CONSTRUCTION-FREE MEDIAN QUASI-MONTE CARLO RULES FOR FUNCTION SPACES WITH UNSPECIFIED SMOOTHNESS AND GENERAL WEIGHTS *

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Abstract. We study quasi-Monte Carlo (QMC) integration of smooth functions defined over the multi-dimensional unit cube. Inspired by a recent work of Pan and Owen, we study a new construction-free median QMC rule which can exploit the smoothness and the weights of function spaces adaptively. For weighted Korobov spaces, we draw a sample of r independent generating vectors of rank-1 lattice rules, compute the integral estimate for each, and approximate the true integral by the median of these r estimates. For weighted Sobolev spaces, we use the same approach but with the rank-1 lattice rules replaced by high-order polynomial lattice rules. A major advantage over the existing approaches is that we do not need to construct good generating vectors by a computer search algorithm, while our median QMC rule achieves almost the optimal worst-case error rate for the respective function space with any smoothness and weights, with a probability that converges to 1 exponentially fast as r increases. Numerical experiments illustrate and support our theoretical findings.

Key words. Numerical integration; quasi-Monte Carlo; rank-1 lattice rule; high-order polynomial lattice rule; weighted function space; median; construction-free

AMS subject classifications. 65D30, 65D32, 41A55, 46E35

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1. Introduction. We consider numerical integration of functions defined over the s-dimensional unit cube $[0,1)^s$. For an integrable function $f:[0,1)^s \to \mathbb{R}$, we denote the integral of f by

$$I_s(f) := \int_{[0,1)^s} f(\boldsymbol{x}) \,\mathrm{d}\boldsymbol{x}.$$

The quasi-Monte Carlo (QMC) method approximates $I_s(f)$ by the equally-weighted average of function evaluations over a deterministic N-element point set $P_{N,s} \subset [0,1)^s$:

$$Q_{P_{N,s}}(f) = \frac{1}{N} \sum_{\boldsymbol{x} \in P_{N,s}} f(\boldsymbol{x}).$$

The worst-case error for a given normed function space \mathcal{F} and point set $P_{N,s}$ is

$$e^{\text{wor}}(Q_{P_{N,s}}; \mathcal{F}) = \sup_{f \in \mathcal{F}; \|f\| \le 1} |Q_{P_{N,s}}(f) - I_s(f)|$$

where ||f|| is the norm of f in this space. The key to success of the QMC method lies in a proper choice of the point set depending on a target class of functions. One wants to construct point sets for which this worst-case error is small and converges at the fastest possible rate as a function of N, for the given space \mathcal{F} . In randomized QMC, the point set $P_{N,s}$ is randomized in a way that $Q_{P_{N,s}}(f)$ becomes an unbiased

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estimator of $I_s(f)$ and one wishes to minimize its variance [24, 25, 29]. In this paper, we focus on deterministic QMC point sets only.

There are two main families of QMC point sets: digital nets and sequences [10, 35] and lattice point sets [35, 42]. We refer the reader to [7, 29, 31] for further introductory details. In this paper, we consider rank-1 lattice point sets for Korobov spaces of periodic functions, and high-order polynomial lattice point sets [9, 34, 40] (which are a special type of digital nets) for Sobolev spaces of non-periodic functions. Each point set from these types is defined by an s-dimensional generating vector, with integer coordinates in the ordinary lattice case and with polynomial coordinates in the polynomial lattice case.

In both cases, the weighted spaces of functions are defined by selecting a positive smoothness parameter α and a positive weight γ_u for each subset of coordinates $u \subseteq \{1, \ldots, s\}$, with $\gamma_{\emptyset} = 1$. The parameter α determines how smooth the admissible functions are required to be. For the Korobov spaces, it tells the minimal rate at which the Fourier coefficients of f are required to decay, and when it is an integer it corresponds to the minimal number of square-integrable mixed partial derivatives of f with respect to each coordinate; see [36, Appendix A]. For the Sobolev spaces, α is a positive integer which also imposes integrability conditions on the partial derivatives of f. The weights γ_u act as constant importance factors given to the subsets of coordinates [11, 44]. A larger γ_u means that the projection of f over the subset of coordinates in u can have a larger variation in some sense, so that more importance should be given to the uniformity of the points over this projection.

