mean. Provided with the standard assumptions on coercivity and continuity related to the random coefficients a and f, the solution to (1) *exists and is unique. Actually, u depends continuously on the coefficients of* (1)*. A standard approach to approximate the solution to* (1) *is to use Finite Elements on Cartesian meshes. In such a setting, the vector parameter $\boldsymbol{h} = (h_1, \ldots, h_d) > 0$ contains the mesh sizes in the different canonical directions and the corresponding approximate solution is denoted by $u_h(\omega)$. Let $r : \mathcal{D} \to \mathbb{R}$ be a smooth function and let $\Psi(u) = \int_{\mathcal{D}} u(x)r(x)dx$ be a linear functional. Our goal here then is to approximate* $\mathrm{E}\left[\int_{\mathcal{D}} u(x)r(x)dx\right]$.

To particularize our set of discretizations, let us now introduce integer multi indices, $\boldsymbol{\alpha} \in \mathbb{N}^d$. Throughout this work, we use discretization vectors of the form

(2)
$$h_i = h_{i,0}\beta_i^{-\alpha_i} \text{ with given constants } h_{0,i} > 0 \text{ and } \beta_i > 1 \text{ for } i = 1, \ldots, d.$$

Correspondingly, we index our discrete approximations to S by $\boldsymbol{\alpha}$, denoting them as $\{S_{\boldsymbol{\alpha}}\}_{\boldsymbol{\alpha} \in \mathbb{N}^d}$. In addition, we make the standard assumption that $\mathrm{E}[S_{\boldsymbol{\alpha}}] \to \mathrm{E}[S]$ as $\min_{1 \le i \le d} \alpha_i \to \infty$. Finally, for later use, we define $|\boldsymbol{\alpha}| = \sum_{i=1}^d \alpha_i$.

2. Multi Index Monte Carlo

Here we introduce the MIMC discretization. To this end, we begin by defining a first-order difference operator along direction $1 \le i \le d$, denoted by Δ_i, as follows:

$$\Delta_i S_{\boldsymbol{\alpha}} = \begin{cases} S_{\boldsymbol{\alpha}} - S_{\boldsymbol{\alpha} - \boldsymbol{e}_i}, & \text{if } \alpha_i > 0, \\ S_{\boldsymbol{\alpha}} & \text{if } \alpha_i = 0, \end{cases}$$

with $\boldsymbol{e}_i$ being the canonical vectors in $\mathbb{R}^d$, i.e. $(\boldsymbol{e}_i)_j = 1$ if $j = i$ and zero otherwise. For later use, we also define recursively the first-order mixed difference operator, $\Delta = \otimes_{i=1}^d \Delta_i = \Delta_1(\otimes_{i=2}^d \Delta_i) = \Delta_d(\otimes_{i=1}^{d-1} \Delta_i)$.

Example $(d = 2)$**.** *In this case, letting $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$, we have*

$$\begin{aligned} \Delta S_{(\alpha_1,\alpha_2)} &= \Delta_2(\Delta_1 S_{(\alpha_1,\alpha_2)}) \\ &= \Delta_2 \left(S_{\alpha_1,\alpha_2} - S_{\alpha_1-1,\alpha_2}\right) \\ &= \left(S_{\alpha_1,\alpha_2} - S_{\alpha_1-1,\alpha_2}\right) - \left(S_{\alpha_1,\alpha_2-1} - S_{\alpha_1-1,\alpha_2-1}\right). \end{aligned}$$

Notice that in general, $\Delta S_{\boldsymbol{\alpha}}$ requires 2^d evaluations of S at different discretization parameters, the largest work of which corresponds precisely to the index appearing in $\Delta S_{\boldsymbol{\alpha}}$, namely $\boldsymbol{\alpha} = (\alpha_1, \alpha_2)$.

Let $\Delta\mathcal{S}_{\boldsymbol{\alpha}}$ be an *unbiased* estimator of $\Delta S_{\boldsymbol{\alpha}}$. In the trivial case, $\Delta\mathcal{S}_{\boldsymbol{\alpha}} = \Delta S_{\boldsymbol{\alpha}}$ for all $\boldsymbol{\alpha} \in \mathbb{N}^d$. However, $\Delta\mathcal{S}_{\boldsymbol{\alpha}}$ can be taken to be more complicated such that it has a smaller variance than that of $\Delta S_{\boldsymbol{\alpha}}$, for example by constructing an antithetic estimator similar to [14]. In any case, the MIMC estimator can be written as:

$$\mathcal{A} = \sum_{\boldsymbol{\alpha}\in\mathcal{I}} \frac{1}{M_{\boldsymbol{\alpha}}} \sum_{m=1}^{M_{\boldsymbol{\alpha}}} \Delta\mathcal{S}_{\boldsymbol{\alpha}}(\omega_{\boldsymbol{\alpha},m}), \tag{3}$$

where $\mathcal{I}\subset \mathbb{N}^d$ is an index set and $M_{\boldsymbol{\alpha}}$ is an integer number of samples for each $\boldsymbol{\alpha} \in \mathcal{I}$. Here, $\omega_{\boldsymbol{\alpha},m}$ are independent, identically distributed (i.i.d.) realizations of the underlying random inputs, ω. Denote $\mathrm{Var}[\Delta\mathcal{S}_{\boldsymbol{\alpha}}] = V_{\boldsymbol{\alpha}}$ and $|\mathrm{E}[\Delta\mathcal{S}_{\boldsymbol{\alpha}}]| = |\mathrm{E}[\Delta S_{\boldsymbol{\alpha}}]| = E_{\boldsymbol{\alpha}}$. Moreover, denote by $W_{\boldsymbol{\alpha}}$ the average work required to compute a realization of $\Delta\mathcal{S}_{\boldsymbol{\alpha}}$. Then, the expected value of the total work corresponding to the estimator, $\mathcal{A}$, is

$$\text{Total work} = W = \sum_{\boldsymbol{\alpha}\in\mathcal{I}} W_{\boldsymbol{\alpha}} M_{\boldsymbol{\alpha}}. \tag{4}$$

Moreover, by independence, the total variance of the estimator is

$$\mathrm{Var}[\mathcal{A}] = \sum_{\boldsymbol{\alpha}\in\mathcal{I}} V_{\boldsymbol{\alpha}} {M_{\boldsymbol{\alpha}}}^{-1}. \tag{5}$$

The objective of the MIMC estimator, $\mathcal{A}$, is to achieve a certain accuracy constraint of the form

$$P(|\mathcal{A} - \mathrm{E}[S]| \leq \mathrm{TOL}) \ \geq 1 - \epsilon \tag{6}$$

for a given accuracy TOL and a given confidence level determined by $0 < \epsilon \ll 1$. Here, we further split the accuracy budget between the bias and statistical errors, imposing the following, more restrictive, two constraints instead:

$$\text{Bias constraint:} \qquad |\mathrm{E}[\mathcal{A} - S]| \leq (1-\theta)\mathrm{TOL}, \tag{7}$$

$$\text{Statistical constraint:} \qquad P\left(|\mathcal{A} - \mathrm{E}[\mathcal{A}]| \leq \theta\mathrm{TOL}\right) \geq 1 - \epsilon. \tag{8}$$

Throughout this work, the value of the splitting parameter, $\theta \in (0,1)$, is assumed to be given and remains fixed; satisfying (7) and (8) thus implies that (6) is satisfied. We refer to [10, 17] for an analysis of the role of θ on standard MLMC simulations. Moreover, motivated by the asymptotic normality of the estimator, $\mathcal{A}$, shown in Appendix A, we replace (8) by

$$\mathrm{Var}[\mathcal{A}] \leq \left(\frac{\theta\mathrm{TOL}}{C_\epsilon}\right)^2. \tag{9}$$

Here, $0 < C_\epsilon$ is such that $\Phi(C_\epsilon) = 1 - \frac{\epsilon}{2}$, where Φ is the cumulative density function of a standard normal random variable. Using the following notation

$$\mathrm{TOL}_S = \frac{\theta\mathrm{TOL}}{C_\epsilon}, \tag{10}$$

and optimizing the total work (4) with respect to $M_{\boldsymbol{\alpha}} \in \mathbb{R}_+$ subject to the statistical constraint (9) yields

$$M_{\boldsymbol{\alpha}} = \mathrm{TOL}_S^{-2} \left(\sum_{\boldsymbol{\tau} \in \mathcal{I}} \sqrt{V_{\boldsymbol{\tau}} W_{\boldsymbol{\tau}}} \right) \sqrt{\frac{V_{\boldsymbol{\alpha}}}{W_{\boldsymbol{\alpha}}}}, \text{ for all } \boldsymbol{\alpha} \in \mathcal{I}. \tag{11}$$

Thus, with this choice of $M_{\boldsymbol{\alpha}}$, the total work becomes

$$W = \mathrm{TOL}_S^{-2} \left(\sum_{\boldsymbol{\alpha} \in \mathcal{I}} \sqrt{V_{\boldsymbol{\alpha}} W_{\boldsymbol{\alpha}}} \right)^2. \tag{12}$$

Of course, in numerical computations, we usually have to take the integer ceiling of $M_{\boldsymbol{\alpha}}$ in expression (11) or perform some kind of integer optimization to find $M_{\boldsymbol{\alpha}} \in \mathbb{N}$ for all $\boldsymbol{\alpha}$, cf. [17]. In the current work, we assume the following

- **Assumption 1**: The absolute value of the expected value of $\Delta \mathcal{S}_{\boldsymbol{\alpha}}$, denoted by $E_{\boldsymbol{\alpha}}$, satisfies

$$E_{\boldsymbol{\alpha}} = |\mathrm{E}[\Delta \mathcal{S}_{\boldsymbol{\alpha}}]| \leq Q_W \prod_{i=1}^{d} \beta_i^{-\alpha_i w_i} \tag{13}$$

  for constants Q_W and $w_i > 0$ for $i = 1 \ldots d$.
- **Assumption 2**: The variance of $\Delta \mathcal{S}_{\boldsymbol{\alpha}}$, denoted by $V_{\boldsymbol{\alpha}}$, satisfies

$$V_{\boldsymbol{\alpha}} = \mathrm{Var}[\Delta \mathcal{S}_{\boldsymbol{\alpha}}] \leq Q_S \prod_{i=1}^{d} \beta_i^{-\alpha_i s_i}, \tag{14}$$

  for constants Q_S and $0 < s_i \leq 2w_i$ for $i = 1 \ldots d$.
- **Assumption 3**: The average work required to compute a realization of $\Delta \mathcal{S}_{\boldsymbol{\alpha}}$, denoted by $W_{\boldsymbol{\alpha}}$, satisfies

$$W_{\boldsymbol{\alpha}} \leq C_{\mathrm{work}} \prod_{i=1}^{d} \beta_i^{\alpha_i \gamma_i}, \tag{15}$$

  for constants C_{work} and $\gamma_i > 0$ for $i = 1 \ldots d$.

Remark 2.1 (On Assumptions 1, 2 and 3)**.** *With sufficient coefficient regularity, Assumptions 1 and 2 hold for the random linear elliptic PDE in Example 1 when discretized by piecewise multilinear continuous finite elements. Indeed, there is extensive work on this problem based on mixed regularity analysis, by several authors who have developed combination techniques through the years. Here, we refer to the works* [29, 30, 15] *and the references therein. In Example 1, it is enough to apply such estimates point wise in* ω *and then to observe that they can be integrated in* Ω*, yielding the desired moment estimates in* (13) *and* (14)*. In Section 3.1, the numerical example has isotropic behavior over* $d = 3$ *dimensions, the work exponent appearing in Assumption 3 satisfies* $\gamma_i = \gamma \approx 1.5$*, and the error exponents are* $w_i = s_i/2 = 2$ *for* $i = 1, \ldots, 3,$ *respectively. These exponents have also been confirmed by numerical experiments cf. Figures 1, 5 and 6.*

Under **Assumptions 2-3**, we estimate the total work, W, by

$$W(\mathcal{I}) \le \mathrm{TOL}_S^{-2} Q_S C_{\mathrm{work}} \left(\sum_{\boldsymbol{\alpha}\in\mathcal{I}} \prod_{i=1}^{d} \exp\left(\frac{\alpha_i \log(\beta_i)(\gamma_i - s_i)}{2} \right) \right)^2. \tag{16}$$

We define $\boldsymbol{g} \in \mathbb{R}^d$ with entries $g_i = \frac{\log(\beta_i)(\gamma_i - s_i)}{2}$, for $i \in \{1, 2, \ldots, d\}$ and estimate

$$\frac{\mathrm{TOL}_S \sqrt{W(\mathcal{I})}}{\sqrt{Q_S C_{\mathrm{work}}}} \le \sum_{\boldsymbol{\alpha}\in\mathcal{I}} \exp\left(\boldsymbol{g}\cdot\boldsymbol{\alpha}\right) = \widetilde{W}(\mathcal{I}), \tag{17}$$

instead of estimating the total work $W(\mathcal{I})$. We also minimize $\widetilde{W}(\mathcal{I})$ instead of minimizing $W(\mathcal{I})$. One of our goals in this work is to motivate a choice for the set of multi indices, $\mathcal{I} = \mathcal{I}(\mathrm{TOL})$, to minimize $\widetilde{W}(\mathcal{I})$ (or equivalently the total work $W(\mathcal{I})$) subject to the constraint

$$\mathrm{Bias}(\mathcal{I}) = \left| \sum_{\boldsymbol{\alpha}\notin\mathcal{I}} \mathrm{E}[\Delta \mathcal{S}_{\boldsymbol{\alpha}}] \right| \le \sum_{\boldsymbol{\alpha}\notin\mathcal{I}} E_{\boldsymbol{\alpha}} \le (1-\theta)\mathrm{TOL}. \tag{18}$$

Or equivalently, due to **Assumption 1**, we aim to satisfy the following:

$$\widetilde{B}(\mathcal{I}) = \sum_{\boldsymbol{\alpha}\notin\mathcal{I}} \exp(-\overline{\boldsymbol{w}}\cdot\boldsymbol{\alpha}) \le \frac{(1-\theta)\mathrm{TOL}}{Q_W}, \tag{19}$$

where we define $\overline{\boldsymbol{w}} \in \mathbb{R}^d$ with entries $\log(\beta_i) w_i$, for $1 \le i \le d$. Moreover, we introduce the following notation

$$\mathrm{TOL}_B = \frac{(1-\theta)\mathrm{TOL}}{Q_W}. \tag{20}$$

For later use, we introduce the notation $I = \{1, 2, \ldots, d\}$ and we define the following sets of dimension indices,

$$\begin{aligned} I_1 &= \{i \in I : s_i > \gamma_i\}, \\ I_2 &= \{i \in I : s_i = \gamma_i\}, \\ I_3 &= \{i \in I : s_i < \gamma_i\}, \\ \hat{I} &= I_2 \cup I_3 = \{i \in I : s_i \le \gamma_i\} \end{aligned} \tag{21}$$

to distinguish between dimensions based on the speed of variance convergence in a dimension compared with the rate of the computational complexity in that dimension. We define $\hat{d}$ to be the size of $\hat{I}$. We also define d_i to be the size of I_i for $i = 1, 2, 3$ and thus it is clear that $d_1 + d_2 + d_3 = d$ and $\hat{d} = d_2 + d_3$.

2.1. **Full Tensor Set.** This section focuses on the special case of a full tensor set. Namely, for a given vector $\boldsymbol{L} = (L_1, L_2, \ldots, L_d)$ we consider the set $\mathcal{I}(\boldsymbol{L}) = \{\boldsymbol{\alpha} \in \mathbb{N}^d \ : \ \alpha_i \le L_i \text{ for all } i \in I\}$. Note that in this case, $\mathrm{E}[\mathcal{A}] = S_{\boldsymbol{L}}$, since the sum telescopes. Under **Assumptions 1-3**, the following theorem outlines the total work of the MIMC estimator when using a full tensor index set.

Theorem 2.1 (Full Tensor Work Complexity). *Under* ***Assumptions 1-3****, for* $\mathcal{I}(\boldsymbol{L}) = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \alpha_i \leq L_i \text{ for } i \in I\}$ *where* $L_i \in \mathbb{R}_+ \cup \{0\}$ *for all* $i \in I$*, the following choice of* $(L_i)_{i=1}^d$ *satisfies the constraint* (7)

$$L_i \geq \frac{\log(\mathrm{TOL}_B^{-1}) + \log(\mathcal{C}_\mathcal{B})}{\log(\beta_i) w_i} \quad \text{for all } i \in I. \tag{22}$$

$$\text{where} \qquad \mathcal{C}_\mathcal{B} = d \left(\prod_{j=1}^d \left(1 - \beta_j^{-w_j}\right) \right)^{-1}.$$

Moreover, taking L_i *as the lower bound of* (22)*, the optimal total work,* $W(\mathcal{I})$*, of the MIMC estimator,* $\mathcal{A}$*, subject to constraint* (9) *satisfies*

$$\limsup_{\mathrm{TOL}\downarrow 0} \frac{W(\mathcal{I})}{\mathrm{TOL}^{-2} \left(\prod_{i=1}^d \mathfrak{r}_i \right)^2} \leq \frac{C_\epsilon^2 Q_S C_{\text{work}}}{\theta^2} \prod_{i=1}^d \mathfrak{K}_i^{-2} < \infty, \tag{23}$$

$$\text{where} \qquad \mathfrak{r}_i = \begin{cases} 1 & \text{if } s_i > \gamma_i, \\ \log(\mathrm{TOL}^{-1}) & \text{if } s_i = \gamma_i, \\ \mathrm{TOL}^{\frac{-(\gamma_i - s_i)}{2w_i}} & \text{if } s_i < \gamma_i, \end{cases} \tag{24a}$$

$$\text{and} \qquad \mathfrak{K}_i = \begin{cases} 1 - \beta_i^{-\frac{s_i - \gamma_i}{2}} & \text{if } s_i > \gamma_i, \\ \log(\beta_i) w_i & \text{if } s_i = \gamma_i, \\ \left(1 - \beta_i^{-\frac{\gamma_i - s_i}{2}}\right) \left(\frac{\mathcal{C}_\mathcal{B} Q_W}{(1-\theta)}\right)^{\frac{-(\gamma_i - s_i)}{2w_i}} & \text{if } s_i < \gamma_i. \end{cases} \tag{24b}$$

Proof. First, for convenience, we introduce the following notation:

$$\overline{s}_i = \log(\beta_i) s_i, \quad \overline{w}_i = \log(\beta_i) w_i, \quad \overline{\gamma}_i = \log(\beta_i) \gamma_i. \tag{25}$$

Then, by **Assumption 1**, starting from (19), we have

$$\begin{aligned}
\widetilde{B}(\mathcal{I}(\boldsymbol{L})) &= \sum_{\boldsymbol{\alpha} \notin \mathcal{I}(\boldsymbol{L})} \prod_{i=1}^d \exp(-\overline{w}_i \alpha_i) \\
&\leq \sum_{i=1}^d \left(\prod_{j \neq i} \frac{\exp(\overline{w}_j)}{\exp(\overline{w}_j) - 1} \right) \sum_{\alpha_i > L_i} \exp(-\overline{w}_i \alpha_i) \\
&\leq \left(\prod_{j=1}^d \frac{\exp(\overline{w}_j)}{\exp(\overline{w}_j) - 1} \right) \sum_{i=1}^d \exp(-\overline{w}_i L_i).
\end{aligned}$$

Recall (20). Then making each of the terms in the previous sum less than TOL_B/d to satisfy (19) yields (22). On the other hand, using definition

(17), we have

$$
\begin{aligned}
\widetilde{W}(\mathcal{I}(\boldsymbol{L})) &= \sum_{\boldsymbol{\alpha}\in\mathcal{I}} \prod_{i=1}^{d} \exp(g_i\alpha_i) \le \prod_{i=1}^{d} \sum_{\alpha_i=0}^{\lfloor L_i \rfloor} \exp\left(g_i\alpha_i\right) \\
&\le \prod_{i\in I_1} \frac{1}{1-\exp(g_i)} \prod_{i\in I_2} \left(L_i+1\right) \prod_{i\in I_3} \frac{\exp(g_iL_i)-\exp(-g_i)}{1-\exp(-g_i)}.
\end{aligned} \tag{26}
$$

The proof finishes by combining (22) with (26) and (17) and taking the limit of the resulting expression as $\mathrm{TOL} \downarrow 0$. □

Remark 2.2 (Isotropic Full Tensor)**.** *Of particular interest is the case* $\gamma_i = \gamma$, $s_i = s$, $w_i = w$ *and* $\beta_i = \beta$ *for all* $i \in I$ *and for positive constants* γ, s, w *and* β*. In this case, we have*

$$
\textit{Work of MIMC} = \begin{cases} \mathcal{O}\left(\mathrm{TOL}^{-2}\right), & s > \gamma, \\ \mathcal{O}\left(\mathrm{TOL}^{-2}\left(\log(\mathrm{TOL}^{-1})\right)^{2d}\right), & s = \gamma, \\ \mathcal{O}\left(\mathrm{TOL}^{-\left(2+\frac{d(\gamma-s)}{w}\right)}\right), & s < \gamma, \end{cases} \tag{27}
$$

asymptotically as $\mathrm{TOL} \to 0$*. When comparing* (27) *to the asymptotic work of MLMC* [8]*, we have*

$$
\textit{Work of MLMC} = \begin{cases} \mathcal{O}\left(\mathrm{TOL}^{-2}\right), & s > d\gamma, \\ \mathcal{O}\left(\mathrm{TOL}^{-2}\left(\log(\mathrm{TOL}^{-1})\right)^{2}\right), & s = d\gamma, \\ \mathcal{O}\left(\mathrm{TOL}^{-\left(2+\frac{(d\gamma-s)}{w}\right)}\right), & s < d\gamma. \end{cases} \tag{28}
$$

We notice that the condition in (27) *for the optimal convergence rate* $\mathcal{O}\left(\mathrm{TOL}^{-2}\right)$ *does not depend on the dimensionality of the underlying problem. Moreover, for the case where the variance convergence is slower than the work increase rate, the work complexity of the MIMC estimator is better than that of MLMC whenever we work with multidimensional problems, i.e.,* $d > 1$*.*

It should be noted, however, that the MIMC results require mixed *regularity (in the sense of* ***Assumptions 1,2****) of certain order. On the other hand, the MLMC results require only* ordinary *regularity of the same order.*

Remark 2.3 (Lower mixed regularity)**.** *In some cases, we might have enough mixed regularity in the sense of* ***Assumptions 1-2*** *along some directions but not along others. For example, assume that, out of d directions, the first* $\tilde{d}$ *directions do not have mixed regularity among each other. Our MIMC estimator can still be applied by considering all first* $\tilde{d}$ *directions as a single direction. This is done by using the same discretization parameter,* $\tilde{\alpha}$*, for all* $\tilde{d}$ *directions, then finding the new rates,* $\tilde{\gamma}$*,* $\tilde{s}$ *and* $\tilde{w}$*, of the resulting direction. This can be thought of as combining MLMC in the first* $\tilde{d}$ *directions with MIMC in the rest of the directions and in the case* $d = \tilde{d}$*, i.e., the problem has no mixed regularity, MIMC reduces to standard MLMC. All* *results derived in the current work can still be applied to this new setting, which conceptually corresponds to* $d - \tilde{d} + 1$ *directions in the MIMC results presented here. In particular, if we assume that the first* $\tilde{d}$ *directions are isotropic with the same variance convergence rate,* s*, and work rate,* γ*, then the results in Theorem 2.1 deteriorate in the sense that for the grouped direction, the conditions relating* s *and* γ *in* (24) *are replaced by the more stringent conditions relating* s *and* $\tilde{d}\gamma$*.*

2.2. **Optimal Sets.** We discuss in this section how to find optimal index sets, $\mathcal{I}$. The objective is to solve an optimization problem of the form

$$\min_{\mathcal{I} \subset \mathbb{N}^d} \widetilde{W}(\mathcal{I}) \quad \text{such that} \quad \widetilde{B}(\mathcal{I}) \leq \mathrm{TOL}_B,$$

where $\widetilde{W}$ and $\widetilde{B}$ were defined in (17) and (19) in terms of $\mathcal{I}$, respectively.