It is known that the best possible QMC point sets cannot provide a better convergence rate than $\mathcal{O}(N^{-\alpha})$ for the worst-case error for these two function spaces. On the other hand, there are effective search algorithms which, for a given α and a given selection of weights γ_u , can construct good rank-1 lattice or polynomial lattice point sets for the function spaces determined by these parameters, and for which the worst-case error converges as $\mathcal{O}(N^{-\alpha+\epsilon})$ for any $\epsilon > 0$ [10, 21]. Software that implement such algorithms is also freely available [26, 28, 37]. These algorithms typically use a greedy component-by-component (CBC) construction approach proposed originally by [19], then re-introduced and popularized by [43]. With the CBC approach, the generating vector is determined one coordinate at a time by optimizing a figure of merit that depends only on this new coordinate and the previous ones, and where the previous coordinates can no longer be changed.

In general, the number of weights γ_u to specify is $2^s - 1$. When s is large, specifying all these weights individually becomes impractical, so it is common practice to "parameterize" the weights by a smaller number of parameters, usually linear instead of exponential in s. The most popular forms of parameterizations are the product weights, the order-dependent weights, and their combination. For the product weights, one specifies a weight $\gamma_j > 0$ for each coordinate $j = 1, \ldots, s$, and the γ_u 's are defined as $\gamma_u = \prod_{j \in u} \gamma_j$. For the order-dependent weights, γ_u depends only on the cardinality of u: $\gamma_u = \Gamma_{|u|}$, where $\Gamma_1, \Gamma_2, \ldots, \Gamma_s$ are selected positive constants. Their combination gives the product and order-dependent (POD) weights, for which $\gamma_u = \Gamma_{|u|} \prod_{j \in u} \gamma_j$ [33]. The main reason why the most popular choices of weights have this form is that the existing search algorithms are truly efficient for large s only when the weights have this specific POD form [11, 23, 26, 28, 33, 38]. Then, by using a fast-CBC approach that speeds up the search by exploiting a fast Fourier transform [28, 38], one can find a generating vector that gives a worst-case error of $\mathcal{O}(N^{-\alpha+\epsilon})$ in $\mathcal{O}(sN\log N)$ operations for ordinary lattices and $\mathcal{O}(\alpha sN\log N)$ for polynomial lattices (with interlacing).

Although this form is convenient, the restriction to POD weights is <u>limiting</u>: for a given application, the appropriate weights may be quite far from the POD form. In this case, imposing POD implies that the point sets are constructed with the wrong weights. Moreover, even without constraints imposed on the form of weights, finding or approximating appropriate weights and the appropriate α for a given application is generally very difficult [27]. When the points are constructed with the wrong weights, the QMC method can be quite ineffective in general. These drawbacks have been addressed very partially in recent papers. In [12], the authors introduces a construction algorithm that does not require the knowledge of α . It uses a CBC construction algorithm with a figure of merit that assumes $\alpha = 1$, and for each coordinate it also constructs the generating vector one binary digit at a time. The method provides a convergence rate of $\mathcal{O}(N^{-\alpha+\epsilon})$. In [4], the authors study the stability of rank-1 lattice rules and polynomial lattice rules to a (limited) misspecification of α and the weights, for product and POD weights. They obtain worst-case error bounds for function spaces determined by parameters α' and $\gamma' = \{\gamma'_n\}$ when the rules are constructed using parameters α and $\gamma = {\gamma_u}$ instead, under certain conditions on those weights. These results are interesting but they do not completely eliminate the need to specify the weights.