Similar to [28], the problem of constructing an optimal index set, $\mathcal{I}$, can be recast into a knapsack problem where a "profit" indicator is assigned to each index and only the most profitable indices are added to $\mathcal{I}$. Let us define the profit, $\mathcal{P}_{\boldsymbol{\alpha}} = \frac{\varepsilon_{\boldsymbol{\alpha}}}{\varpi_{\boldsymbol{\alpha}}}$, of a multi index, $\boldsymbol{\alpha}$, in terms of its error contribution, denoted here by $\varepsilon_{\boldsymbol{\alpha}}$, and its the work contribution, denoted here by $\varpi_{\boldsymbol{\alpha}}$. Moreover, define the total error associated with an index set $\mathcal{I}$ as

$$\mathfrak{E}(\mathcal{I}) = \sum_{\boldsymbol{\alpha} \notin \mathcal{I}} \varepsilon_{\boldsymbol{\alpha}}$$

and the corresponding total work as

$$\mathfrak{W}(\mathcal{I}) = \sum_{\boldsymbol{\alpha} \in \mathcal{I}} \varpi_{\boldsymbol{\alpha}}.$$

Intuitively, we may think of $\mathfrak{E}(\mathcal{I})$ as a sharp upper bound for $\widetilde{B}(\mathcal{I})$, and think of $\mathfrak{W}(\mathcal{I})$ as a correspondingly sharp lower bound for $\widetilde{W}(\mathcal{I})$. Then we can show the following optimality result with respect to $\mathfrak{E}(\mathcal{I})$ and $\mathfrak{W}(\mathcal{I})$, namely:

Lemma 2.1 (Optimal profit sets)**.** *The set* $\mathcal{I}(\nu) = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \mathcal{P}_{\boldsymbol{\alpha}} \geq \nu\}$ *is optimal in the sense that any other set,* $\tilde{\mathcal{I}}$*, with smaller work,* $\mathfrak{W}(\tilde{\mathcal{I}}) < \mathfrak{W}(\mathcal{I}(\nu))$*, leads to a larger error,* $\mathfrak{E}(\tilde{\mathcal{I}}) > \mathfrak{E}(\mathcal{I}(\nu))$*.*

Proof. We have that for any $\boldsymbol{\alpha} \in \mathcal{I}(\nu)$ and $\hat{\boldsymbol{\alpha}} \notin \mathcal{I}(\nu)$

$$\mathcal{P}_{\boldsymbol{\alpha}} \geq \nu \qquad \text{and} \qquad \mathcal{P}_{\hat{\boldsymbol{\alpha}}} < \nu.$$

Now, take an arbitrary index set, $\tilde{\mathcal{I}}$, such that $\mathfrak{W}(\tilde{\mathcal{I}}) < \mathfrak{W}(\mathcal{I}(\nu))$ and set

$$\mathcal{J}_1 = \mathcal{I}(\nu) \cap \tilde{\mathcal{I}}^c, \qquad \mathcal{J}_2 = \mathcal{I}(\nu) \cap \tilde{\mathcal{I}},$$
$$\mathcal{J}_3 = \mathcal{I}(\nu)^c \cap \tilde{\mathcal{I}}, \qquad \mathcal{J}_4 = \mathcal{I}(\nu)^c \cup \tilde{\mathcal{I}}^c.$$

where $\mathcal{I}(\nu)^c$ is the complement of the set $\mathcal{I}(\nu)$. Then,

$$\mathfrak{W}(\mathcal{I}(\nu)) - \mathfrak{W}(\tilde{\mathcal{I}}) = \sum_{\boldsymbol{\alpha} \in \mathcal{J}_1 \cup \mathcal{J}_2} \varpi_{\boldsymbol{\alpha}} - \sum_{\boldsymbol{\alpha} \in J_2 \cup J_3} \varpi_{\boldsymbol{\alpha}} = \sum_{\boldsymbol{\alpha} \in \mathcal{J}_1} \varpi_{\boldsymbol{\alpha}} - \sum_{\boldsymbol{\alpha} \in \mathcal{J}_3} \varpi_{\boldsymbol{\alpha}} > 0,$$

and

$$\mathfrak{E}(\mathcal{I}(\nu)) - \mathfrak{E}(\tilde{\mathcal{I}}) = \sum_{\boldsymbol{\alpha} \in \mathcal{J}_3 \cup \mathcal{J}_4} \varepsilon_{\boldsymbol{\alpha}} - \sum_{\boldsymbol{\alpha} \in \mathcal{J}_1 \cup \mathcal{J}_4} \varepsilon_{\boldsymbol{\alpha}} = \sum_{\boldsymbol{\alpha} \in \mathcal{J}_3} \mathcal{P}_{\boldsymbol{\alpha}} \varpi_{\boldsymbol{\alpha}} - \sum_{\boldsymbol{\alpha} \in \mathcal{J}_1} \mathcal{P}_{\boldsymbol{\alpha}} \varpi_{\boldsymbol{\alpha}}.$$

Then,

$$\mathfrak{E}(\mathcal{I}(\nu)) - \mathfrak{E}(\tilde{\mathcal{I}}) \leq \nu \left(\sum_{\boldsymbol{\alpha} \in \mathcal{J}_3} \varpi_{\boldsymbol{\alpha}} - \sum_{\boldsymbol{\alpha} \in \mathcal{J}_1} \varpi_{\boldsymbol{\alpha}} \right) < 0$$

□

For MIMC, under **Assumptions 1-3**, $\varepsilon_{\boldsymbol{\alpha}}$ can be taken to be the bias contribution of the term $\Delta \mathcal{S}_{\boldsymbol{\alpha}}$, i.e., $\varepsilon_{\boldsymbol{\alpha}} = E_{\boldsymbol{\alpha}}$. Additionally, the work contribution can also be taken as $\varpi_{\boldsymbol{\alpha}} = \sqrt{V_{\boldsymbol{\alpha}} W_{\boldsymbol{\alpha}}}$. Using the estimates in **Assumptions 1-3** as sharp approximations to their counterparts, the profits in our problem are approximated correspondingly by

$$\mathcal{P}_{\boldsymbol{\alpha}} \approx C_P \prod_{i=1}^{d} e^{-\alpha_i \log(\beta_i)(w_i + \frac{\gamma_i - s_i}{2})},$$

for some constant C_P. Therefore, ordering the profits according to level sets as in Lemma 2.1, yields optimal sets of multi indices that are of anisotropic Total Degree (TD) type. Let us introduce strictly positive normalized weights defined by

$$\delta_i = \frac{\log(\beta_i)(w_i + \frac{\gamma_i - s_i}{2})}{C_{\boldsymbol{\delta}}}, \quad \text{for all } i \in I, \tag{29}$$
$$\text{where} \qquad C_{\boldsymbol{\delta}} = \sum_{j=1}^{d} \log(\beta_j)(w_j + \frac{\gamma_j - s_j}{2}).$$

Observe that $0 < \delta_i \leq 1$, since $s_i \leq 2w_i$ and $\gamma_i > 0$. Then, for $L = 0, 1, \ldots,$ introduce a family of TD index sets:

$$\mathcal{I}_{\boldsymbol{\delta}}(L) = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \boldsymbol{\alpha} \cdot \boldsymbol{\delta} = \sum_{i=1}^{d} \delta_i \alpha_i \leq L\}. \tag{30}$$

In our numerical example, presented in Section 3, Figure 2 suggests that the TD set is indeed the optimal index set in this case.

The current section continues by first considering a general vector of weights, $\boldsymbol{\delta}$, and finding a value of L that satisfies the bias constraint in Lemma 2.2, then deriving the resulting computational complexity in Lemma 2.3. Next, we present our main result in Theorem 2.2 when using the optimal weights of (29). Finally, we conclude this section with a few remarks about special cases.

Lemma 2.2 (L of MIMC with general $\boldsymbol{\delta}$)**.** *Consider the multi-index sets* $\mathcal{I}_{\boldsymbol{\delta}}(L) = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \boldsymbol{\delta} \cdot \boldsymbol{\alpha} \leq L\}$ *with given weights* $\boldsymbol{\delta} \in \mathbb{R}_+^d$ *such that* $|\boldsymbol{\delta}| = 1$

and $L \in \mathbb{R}_+ \cup \{0\}$*. Let*

$$\eta = \min_{i \in I} \delta_i^{-1} \overline{w}_i, \text{ and } \qquad \underline{\eta} = \min_{\substack{i \in I \\ \delta_i^{-1}\overline{w}_i > \eta}} \delta_i^{-1} \overline{w}_i.$$

Moreover, let $l_1 = \#\{i \in I : \delta_i^{-1}\overline{w}_i = \eta\}$ *and* $l_2 = d - l_1$*. If* ***Assumption 1*** *holds, then, to satisfy the following bias inequality,*

$$\lim_{\mathrm{TOL}\downarrow 0} \frac{\widetilde{B}(\mathcal{I}_{\boldsymbol{\delta}}(L))}{\mathrm{TOL}_B} \le 1, \tag{31}$$

it is enough to take L *as follows:*

$$L \ge \frac{1}{\eta}\left(\log(\mathrm{TOL}_B^{-1}) + (l_1 - 1)\log\left(\frac{1}{\eta}\log(\mathrm{TOL}_B^{-1})\right) + \log(\mathfrak{C}_{\mathfrak{B}})\right) \tag{32}$$

where

$$\mathfrak{C}_{\mathfrak{B}} = \exp(|\overline{\boldsymbol{w}}|)\left(\prod_{i=1}^{d} \delta_i^{-1}\right)\left[\eta^{-l_1}\underline{\eta}^{-l_2}\sum_{j=0}^{l_1-1}\frac{\eta^j}{j!} + \frac{\underline{\eta}^{-l_2}}{(l_1-1)!}\left(\frac{2}{\underline{\eta}-\eta}\right)\left(\sum_{j=0}^{l_2-1}\exp(-j)\left(\frac{2j}{\underline{\eta}-\eta}\right)^j\frac{\underline{\eta}^j}{j!}\right)\right]$$

Proof. In this proof, we use the identity of Lemma B.1 and the following bound that holds for any $x \in \mathbb{R}_+, b > 0$ and $j \in \mathbb{N}$:

$$x^j \le \left(\frac{j}{b}\right)^j \exp(-j)\exp(bx). \tag{33}$$

For convenience, we reorder the indices so that

$$\begin{aligned} \frac{\overline{w}_i}{\delta_i} &= \eta \qquad \text{for } i = 1, \ldots, l_1, \\ \frac{\overline{w}_i}{\delta_i} &\ge \eta \qquad \text{for } i = l_1 + 1, \ldots, d. \end{aligned}$$

We have

$$
\begin{aligned}
\widetilde{B}(\mathcal{I}_{\boldsymbol{\delta}}(L)) &= \sum_{\{\boldsymbol{\alpha}\in\mathbb{N}^d\,:\,\boldsymbol{\alpha}\cdot\boldsymbol{\delta}>L\}} \exp(-\overline{\boldsymbol{w}}\cdot\boldsymbol{\alpha}) \\
&\leq \int_{\{\boldsymbol{x}\in\mathbb{R}^d_+\,:\,\boldsymbol{x}\cdot\boldsymbol{\delta}\geq L\}} \exp(-\overline{\boldsymbol{w}}\cdot(\boldsymbol{x}-\mathbf{1}))\,\mathrm{d}\boldsymbol{x} \\
&= \exp(|\overline{\boldsymbol{w}}|)\left(\prod_{i=1}^d \delta_i^{-1}\right)\int_{\{\boldsymbol{x}\in\mathbb{R}^d_+\,:\,|\boldsymbol{x}|\geq L\}} \exp\left(-\sum_{i=1}^d \delta_i^{-1}x_i\overline{w}_i\right)\,\mathrm{d}\boldsymbol{x} \\
&\leq \exp(|\overline{\boldsymbol{w}}|)\left(\prod_{i=1}^d \delta_i^{-1}\right)\int_{\{\boldsymbol{x}\in\mathbb{R}^d_+\,:\,|\boldsymbol{x}|\geq L\}} \exp\left(-\eta\sum_{i=1}^{l_1} x_i - \underline{\eta}\sum_{i=l_1+1}^d x_i\right)\,\mathrm{d}\boldsymbol{x} \\
&= \exp(|\overline{\boldsymbol{w}}|)\left(\prod_{i=1}^d \delta_i^{-1}\right)\Bigg[\int_{\boldsymbol{x}\in\mathbb{R}^d_+} \exp\left(-\eta\sum_{i=1}^{l_1} x_i - \underline{\eta}\sum_{i=l_1+1}^d x_i\right) - \\
&\qquad \int_{\{\boldsymbol{x}\in\mathbb{R}^d_+\,:\,|\boldsymbol{x}|\leq L\}} \exp\left(-\eta\sum_{i=1}^{l_1} x_i - \underline{\eta}\sum_{i=l_1+1}^d x_i\right)\,\mathrm{d}\boldsymbol{x}\Bigg],
\end{aligned}
$$

where

$$
\int_{\boldsymbol{x}\in\mathbb{R}^d_+} \exp\left(-\eta\sum_{i=1}^{l_1} x_i - \underline{\eta}\sum_{i=l_1+1}^d x_i\right) = \eta^{-l_1}\underline{\eta}^{-l_2}.
$$

Now consider

$$
\begin{aligned}
&\int_{\{\boldsymbol{x}\in\mathbb{R}^d_+\,:\,|\boldsymbol{x}|\leq L\}} \exp\left(-\eta\sum_{i=1}^{l_1} x_i - \underline{\eta}\sum_{i=l_1+1}^d x_i\right)\,\mathrm{d}\boldsymbol{x} \\
&= \int_{\{\boldsymbol{x}_2\in\mathbb{R}^{l_2}_+\,:\,|\boldsymbol{x}_2|\leq L\}} \exp\left(-\underline{\eta}|\boldsymbol{x}_2|\right) \\
&\qquad\qquad \left(\int_{\{\boldsymbol{x}_1\in\mathbb{R}^{l_1}_+\,:\,|\boldsymbol{x}_1|\leq L-|\boldsymbol{x}_2|\}} \exp\left(-\eta|\boldsymbol{x}_1|\right)\,\mathrm{d}\boldsymbol{x}_1\right)\,\mathrm{d}\boldsymbol{x}_2 \\
&= \frac{1}{(l_1-1)!}\int_{\{\boldsymbol{x}_2\in\mathbb{R}^{l_2}_+\,:\,|\boldsymbol{x}_2|\leq L\}} \exp\left(-\underline{\eta}|\boldsymbol{x}_2|\right)\left(\int_0^{L-|\boldsymbol{x}_2|} \exp(-\eta t)t^{l_1-1}\mathrm{d}t\right)\mathrm{d}\boldsymbol{x}_2 \\
&= \frac{1}{(l_1-1)!}\int_0^L \exp(-\eta t)t^{l_1-1}\left(\int_{\{\boldsymbol{x}_2\in\mathbb{R}^{l_2}_+\,:\,|\boldsymbol{x}_2|\leq L-t\}} \exp\left(-\underline{\eta}|\boldsymbol{x}_2|\right)\mathrm{d}\boldsymbol{x}_2\right)\mathrm{d}t \\
&= \frac{1}{(l_1-1)!(l_2-1)!}\int_0^L \exp(-\eta t)t^{l_1-1}\left(\int_0^{L-t} \exp(-\underline{\eta}z)z^{l_2-1}\,\mathrm{d}z\right)\mathrm{d}t \\
&= \frac{\underline{\eta}^{-l_2}}{(l_1-1)!}\int_0^L \exp(-\eta t)t^{l_1-1}\left(1-\exp(-\underline{\eta}(L-t))\sum_{j=0}^{l_2-1}\frac{(\underline{\eta}(L-t))^j}{j!}\right)\mathrm{d}t
\end{aligned}
$$

$$= \eta^{-l_1}\underline{\eta}^{-l_2} - \eta^{-l_1}\underline{\eta}^{-l_2}\left(\exp(-\eta L)\sum_{j=0}^{l_1-1}\frac{(\eta L)^j}{j!}\right)$$
$$- \frac{\underline{\eta}^{-l_2}}{(l_1-1)!}\int_0^L \exp(-\eta t)t^{l_1-1}\left(\exp(-\underline{\eta}(L-t))\sum_{j=0}^{l_2-1}\frac{(\underline{\eta}(L-t))^j}{j!}\right).\mathrm{d}t$$

Here, we can bound

$$\eta^{-l_1}\underline{\eta}^{-l_2}\left(\exp(-\eta L)\sum_{j=0}^{l_1-1}\frac{(\eta L)^j}{j!}\right) \le \eta^{-l_1}\underline{\eta}^{-l_2}\exp(-\eta L)L^{l_1-1}\sum_{j=0}^{l_1-1}\frac{\eta^j}{j!}.$$

Recall that $\underline{\eta} > \eta$ and bound, using (33) for $(L-t)^j$ with $b = \frac{\underline{\eta}-\eta}{2}$,

$$\frac{\underline{\eta}^{-l_2}}{(l_1-1)!}\int_0^L \exp(-\eta t)t^{l_1-1}\left(\exp(-\underline{\eta}(L-t))\sum_{j=0}^{l_2-1}\frac{(\underline{\eta}(L-t))^j}{j!}\right)\mathrm{d}t$$
$$\le \frac{\underline{\eta}^{-l_2}}{(l_1-1)!}\left(\sum_{j=0}^{l_2-1}\exp(-j)\left(\frac{2j}{\underline{\eta}-\eta}\right)^j\frac{\underline{\eta}^j}{j!}\right)$$
$$\exp\left(-L\left(\frac{\underline{\eta}+\eta}{2}\right)\right)\int_0^L \exp\left(t\frac{\underline{\eta}-\eta}{2}\right)t^{l_1-1}\mathrm{d}t$$
$$\le \frac{\underline{\eta}^{-l_2}}{(l_1-1)!}\left(\frac{2}{\underline{\eta}-\eta}\right)\left(\sum_{j=0}^{l_2-1}\exp(-j)\left(\frac{2j}{\underline{\eta}-\eta}\right)^j\frac{\underline{\eta}^j}{j!}\right)\exp\left(-\eta L\right)L^{l_1-1}.$$

Substituting everything back, we can bound the bias as follows

$$\widetilde{B}(\mathcal{I}_{\boldsymbol{\delta}}(L)) \le \mathfrak{C}_{\mathfrak{B}}\exp\left(-\eta L\right)L^{l_1-1}.$$

Choosing L as in (32) yields

$$\lim_{\mathrm{TOL}\downarrow 0}\frac{\widetilde{B}(\mathcal{I}_{\boldsymbol{\delta}})}{\mathrm{TOL}_B} \le 1 + \lim_{\mathrm{TOL}\downarrow 0}\left(\frac{(l_1-1)\log\left(\frac{1}{\eta}\log(\mathrm{TOL}_B^{-1})\right)+\log(\mathfrak{C}_{\mathfrak{B}})}{\log\left(\mathrm{TOL}_B^{-1}\right)}\right)^{l_1-1} = 1,$$

which finishes the proof. □

Lemma 2.3 (Work estimate of MIMC with general $\boldsymbol{\delta}$)**.** *Let the approximation set be* $\mathcal{I}_{\boldsymbol{\delta}}(L) = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \boldsymbol{\delta}\cdot\boldsymbol{\alpha} \le L\}$ *for a given* $\boldsymbol{\delta} \in \mathbb{R}_+^d$ *with* $|\boldsymbol{\delta}| = 1$ *and take* L *as the lower bound in* (32)*. Under* ***Assumptions 2-3****, denoting*

$$\chi = \max_{i\in I}\frac{\log(\beta_i)(\gamma_i - s_i)}{2\delta_i} = \max_{i\in I}\frac{g_i}{\delta_i}, \quad (34)$$

the total work, $W(\mathcal{I}_{\boldsymbol{\delta}})$*, of the MIMC estimator,* $\mathcal{A}$*, subject to constraint* (9) *satisfies the following cases:*

Case A) If $\chi \leq 0$, then

$$\limsup_{\mathrm{TOL}\downarrow 0} \frac{W(\mathcal{I}_{\boldsymbol{\delta}})}{\mathrm{TOL}^{-2}\left(\log\left(\mathrm{TOL}^{-1}\right)\right)^{2d_2}} \leq \frac{C_\epsilon^2 Q_S C_{\mathrm{work}}}{\theta^2 {\mathfrak{C}_1}^2 {\mathfrak{C}_2}^2} < \infty, \tag{35}$$

$$\begin{aligned} &\textit{where} \qquad \mathfrak{C}_1 = \prod_{i\in I_1}\left(1-\beta_i^{-\frac{s_i-\gamma_i}{2}}\right) \\ &\textit{and} \qquad \mathfrak{C}_2 = \eta^{d_2} d_2! \left(\prod_{j\in I_2}\delta_j\right). \end{aligned} \tag{36}$$

Case B) If $\chi > 0$, let

$$\underline{\chi} = \max_{\substack{i\in\hat{I} \\ 0\leq \frac{\log(\beta_i)(\gamma_i-s_i)}{2\delta_i}<\chi}} \frac{\log(\beta_i)(\gamma_i-s_i)}{2\delta_i}.$$

Moreover, denote $n_1 = \#\{i\in I : \delta_i^{-1}g_i = \chi\}$, $n_2 = d_2+d_3-n_1$, and $\mathfrak{j} = \frac{2(n_1-1)\chi+2(l_1-1)\eta}{\eta}$. Then, we have

$$\limsup_{\mathrm{TOL}\downarrow 0} \frac{W(\mathcal{I}_{\boldsymbol{\delta}})}{\mathrm{TOL}^{-2-2\frac{\chi}{\eta}}\left(\log\left(\mathrm{TOL}^{-1}\right)\right)^{\mathfrak{j}}} \leq \frac{C_\epsilon^2 Q_S C_{\mathrm{work}} {\mathfrak{C}_3}^2}{\eta^{\mathfrak{j}} {\mathfrak{C}_1}^2 \theta^2}\left(\frac{\mathfrak{C}_{\mathfrak{B}} Q_W}{1-\theta}\right)^{2\frac{\chi}{\eta}} < \infty, \tag{37}$$

where

$$\mathfrak{C}_3 = \frac{\prod_{i\in\hat{I}}\delta_i^{-1}}{(n_1-1)!(n_2-1)!}\exp(1-n_2)\left(\frac{2(n_2-1)}{\chi-\underline{\chi}}\right)^{n_2-1}\frac{4\exp(\chi)}{\chi^2-\underline{\chi}^2}. \tag{38}$$

Proof. Define $\tilde{\boldsymbol{\delta}}_1 = (\delta_i)_{i\in I_1}$ and $\tilde{\boldsymbol{g}}_1 = (g_i)_{i\in I_1}$ to be the entries of $\boldsymbol{\delta}$ and $\boldsymbol{g}$ corresponding to I_1, respectively. Similarly define $\hat{\boldsymbol{\delta}}$ and $\hat{\boldsymbol{g}}$ to be the entries of $\boldsymbol{\delta}$ and $\boldsymbol{g}$ corresponding to $\hat{I}$, respectively. Then, starting from (17), we have

$$\begin{aligned} \widetilde{W}(\mathcal{I}_{\boldsymbol{\delta}}(L)) &= \sum_{\boldsymbol{\alpha}\in\mathcal{I}_{\boldsymbol{\delta}}}\exp(\boldsymbol{g}\cdot\boldsymbol{\alpha}) \\ &\leq \underbrace{\left(\sum_{\boldsymbol{\alpha}\in\mathbb{N}^{d_1},\boldsymbol{\alpha}\cdot\tilde{\boldsymbol{\delta}}_1\leq L}\exp(\tilde{\boldsymbol{g}}_1\cdot\boldsymbol{\alpha})\right)}_{:=P_1}\underbrace{\left(\sum_{\boldsymbol{\alpha}\in\mathbb{N}^{\hat{d}},\boldsymbol{\alpha}\cdot\hat{\boldsymbol{\delta}}\leq L}\exp(\hat{\boldsymbol{g}}\cdot\boldsymbol{\alpha})\right)}_{:=\hat{P}}. \end{aligned} \tag{39}$$

Now, for the term P_1, since $g_j < 0$, $\forall j\in I_1$, we have

$$P_1 \leq \frac{1}{\prod_{j\in I_1}(1-e^{g_j})}. \tag{40}$$

For the term $\hat{P}$, we distinguish between two cases:

Case A) If $\chi \leq 0$, then $\max_i g_i \leq 0$ and $I_3 = \emptyset$ and $\hat{I} = I_2$. Then, since $g_j = 0$ for all $j \in I_2$, we have

$$
\begin{aligned}
\hat{P} &= \sum_{\{\boldsymbol{\alpha} \in \mathbb{N}^{d_2} \,:\, \tilde{\boldsymbol{\delta}}_2 \cdot \boldsymbol{\alpha} \leq L\}} 1 \\
&\leq \int_{\{\boldsymbol{x} \in \mathbb{R}_+^{d_2} \,:\, \boldsymbol{x} \cdot \tilde{\boldsymbol{\delta}}_2 \leq L + |\tilde{\boldsymbol{\delta}}_2|\}} 1 \,\mathrm{d}\boldsymbol{x} \\
&\leq \frac{1}{\prod_{j \in I_2} \delta_j} \int_{\{\boldsymbol{y} \in \mathbb{R}_+^{d} \,:\, |\boldsymbol{y}| \leq L + |\tilde{\boldsymbol{\delta}}_2|\}} 1 \,\mathrm{d}\boldsymbol{y} \\
&= \frac{1}{\prod_{j \in I_2} \delta_j} \frac{(L + |\tilde{\boldsymbol{\delta}}_2|)^{d_2}}{d_2!}.
\end{aligned}
$$

The proof finishes for this case by combining the previous inequality with (39), (40), (17) and (32) and taking the limit of the resulting expression as $\mathrm{TOL} \downarrow 0$.

Case B) If $\chi > 0$, then using the identity of Lemma B.1 and the bound (33), we have

$$
\begin{aligned}
\hat{P} &\leq \int_{\{\boldsymbol{x} \in \mathbb{R}_+^{\hat{d}} \,:\, \boldsymbol{x} \cdot \hat{\boldsymbol{\delta}} \leq L + |\hat{\boldsymbol{\delta}}|\}} \exp(\hat{\boldsymbol{g}} \cdot \boldsymbol{x}) \mathrm{d}\boldsymbol{x} \\
&\leq \left(\prod_{i \in \hat{I}} \delta_i^{-1} \right) \int_{\{\boldsymbol{x}_2 \in \mathbb{R}_+^{n_2} \,:\, |\boldsymbol{x}_2| \leq L + |\hat{\boldsymbol{\delta}}|\}} \exp(\underline{\chi} |\boldsymbol{x}_2|) \\
&\qquad \left(\int_{\{\boldsymbol{x}_1 \in \mathbb{R}_+^{n_1} \,:\, |\boldsymbol{x}_1| \leq L + |\hat{\boldsymbol{\delta}}| - |\boldsymbol{x}_2|\}} \exp(\chi |\boldsymbol{x}_1|) \mathrm{d}\boldsymbol{x}_1 \right) \mathrm{d}\boldsymbol{x}_2 \\
&= \frac{\prod_{i \in \hat{I}} \delta_i^{-1}}{(n_1 - 1)!} \int_{\{\boldsymbol{x}_2 \in \mathbb{R}_+^{n_2} \,:\, |\boldsymbol{x}_2| \leq L + |\hat{\boldsymbol{\delta}}|\}} \exp(\underline{\chi} |\boldsymbol{x}_2|) \\
&\qquad \left(\int_0^{L + |\hat{\boldsymbol{\delta}}| - |\boldsymbol{x}_2|} \exp(\chi t) t^{n_1 - 1} \mathrm{d}t \right) \mathrm{d}\boldsymbol{x}_2 \\
&= \frac{\prod_{i \in \hat{I}} \delta_i^{-1}}{(n_1 - 1)!} \int_0^{L + |\hat{\boldsymbol{\delta}}|} \exp(\chi t) t^{n_1 - 1} \\
&\qquad \left(\int_{\{\boldsymbol{x}_2 \in \mathbb{R}_+^{n_2} \,:\, |\boldsymbol{x}_2| \leq L + |\hat{\boldsymbol{\delta}}| - t\}} \exp(\underline{\chi} |\boldsymbol{x}_2|) \mathrm{d}\boldsymbol{x}_2 \right) \mathrm{d}t \\
&= \frac{\prod_{i \in \hat{I}} \delta_i^{-1}}{(n_1 - 1)!(n_2 - 1)!} \int_0^{L + |\hat{\boldsymbol{\delta}}|} \exp(\chi t) t^{n_1 - 1} \left(\int_0^{L + |\hat{\boldsymbol{\delta}}| - t} \exp(\underline{\chi} z) z^{n_2 - 1} \mathrm{d}z \right) \mathrm{d}t \\
&\leq \mathfrak{C} \int_0^{L + |\hat{\boldsymbol{\delta}}|} \exp(\chi t) t^{n_1 - 1} \left(\int_0^{L + |\hat{\boldsymbol{\delta}}| - t} \exp\left(z \frac{\underline{\chi} + \chi}{2} \right) \mathrm{d}z \right) \mathrm{d}t,
\end{aligned}
$$

$$\text{where} \qquad \mathfrak{C} = \frac{\prod_{i \in \hat{I}} \delta_i^{-1}}{(n_1-1)!(n_2-1)!} \exp(1-n_2) \left(\frac{2(n_2-1)}{\chi - \underline{\chi}}\right)^{n_2-1},$$

continuing

$$\begin{aligned}
\hat{P} &\leq \mathfrak{C} \exp\left(\frac{\underline{\chi}+\chi}{2}\left(L+|\hat{\boldsymbol{\delta}}|\right)\right) \frac{2}{\underline{\chi}+\chi} \int_0^{L+|\hat{\boldsymbol{\delta}}|} t^{n_1-1} \exp\left(t \frac{\chi-\underline{\chi}}{2}\right) \mathrm{d}t \\
&\leq \mathfrak{C} \exp\left(\frac{\underline{\chi}+\chi}{2}\left(L+|\hat{\boldsymbol{\delta}}|\right)\right) \frac{2\left(L+|\hat{\boldsymbol{\delta}}|\right)^{n_1-1}}{\underline{\chi}+\chi} \int_0^{L+|\hat{\boldsymbol{\delta}}|} \exp\left(t \frac{\chi-\underline{\chi}}{2}\right) \mathrm{d}t \\
&\leq \frac{2\mathfrak{C} \exp\left(\chi|\hat{\boldsymbol{\delta}}|\right)}{\chi - \underline{\chi}} \exp\left(\chi L\right) \frac{2\left(L+|\hat{\boldsymbol{\delta}}|\right)^{n_1-1}}{\underline{\chi}+\chi} \\
&\leq \frac{4\mathfrak{C}\exp\left(\chi\right)}{\chi^2 - \underline{\chi}^2} \exp\left(\chi L\right) \left(L+1\right)^{n_1-1}.
\end{aligned}$$

The proof finishes for this case by combining the previous inequality with (39), (40), (17) and (32) and taking the limit of the resulting expression as $\mathrm{TOL} \downarrow 0$.

□

Theorem 2.2 (Work estimate with optimal weights)**.** *Let the approximation set be* $\mathcal{I}_{\boldsymbol{\delta}}(L) = \{\boldsymbol{\alpha} \in \mathbb{N}^d : \boldsymbol{\delta} \cdot \boldsymbol{\alpha} \leq L\}$ *for* $\boldsymbol{\delta} \in \mathbb{R}_+^d$ *given by* (29) *and take* L *as the lower bound in* (32) *to satisfy the bias constraint* (18) *under **Assumption 1**. Then, under **Assumptions 2-3** and using the following notation:*

$$\zeta = \max_{i \in I} \frac{\gamma_i - s_i}{2w_i}, \tag{41}$$

the total work, $W(\mathcal{I}_{\boldsymbol{\delta}})$*, of the MIMC estimator,* $\mathcal{A}$*, subject to constraint* (9)*, satisfies the following cases:*

Case A) If $\zeta \leq 0$*, then*

$$\limsup_{\mathrm{TOL}\downarrow 0} \frac{W(\mathcal{I}_{\boldsymbol{\delta}})}{\mathrm{TOL}^{-2}\left(\log\left(\mathrm{TOL}^{-1}\right)\right)^{2d_2}} \leq \frac{C_\epsilon^2 Q_S C_{\mathrm{work}}}{\theta^2 {\mathfrak{C}_1}^2 {\mathfrak{C}_2}^2} < \infty, \tag{42}$$

where $\mathfrak{C}_1$ *and* $\mathfrak{C}_2$ *are from* (36)*.*

Case B) if $\zeta > 0$*, then let* $k_1 = \#\{i \in I : \frac{\gamma_i - s_i}{2w_i} = \zeta\}$*, and* $\mathfrak{k} = 2(k_1-1)(\zeta+1)$*. Then, we have*

$$\limsup_{\mathrm{TOL}\downarrow 0} \frac{W(\mathcal{I}_{\boldsymbol{\delta}})}{\mathrm{TOL}^{-2-2\zeta}\left(\log\left(\mathrm{TOL}^{-1}\right)\right)^{\mathfrak{k}}} \leq \frac{C_\epsilon^2 Q_S C_{\mathrm{work}} {\mathfrak{C}_3}^2}{\eta^{\mathfrak{k}} {\mathfrak{C}_1}^2 \theta^2} \left(\frac{Q_W \mathfrak{C}_{\mathfrak{B}}}{1-\theta}\right)^{2\zeta} < \infty, \tag{43}$$

where $\mathfrak{C}_3$ *is from* (38)*.*

Proof. We prove this theorem by using Lemma 2.3 and proving that using $\boldsymbol{\delta}$ in (29) yields $k_1 = l_1 = n_1$ and

$$\zeta = \frac{\chi}{\eta} = \frac{\max_{i\in I}\left(g_i \delta_i^{-1}\right)}{\min_{i\in I}\left(\overline{w}_i \delta_i^{-1}\right)}.$$

Recall that $\delta_j = \frac{\overline{w}_j + g_j}{C_{\boldsymbol{\delta}}}$. Then

$$\begin{aligned} l_1 &= \#\{i \in I : \delta_i^{-1}\overline{w}_i = \min_{j\in I} \delta_j^{-1}\overline{w}_j\} \\ &= \#\{i \in I : \frac{\overline{w}_i}{\overline{w}_i + g_i} = \min_{j\in I} \frac{\overline{w}_j}{\overline{w}_j + g_j}\} \\ &= \#\{i \in I : 1 + \frac{g_i}{\overline{w}_i} = 1 + \max_{j\in I} \frac{g_j}{\overline{w}_j}\} = k_1 \end{aligned}$$

$$\begin{aligned} n_1 &= \#\{i \in I : \delta_i^{-1} g_i = \max_{j\in I} \delta_j^{-1} g_j\} \\ &= \#\{i \in I : \frac{g_i}{\overline{w}_i + g_i} = \max_{j\in I} \frac{g_j}{\overline{w}_j + g_j}\} \\ &= \#\{i \in I : 1 + \frac{\overline{w}_i}{g_i} = 1 + \min_{j\in I} \frac{\overline{w}_j}{g_j}\} = k_1. \end{aligned}$$

Next, observe that, on the one hand, by setting $\sigma_j = g_j/\overline{w}_j$, we have

$$\frac{1}{\eta} = \max_{j\in I} \frac{\delta_j}{\overline{w}_j} = \frac{1}{C_{\boldsymbol{\delta}}} \max_{j\in I} \left(1 + \frac{g_j}{\overline{w}_j}\right) = \frac{1}{C_{\boldsymbol{\delta}}} \left(1 + \max_{j\in I} \sigma_j\right)$$

and, on the other hand, we have

$$\chi = \max_{j\in I} \frac{g_j}{\delta_j} = C_{\boldsymbol{\delta}} \max_{j\in I} \frac{\sigma_j}{1+\sigma_j} = C_{\boldsymbol{\delta}} \frac{\max_{j\in I} \sigma_j}{1 + \max_{j\in I} \sigma_j},$$

since $f(x) = x/(1+x)$ is a monotone increasing function. Then,

$$\frac{\chi}{\eta} = \max_{i\in I} \sigma_i = \zeta.$$

□

Remark 2.4 (Choice of $\boldsymbol{\delta}$)**.** *Notice that other choices of $\boldsymbol{\delta}$ may achieve the same optimal rate stated in Theorem 2.2. For instance, when $g_i > 0$ for all $i \in I$, we can choose $\delta_i \propto \sqrt{g_i \overline{w}_i}$. With this choice of weights, we achieve the optimal rate but expect the corresponding constants to be sub-optimal, due to Lemma 2.1.*

Remark 2.5 (On isotropic directions)**.** *In the isotropic case of Remark 2.2, we have $k_1 = d$ and the TD set becomes*

$$\mathcal{I}(L) = \{\boldsymbol{\alpha} \in \mathbb{N}^d \,:\, |\boldsymbol{\alpha}| \le L\}.$$

The same rates of Theorem 2.2 can be obtained, with slightly different constants, namely:

$$\mathfrak{C}_{\mathfrak{B}} = \exp(|\overline{\boldsymbol{w}}|) \left(\prod_{i=1}^{d} \delta_i^{-1} \right) \eta^{-d} \sum_{j=0}^{d-1} \frac{\eta^j}{j!}$$

$$\text{and} \qquad \mathfrak{C}_3 = \frac{1}{\chi(d-1)!} \left(\prod_{i \in \hat{I}} \delta_i^{-1} \right)$$

Also, in this case, $\zeta = \frac{\gamma - s}{2w}$ *and* $\mathfrak{k} = 2(d-1)(\zeta+1)$*. Most importantly, in* Case B *the computational complexity of MIMC with a TD set would be* $\mathcal{O}\left(\mathrm{TOL}^{-2(1+\zeta)} \left(\log(\mathrm{TOL}^{-1})\right)^{\mathfrak{k}}\right)$*. Compare this computational complexity to the one of MIMC based on a full tensor set, namely* $\mathcal{O}\left(\mathrm{TOL}^{-2(1+d\zeta)}\right)$*.*

Remark 2.6 (A unique worst direction)**.** *In Theorem 2.2, consider the special case when* $k_1 = 1$*, i.e. when the directions are dominated by a single direction with the maximum difference between the work rate and the rate of variance convergence. In this case, the value of* L *becomes*

$$L = \frac{1}{\eta} \left(\log(\mathrm{TOL}_B^{-1}) + \log(\mathfrak{C}_{\mathfrak{B}}) \right)$$

and MIMC with a TD set achieves a better rate for the computational complexity, namely $\mathcal{O}\left(\mathrm{TOL}^{2-2\zeta}\right)$*. In other words, the logarithmic term disappears in the computational complexity.*

The same results also holds when the variance convergence is faster than algebraic in all but one direction and, in this case, the overall complexity is dictated by the only direction with an algebraic convergence rate. In this case, the optimal set might be no longer of TD type but it can still be constructed by using the same method and the same profit definition presented in Section 2.2.

3. Numerical Example

This section presents a numerical example illustrating the behavior of the MIMC, which is in agreement with our theoretical analysis. For the sake of comparison, we show the results of applying three different approximations to the same problem: MLMC as outlined in [8], MIMC with a full tensor set as outlined in Section 2.1, and MIMC with a Total Degree index set as outlined in Section 2.2. We begin by describing the numerical example. Then we present the solvers and algorithms and finish by showing the numerical results.

3.1. **Example overview.**

The numerical example is adapted from [17] and is based on Example 1 in Section 1.1 with some particular choices that satisfy the assumptions therein and **Assumptions 1-3**. First, the domain is chosen to be $\mathcal{D} = [0,1]^3$ and the forcing is

$$f(\boldsymbol{x};\omega) = f_0 + \widehat{f} \sum_{i=0}^{K} \sum_{j=0}^{K} \sum_{k=0}^{K} \Phi_{ijk}(\boldsymbol{x}) Z_{ijk},$$

where

$$\Phi_{ijk}(\boldsymbol{x}) = \sqrt{\lambda_i \lambda_j \lambda_k} \phi_i(x_1) \phi_j(x_2) \phi_k(x_3),$$

and

$$\phi_i(x) = \begin{cases} \cos\left(\frac{5\Lambda i}{2}\pi x\right) & i \text{ is even,} \\ \sin\left(\frac{5\Lambda(i+1)}{2}\pi x\right) & i \text{ is odd,} \end{cases}$$

$$\lambda_i = (2\pi)^{\frac{7}{6}} \Lambda^{\frac{11}{6}} \begin{cases} \frac{1}{2} & i = 0, \\ \exp\left(-2\left(\frac{\Lambda i}{4}\pi\right)^2\right) & i \text{ is even,} \\ \exp\left(-2\left(\frac{\Lambda(i+1)}{4}\pi\right)^2\right) & i \text{ is odd,} \end{cases}$$

for given parameters $0 < \Lambda$ and $K \in \mathbb{N}^+$, and $\boldsymbol{Z} = \{Z_{ijk}\}$ a set of $(K+1)^3$ i.i.d. standard normal random variables. Moreover, the diffusion coefficient is chosen to be a function of two random variables as follows:

$$a(\boldsymbol{x};\omega) = a_0 + \exp\Big(4Y_1 \Phi_{121}(\boldsymbol{x}) + 40 Y_2 \Phi_{877}(\boldsymbol{x})\Big). \tag{44}$$

Here, $\boldsymbol{Y} = \{Y_1, Y_2\}$ is a set of i.i.d. standard normal random variables, also independent of $\boldsymbol{Z}$. Finally, the quantity of interest, S, is

$$S = (2\pi\sigma)^{\frac{-3}{2}} \int_{\mathcal{D}} \exp\left(-\frac{\|\boldsymbol{x} - \boldsymbol{x}_0\|_2^2}{2\sigma^2}\right) u(\boldsymbol{x}) d\boldsymbol{x},$$

and the selected parameters are $a_0 = 0.01, f_0 = 50, \widehat{f} = 10, \Lambda = \frac{0.2}{\sqrt{2}}, K = 10, \sigma^2 = 0.02622863$ and $\boldsymbol{x}_0 = [0.5026695, 0.26042876, 0.62141498]$. Since the diffusion coefficient, a, is independent of the forcing, f, a reference solution can be calculated to sufficient accuracy by scaling and taking the expectation of the weak form with respect to $\boldsymbol{Z}$ to obtain a formula with constant forcing for the conditional expectation with respect to Y. We then use stochastic collocation [3] with a sufficiently accurate quadrature to produce the reference value, $\mathrm{E}[S]$. Using this method, the reference value 1.6026 is computed with an error estimate of 10^{-4}.

3.2. **Solvers and Algorithms.**

3.2.1. *Solving the underlying PDE problems.* To solve the underlying PDE problems, uniform meshes with a standard trilinear finite element basis are used to discretize the weak form of the model problem. The number of elements in each dimension is a positive integer, N_i, to give a mesh size of $h_i = N_i^{-1}$ for all $i = 1,2,3$. Moreover, we use the same $\beta = 2$ in all dimensions. In other words, given a multi index $\boldsymbol{\alpha}$, we use $N_i = 2^{\alpha_i}$ in each dimension and the resulting problem is isotropic with $w_i = 2$ and $s_i = 4$

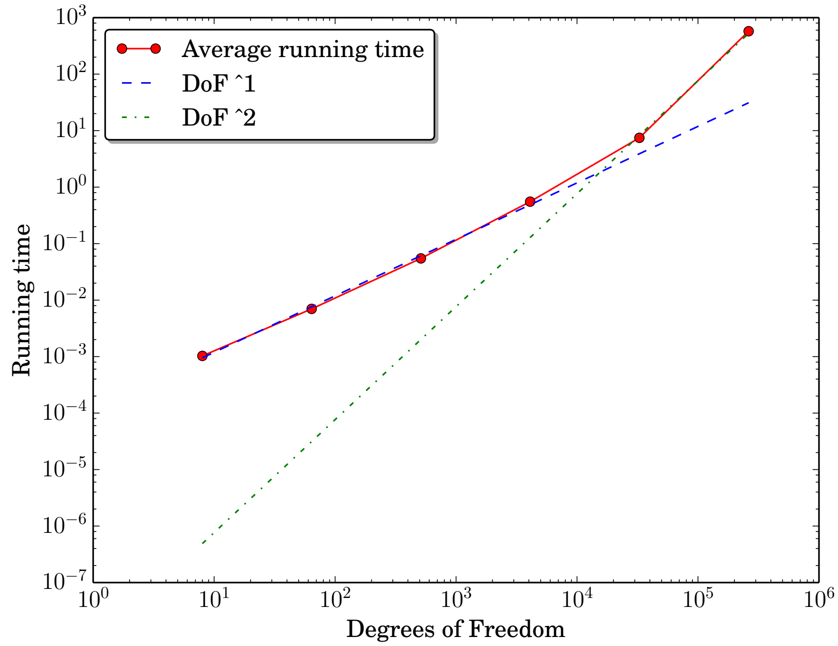

FIGURE 1. Average running time of the MUMPS linear solver versus the number of degrees of freedom. This shows that, for our numerical example, γ_i in (15) is the same for $i = 1 \dots d$ and ranges from 1 to 2.

for all $i = 1, 2, 3$ (the same case as Remarks 2.2 and 2.5). The linear solver MUMPS [1, 2] was used for solving the linear problem. For the mesh sizes of interest, the running time of MUMPS varies from quadratic to linear in the total number of degrees of freedom (cf. Figure 1). As such, γ_i in (15) is the same for all $i = 1, 2, 3$ and ranges from 1 to 2. We use a value of $\gamma_i = 1.5$ to predict the rates of computational complexity in (28) and Theorems 2.1 and 2.2.

3.2.2. *MIMC Algorithm.* The algorithm used to generate the results presented in the next section is a slight modification and extension of the MLMC algorithm first outlined in [12]. Specifically, the sample variance was used to calculate the required number of samples on each level in MIMC, with a minimum of three samples per level. Moreover, we used fixed tolerance-splitting, $\theta = 0.66$. This is the asymptotic optimal choice for the MLMC method in discussed in [17]. Note that this choice might be sub-optimal for MIMC and further work needs to be done in this case. In summary, the algorithm can be summarized as follows:

Step 1. Start with empty index set $\mathcal{I}$
Step 2. Expand index set $\mathcal{I}$
Step 3. Ensure that at least M_0 samples are calculated for all $\boldsymbol{\alpha} \in \mathcal{I}$.

Step 4. Using sample variances as estimates for $V_{\boldsymbol{\alpha}}$; calculate (11) for all $\boldsymbol{\alpha} \in \mathcal{I}$.
Step 5. Calculate extra samples to have at least $M_{\boldsymbol{\alpha}}$ samples for each $\boldsymbol{\alpha}$.
Step 6. Estimate the bias as $\sum_{\boldsymbol{\alpha} \in \partial \mathcal{I}} E_{\boldsymbol{\alpha}}$, where $\partial \mathcal{I}$ is the outer boundary of $\mathcal{I}$.
Step 7. Stop if the error estimate is less than TOL; otherwise, go to Step 2.

This algorithm is general and can be used for MIMC with both TD and full tensor sets. For TD sets, we simply increase the value of L in (30) to expand the set in Step 2. For full tensor sets, we successively increase the value of L_i for $i = 1 \ldots d$ allowing for anisotropic full tensor sets.

3.3. **Results.** Three methods were tested: MLMC as outlined in [8], MIMC with full tensor sets (referred to as "FT" in the figures), and MIMC with isotropic total degree set (referred to as "TD" in the figures). In this isotropic example, following Remark 2.5, the total degree sets defined in Section 2.2 becomes

$$\mathcal{I}(L) = \{\boldsymbol{\alpha} \in \mathbb{N}^3 : |\boldsymbol{\alpha}| \leq L\}.$$

Figures 2 and 3 provide numerical evidence that this TD set is indeed (at least for sufficiently small TOL) a nearly optimal index set for MIMC approximation. On the other hand, Figures 5 and 6 show numerical results that are in agreement with the convergence rates claimed in Remark 2.1. Specifically, these figures show consistent results with the values $s_i = 4$ and $w_i = 2$ for all $i = 1, 2, 3$. Moreover, Figure 4 shows numerical evidence of the normality of the statistical error of the MIMC estimator.

Figure 7 shows the running time for different tolerances. The MIMC method with a full tensor set or a total degree set seems to exhibit the expected rate of TOL^{-2} in the computational time. On the other hand, MLMC seems to exhibit a rate closer to $\mathrm{TOL}^{-2.25}$, in agreement with (28). Recall that in this example, $d = 3, \gamma_i = 1.5, s_i = 4$ and $w_i = 2$ for all $i = 1, 2, 3$. The increase in running time for certain tolerances in MLMC and MIMC with a full tensor set is due to two effects: a) In MIMC with a full tensor set, the optimal number of samples according to (11) is less than 1 for most $\boldsymbol{\alpha}$ for certain tolerances, and taking the ceiling of these values increases the work. b) For both methods, the increase in running time corresponds to the discrete increments of the maximum number of degrees of freedom per level (cf. Figure 9). Since a fixed tolerance-splitting parameter, θ, was used, this means that the statistical constraint is not relaxed when the bias becomes smaller and the algorithm ends up solving for a slightly smaller tolerance than the required TOL (cf. Figure 8). Notice that although the fixed tolerance splitting parameter was also used for MIMC with total degree sets, the running time does not exhibit the same jumps. This is because the discrete increments in the number of degrees of freedom are not as significant in this method (cf. Figure 9).

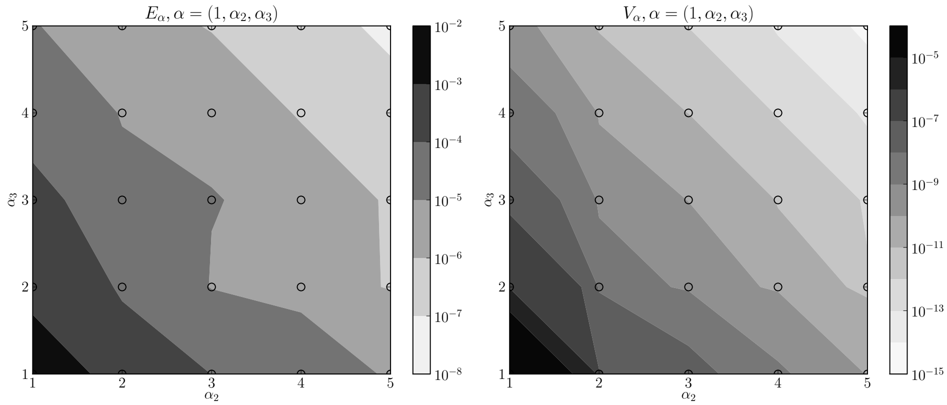

Figure 2. Numerical example, rate verification: contour plots of sample mean (left) and variance (right) of mixed differences used in MIMC for a slice of multi indices. The parallel lines, asymptotically, suggest that isotropic TD sets are nearly optimal in this example.

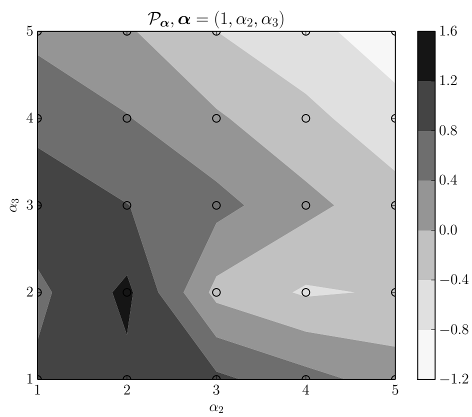

Figure 3. Numerical example, rate verification: contour plots of profits used in MIMC for a slice of multi indices. Numerical results indicate that, asymptotically, the isotropic TD sets are nearly optimal in this example.

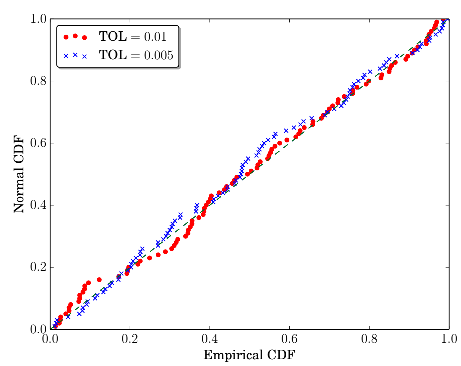

Figure 4. QQ-plot of the normalized error of the MIMC estimator with a TD set for different values of TOL. Similar results were obtained for other tolerances using either MLMC or MIMC with full tensor sets. This is in agreement with Lemma A.1.

4. Conclusions

We have proposed and analyzed a novel Multi Index Monte Carlo (MIMC) method for weak approximation of stochastic models that are described in terms of differential equations either driven by random measures or with

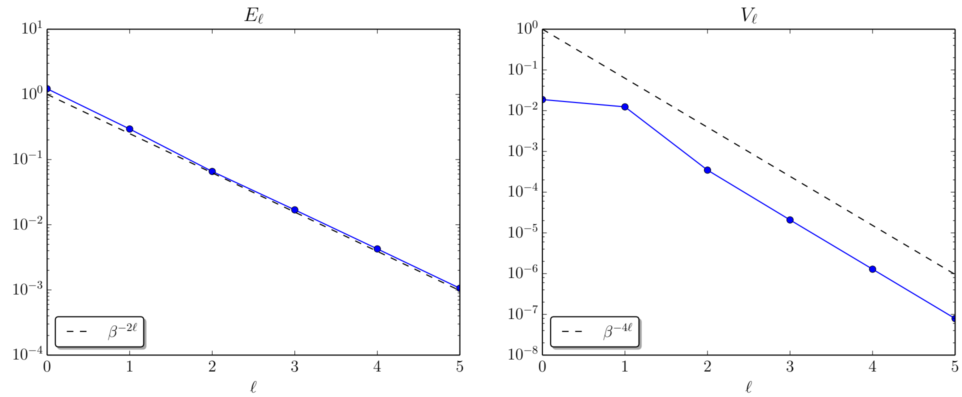

FIGURE 5. Numerical example, rate verification: sample mean (left) and variance (right) of differences versus level ℓ for MLMC. Notice that the observed rates are consistent with Remark 2.1.

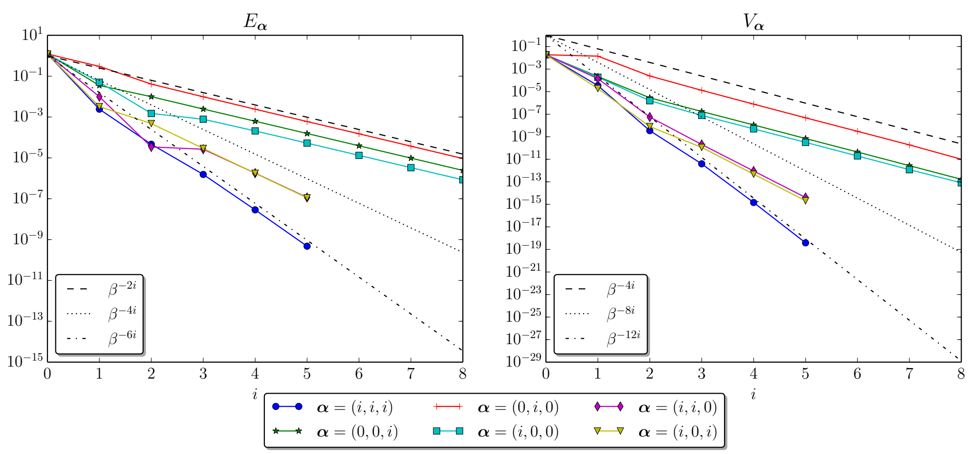

FIGURE 6. Numerical example, rate verification: sample mean (left) and variance (right) of mixed differences used in MIMC. Notice that the observed rates are consistent with Remark 2.1 and are better than those observed for MLMC, cf. Figure 5.

random coefficients. The MIMC method uses a stochastic combination technique to solve the given approximation problem, generalizing the notion of standard MLMC levels into a set of multi indices that should be properly chosen to exploit the available regularity. Indeed, instead of using first-order differences as in standard MLMC, MIMC uses high-order differences to reduce the variance of the hierarchical differences dramatically. This in turn gives a new improved complexity result that increases the domain of the problem parameters for which the method achieves the optimal convergence rate, $\mathcal{O}(\mathrm{TOL}^{-2})$. We have outlined a method for constructing an

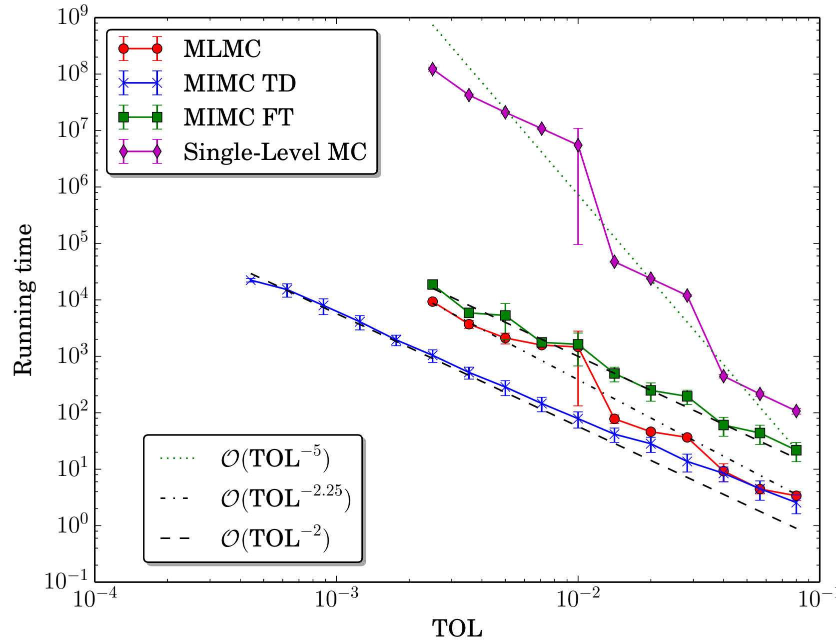

FIGURE 7. Running time for different values of TOL when using MLMC and MIMC with different sets. The error bars extend from the 5% percentile to the 95% percentile. Also included for comparison is a theoretical running time for the single-level Monte Carlo method. Notice that the rate of MIMC is the optimal Monte Carlo rate of $\mathcal{O}\left(\text{TOL}^{-2}\right)$ for this example, while MLMC is closer to $\mathcal{O}\left(\text{TOL}^{-2.25}\right)$, in agreement with the results listed in Remark 2.2 for $d = 3, \gamma_i = 1.5, s_i = 4$ and $w_i = 2$ for all $i = 1, 2, 3$.

optimal set of indices for our MIMC method. Moreover, under our standard assumptions, we showed that the optimal index set turns out to be of Total Degree (TD) type. Using optimal index sets, MIMC achieves a better rate for the computational complexity than when using Full Tensor sets; in fact, in some cases, the rate does not depend on the dimensionality of the underlying problem. We also presented numerical results to substantiate some of the derived computational complexity rates. In Appendix A, using the Lindeberg-Feller theorem, we also show the asymptotic normality of the statistical error in the MIMC estimator and justify in this way our error estimate that allows both the required accuracy and confidence in the final result to be prescribed.

Our method requires more regularity of the underlying solution than does MLMC. If the underlying solution is sufficiently regular only in some directions, then one can still combine MIMC with MLMC by applying mixed first-order differences to the sufficiently regular directions, while applying a single first-order difference to less regular directions.

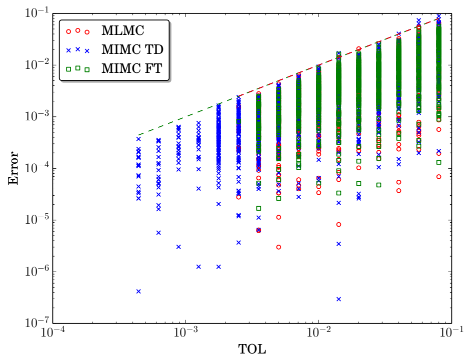

FIGURE 8. The exact computational error for MLMC and MIMC using different index sets. Notice that since we imposed a fixed tolerance splitting parameter, $\theta = 0.66$, in some cases our numerical error is slightly smaller than the required TOL for all methods.

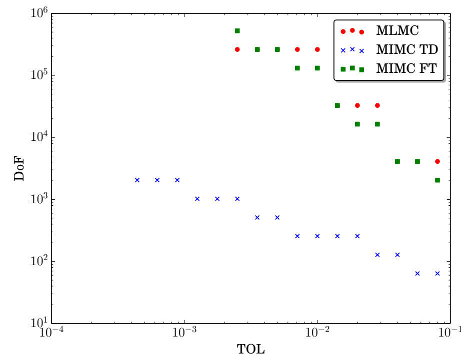

FIGURE 9. The maximum number of degrees of freedom across levels for MLMC and MIMC with different sets. Notice that by using total degree sets, we are able to achieve the same value of TOL with substantially fewer degrees of freedom.

In future work, more has to be done to improve the MIMC algorithm, using the variance convergence model to estimate the variances instead of relying on sample variance only; for example, by applying ideas as those in [10]. Also, a better choice of the splitting parameter, θ, can be derived to improve the computational complexity up to a constant factor; similar to the work done in [17]. Moreover, MIMC can be used to improve the computational complexity rate in the case of PDEs with random fields that are approximated by converging series, such as a Karhunen-Loéve decomposition, cf. [31]. By treating the number of terms in the decomposition as an extra discretization direction and applying MIMC, we might be able to improve the computational complexity. Also, the use of either *a priori* refined non-uniform discretizations or adaptive algorithms based on *a posteriori* error estimates for non-uniform refinement as introduced in [22, 23, 27] can be combined with MIMC to improve efficiency. Finally, ideas from [32] and [18] can be extended by replacing the Monte Carlo sampling of mixed differences in MIMC by a sparse-grid stochastic collocation, effectively including interpolation levels along the different random directions into the combination technique together with the other discretization parameters. Similarly, we can apply Quasi Monte Carlo to replace Monte Carlo sampling of the mixed differences in MIMC as outlined in [25] for a multilevel setting. Provided that there is enough mixed regularity in the problem at hand, we expect to improve again the optimal complexity further from $\mathcal{O}(\mathrm{TOL}^{-2})$ in MIMC to $\mathcal{O}(\mathrm{TOL}^{-r})$ with $r < 2$.

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Appendix A. Asymptotic Normality of the MIMC estimator

Lemma A.1 (Asymptotic Normality of the MIMC Estimator)**.** *Consider the MIMC estimator introduced in* (3)*,* $\mathcal{A}$*, based on a set of multi indices,* $\mathcal{I}(\mathrm{TOL})$*, and given by*

$$\mathcal{A} = \sum_{\boldsymbol{\alpha}\in\mathcal{I}} \sum_{m=1}^{M_{\boldsymbol{\alpha}}} \frac{\Delta \mathcal{S}_{\boldsymbol{\alpha}}(\omega_{\boldsymbol{\alpha},m})}{M_{\boldsymbol{\alpha}}}.$$

Assume that for $1 \le i \le d$ *there exists* $0 < L_i(\mathrm{TOL})$ *such that*

$$\mathcal{I}(\mathrm{TOL}) \subset \{\boldsymbol{\alpha} \in \mathbb{N}^d : \alpha_i \le L_i(\mathrm{TOL}), \ \text{for } 1 \le i \le d\}. \tag{45}$$

Denote $Y_{\boldsymbol{\alpha}} = |\Delta\mathcal{S}_{\boldsymbol{\alpha}} - \mathrm{E}[\Delta\mathcal{S}_{\boldsymbol{\alpha}}]|$ *and assume that the following inequalities*

$$Q_S \prod_{i=1}^{d} \exp(-\alpha_i s_i) \le \mathrm{E}\left[Y_{\boldsymbol{\alpha}}^2\right], \tag{46a}$$

$$\mathrm{E}\left[Y_{\boldsymbol{\alpha}}^{2+\rho}\right] \le Q_R \prod_{i=1}^{d} \exp(-\alpha_i r_i), \tag{46b}$$

hold for strictly positive constants $\rho, \{s_i, r_i\}_{i=1}^d, Q_S$ *and* Q_R*. Choose the number of samples on each level,* $M_{\boldsymbol{\alpha}}(\mathrm{TOL})$*, to satisfy, for strictly positive sequences* $\{\tilde{s}_i\}_{i=1}^d$ *and* $\{H_{\boldsymbol{\tau}}\}_{\boldsymbol{\tau}\in\mathcal{I}(\mathrm{TOL})}$ *and for all* $\boldsymbol{\alpha} \in \mathcal{I}(\mathrm{TOL})$*,*

$$M_{\boldsymbol{\alpha}} \ge \mathrm{TOL}^{-2}\, C_M \left(\prod_{i=1}^{d} \exp(-\alpha_i \tilde{s}_i)\right) H_{\boldsymbol{\alpha}}^{-1} \left(\sum_{\boldsymbol{\tau}\in\mathcal{I}(\mathrm{TOL})} H_{\boldsymbol{\tau}}\right). \tag{47}$$

Denote, for all $1 \le i \le d$*,*

$$p_i = (\rho/2)\tilde{s}_i - r_i + (1 + \rho/2)s_i$$

and choose $0 < c_i$ such that whenever $0 < p_i$, the inequality $c_i < \rho/p_i$ holds. Finally, if we take the quantities $L_i(\mathrm{TOL})$ in (45) to be

$$L_i(\mathrm{TOL}) = c_i \log(\mathrm{TOL}^{-1}) + o\left(\log(\mathrm{TOL}^{-1})\right), \text{ for all } 1 \le i \le d,$$

then we have

$$\lim_{\mathrm{TOL}\downarrow 0} \mathrm{P}\left[\frac{\mathcal{A} - \mathrm{E}[\mathcal{A}]}{\sqrt{\mathrm{Var}[\mathcal{A}]}} \le z\right] = \Phi\left(z\right),$$

where $\Phi(z)$ is the normal cumulative density function of a standard normal random variable.

Proof. We prove this theorem by ensuring that the Lindeberg condition [11, Lindeberg-Feller Theorem, p. 114] (also restated in [10, Theorem A.1]) is satisfied. The condition becomes in this case

$$\lim_{\mathrm{TOL}\downarrow 0} \underbrace{\frac{1}{\mathrm{Var}[\mathcal{A}]} \sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} \sum_{m=1}^{M_{\boldsymbol{\alpha}}} \mathrm{E}\left[\frac{Y_{\boldsymbol{\alpha}}^2}{M_{\boldsymbol{\alpha}}^2} \mathbf{1}_{\frac{Y_{\boldsymbol{\alpha}}}{M_{\boldsymbol{\alpha}}} > \epsilon\sqrt{\mathrm{Var}[\mathcal{A}]}}\right]}_{=F} = 0,$$

for all $\epsilon > 0$. Below we make repeated use of the following identity for non-negative sequences $\{a_{\boldsymbol{\alpha}}\}$ and $\{b_{\boldsymbol{\alpha}}\}$ and $q \ge 0$:

$$\sum_{\boldsymbol{\alpha}} a_{\boldsymbol{\alpha}}^q b_{\boldsymbol{\alpha}} \le \left(\sum_{\boldsymbol{\alpha}} a_{\boldsymbol{\alpha}}\right)^q \sum_{\boldsymbol{\alpha}} b_{\boldsymbol{\alpha}}. \tag{48}$$

First, we use the Markov inequality to bound

$$\begin{aligned} F &= \frac{1}{\mathrm{Var}[\mathcal{A}]} \sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} \sum_{m=1}^{M_{\boldsymbol{\alpha}}} \mathrm{E}\left[\frac{Y_{\boldsymbol{\alpha}}^2}{M_{\boldsymbol{\alpha}}^2} \mathbf{1}_{Y_{\boldsymbol{\alpha}} > \epsilon\sqrt{\mathrm{Var}[\mathcal{A}]} M_{\boldsymbol{\alpha}}}\right] \\ &\le \frac{\epsilon^{-\rho}}{\mathrm{Var}[\mathcal{A}]^{1+\rho/2}} \sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} M_{\boldsymbol{\alpha}}^{-1-\rho} \mathrm{E}\left[Y_{\boldsymbol{\alpha}}^{2+\rho}\right]. \end{aligned}$$

Using (48) and substituting for the variance $\mathrm{Var}[\mathcal{A}]$ where we denote $\mathrm{Var}[\Delta\mathcal{S}_{\boldsymbol{\alpha}}] = \mathrm{E}\left[(\Delta\mathcal{S}_{\boldsymbol{\alpha}} - \mathrm{E}[\Delta\mathcal{S}_{\boldsymbol{\alpha}}])^2\right]$ by $V_{\boldsymbol{\alpha}}$, we find

$$\begin{aligned} F &\le \frac{\epsilon^{-\rho}\left(\sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} M_{\boldsymbol{\alpha}}^{-1} V_{\boldsymbol{\alpha}}\right)^{1+\rho/2}}{\left(\sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} V_{\boldsymbol{\alpha}} M_{\boldsymbol{\alpha}}^{-1}\right)^{1+\rho/2}} \sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} V_{\boldsymbol{\alpha}}^{-1-\rho/2} M_{\boldsymbol{\alpha}}^{-\rho/2} \mathrm{E}\left[Y_{\boldsymbol{\alpha}}^{2+\rho}\right] \\ &= \epsilon^{-\rho} \sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} V_{\boldsymbol{\alpha}}^{-1-\rho/2} M_{\boldsymbol{\alpha}}^{-\rho/2} \mathrm{E}\left[Y_{\boldsymbol{\alpha}}^{2+\rho}\right]. \end{aligned}$$

Using the lower bound in (47) on the number of samples, $M_{\boldsymbol{\alpha}}$, and (48), again yields

$$\begin{aligned} F &\le C_M^{-\rho/2}\epsilon^{-\rho}\mathrm{TOL}^{\rho}\left(\sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} V_{\boldsymbol{\alpha}}^{-1-\rho/2}\left(\prod_{i=1}^{d}\exp\left(\frac{\rho\alpha_i\tilde{s}_i}{2}\right)\right)H_{\boldsymbol{\alpha}}^{\rho/2}\mathrm{E}\left[Y_{\boldsymbol{\alpha}}^{2+\rho}\right]\right) \\ &\qquad\qquad\qquad\left(\sum_{\boldsymbol{\tau}\in\mathcal{I}(\mathrm{TOL})} H_{\boldsymbol{\tau}}\right)^{-\rho/2} \\ &\le C_M^{-\rho/2}\epsilon^{-\rho}\mathrm{TOL}^{\rho}\left(\sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})} V_{\boldsymbol{\alpha}}^{-1-\rho/2}\left(\prod_{i=1}^{d}\exp\left(\frac{\rho\alpha_i\tilde{s}_i}{2}\right)\right)\mathrm{E}\left[Y_{\boldsymbol{\alpha}}^{2+\rho}\right]\right). \end{aligned}$$

Finally, using the bounds (46a) and (46b),

$$F \le \underbrace{C_M^{-\rho/2}\epsilon^{-\rho}Q_S^{-1-\rho/2}Q_R}_{=C_F}\mathrm{TOL}^{\rho}\left(\sum_{\boldsymbol{\alpha}\in\mathcal{I}(\mathrm{TOL})}\left(\prod_{i=1}^{d}\exp\left(p_i\alpha_i\right)\right)\right).$$

Next, define three sets of dimension indices:

$$\begin{aligned} \hat{I}_1 &= \{1 \le i \le d : p_i < 0\}, \\ \hat{I}_2 &= \{1 \le i \le d : p_i = 0\}, \\ \hat{I}_3 &= \{1 \le i \le d : p_i > 0\}. \end{aligned} \tag{49}$$

Then, using (45) yields

$$\begin{aligned} F \le& C_F\mathrm{TOL}^{\rho}\prod_{i=1}^{d}\left(\sum_{\alpha_i=0}^{L_i}\exp\left(p_i\alpha_i\right)\right) \\ \le& C_F\mathrm{TOL}^{\rho}\prod_{i\in\hat{I}_1}\frac{1}{1-\exp(p_i)}\prod_{i\in\hat{I}_2}L_i\prod_{i\in\hat{I}_3}\frac{1-\exp(p_i(L_i+1))}{1-\exp(p_i)}. \end{aligned}$$

To conclude, observe that if $|\hat{I}_3| = 0$ then $\lim_{\mathrm{TOL}\downarrow 0} F = 0$ for any choice of $L_i \ge 0$, $1 \le i \le d$. Similarly, if $|\hat{I}_3| > 0$, since we assumed that $c_i p_i < \rho$ holds for all $i \in \hat{I}_3$ then $\lim_{\mathrm{TOL}\downarrow 0} F = 0$. □

Remark. *The lower bound on the number of samples per index* (47) *mirrors the choice* (11)*, the latter being the optimal number of samples satisfying constraint* (9)*. Specifically,* $H_{\boldsymbol{\alpha}} = \sqrt{V_{\boldsymbol{\alpha}}W_{\boldsymbol{\alpha}}}$ *and* $\tilde{s}_i = s_i$*. Furthermore, notice that the previous Lemma bounds the growth of* L *from above, while Theorem 2.1 and Theorem 2.2 bound the value of* L *from below to satisfy the bias accuracy constraint.*

Appendix B. Integrating an exponential over a simplex

Lemma B.1. *The following identity holds for any $L > 0$ and $a \in \mathbb{R}$*

$$\begin{aligned} \int_{\{\boldsymbol{x}\in\mathbb{R}_+^d\,:\,|\boldsymbol{x}|\leq L\}} \exp(a|\boldsymbol{x}|)\,d\boldsymbol{x} &= (-a)^{-d}\left(1-\exp(La)\sum_{j=0}^{d-1}\frac{(-La)^j}{j!}\right) \\ &= \frac{1}{(d-1)!}\int_0^L \exp(at)t^{d-1}\,dt. \end{aligned} \tag{50}$$

Proof.

$$\int_{\{\boldsymbol{x}\in\mathbb{R}_+^d\,:\,|\boldsymbol{x}|\leq L\}} \exp(a|\boldsymbol{x}|)\mathrm{d}\boldsymbol{x} = L^d \int_{\{\boldsymbol{x}\in\mathbb{R}_+^d\,:\,|\boldsymbol{x}|\leq 1\}} \exp(aL|\boldsymbol{x}|)\mathrm{d}\boldsymbol{x}.$$

Then, we prove, by induction on d and for $b = aL$, the following identity

$$\int_{\{\boldsymbol{x}\in\mathbb{R}_+^d\,:\,|\boldsymbol{x}|\leq 1\}} \exp(b|\boldsymbol{x}|) = (-b)^{-d}\left(1-\exp(b)\sum_{j=0}^{d-1}\frac{(-b)^j}{j!}\right).$$

First, for $d = 1$, we have

$$\int_0^1 \exp(bx)\mathrm{d}x = \frac{\exp(b)-1}{b}.$$

Next, assuming that the identity is true for $d-1$, we prove it for d. Indeed, we have

$$\begin{aligned} &\int_{\{\boldsymbol{x}\in\mathbb{R}_+^d\,:\,|\boldsymbol{x}|\leq 1\}} \exp(b|\boldsymbol{x}|)\mathrm{d}\boldsymbol{x} \\ &= \int_0^1 \exp(by)\left(\int_{\{\boldsymbol{x}\in\mathbb{R}_+^{d-1}\,:\,|\boldsymbol{x}|\leq 1-y\}} \exp(b|\boldsymbol{x}|)\mathrm{d}\boldsymbol{x}\right)\mathrm{d}y \\ &= \int_0^1 \exp(by)\,(1-y)^{d-1}\left(\int_{\{\boldsymbol{x}\in\mathbb{R}_+^{d-1}\,:\,|\boldsymbol{x}|\leq 1\}} \exp((1-y)b|\boldsymbol{x}|)\mathrm{d}\boldsymbol{x}\right)\mathrm{d}y \\ &= \int_0^1 \exp(by)\frac{(1-y)^{d-1}}{(-(1-y)b)^{d-1}}\left(1-\exp((1-y)b)\sum_{j=0}^{d-2}\frac{(-(1-y)b)^j}{j!}\right)\mathrm{d}y \\ &= \int_0^1 \left[\frac{\exp(by)}{(-b)^{d-1}} - \frac{\exp(b)}{(-b)^{d-1}}\sum_{j=0}^{d-2}\frac{(-(1-y)b)^j}{j!}\right]\mathrm{d}y \\ &= \frac{(-1)^{d-1}}{b^d}(\exp(b)-1) - \frac{(-1)^{d-1}\exp(b)}{b^{d-1}}\sum_{j=0}^{d-2}\frac{(-b)^j}{(j+1)!} \\ &= \frac{(-1)^d}{b^d} - \frac{(-1)^d}{b^d}\exp(b) - \frac{(-1)^d\exp(b)}{b^d}\sum_{j=1}^{d-1}\frac{(-b)^j}{(j)!} \end{aligned}$$

$$= (-b)^{-d}\left(1-\exp(b)\sum_{j=0}^{d-1}\frac{(-b)^j}{j!}\right).$$

Finally, the second equality in (50) follows by repeatedly integrating by parts. □

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