The method studied in this paper requires no knowledge at all on α and the weights γ_u . No value needs to be specified for any of these parameters. The algorithm is inspired by recent work from Pan and Owen [39], and works as follows. For a fixed odd integer r > 0, we draw r generating vectors independently and uniformly from the set of all admissible generating vectors. For each of them, we compute the corresponding QMC approximation $Q_{P_{N,s}}(f)$, then we take the median M(f) of these r approximations as our final estimate of $I_s(f)$. Since the method does not require the explicit construction of a good point set, we call it a construction-free median QMC rule.

Our main contribution is to prove that for \mathcal{F} representing either a weighted Korobov or weighted Sobolev space determined by parameters α and γ , the error $|M(f) - I_s(f)|$ obeys the following type of probabilistic bound: For any $\epsilon > 0$ and $0 < \rho < 1$, there is a constant $c_1 = c_1(\alpha, \gamma, \epsilon) > 0$ (which depends on α , the γ_u 's and ϵ) such that

$$\mathbb{P}\left[\sup_{f\in\mathcal{F};\,||f||\leq 1}|M(f)-I_s(f)|\leq \frac{c_1(\alpha,\gamma,\epsilon)}{(\rho N)^{\alpha-\epsilon}}\right]\geq 1-\rho^{(r+1)/2}/4.$$

In other words, the worst-case error of the median estimator is bounded by a quantity that decreases almost at the best possible rate of $\mathcal{O}(N^{-\alpha})$, with a probability that converges to 1 exponentially fast as a function of r. That is, we have a simple method that provides essentially the best possible convergence rate with very high probability, without requiring any knowledge of α and the weights. The key reason why this is possible is that the vast majority of the choices of generating vectors turn out to be quite good and give a QMC approximation which is quite close to $I_s(f)$. Only a small minority give a large error. For the vector giving the median value to be in that small minority, there must be at least (r+1)/2 generating vectors in the sample of size r that belong to this small minority, and the probability that this happens decreases towards zero exponentially in r.

The remainder is organized as follows. In Section 2, we recall some basic facts on lattice rules for Korobov spaces, and we prove our main result for the median estimator in this setting. In Section 3, we do the same for high-order polynomial

lattice rules in Sobolev spaces. In Section 4, we report numerical experiments to support our theoretical findings.

2. Lattice rules for Korobov spaces.

- 2.1. **Definitions.** Lattice point sets are well suited for performing numerical integration of smooth periodic functions. A rank-1 lattice point set is defined as follows:
- DEFINITION 2.1 (rank-1 lattice point set). Let $N \geq 2$ be the number of points and $\mathbf{z} = (z_1, \dots, z_s) \in \{1, \dots, N-1\}^s$. The rank-1 lattice point set defined by N and the generating vector \mathbf{z} is

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$$P_{N,s,z} = \left\{ \left(\left\{ \frac{nz_1}{N} \right\}, \dots, \left\{ \frac{nz_s}{N} \right\} \right) \in [0,1)^s \mid n = 0, 1, \dots, N - 1 \right\},$$

- where $\{x\} := x \lfloor x \rfloor$ denotes the fractional part of a real $x \geq 0$. The QMC algorithm using $P_{N,s,z}$ as a point set is called the rank-1 lattice rule with generating vector z.
- Let $f:[0,1)^s\to\mathbb{R}$ be periodic with an absolutely convergent Fourier series

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathbb{Z}^s} \hat{f}(\boldsymbol{k}) \exp(2\pi i \boldsymbol{k} \cdot \boldsymbol{x}),$$

where the dot product \cdot denotes the usual inner product of two vectors on the Euclidean space \mathbb{R}^s and $\hat{f}(\mathbf{k})$ denotes the \mathbf{k} -th Fourier coefficient of f:

$$\hat{f}(\boldsymbol{k}) := \int_{[0,1)^s} f(\boldsymbol{x}) \exp\left(-2\pi i \boldsymbol{k} \cdot \boldsymbol{x}\right) d\boldsymbol{x}.$$

- Note that $\hat{f}(\mathbf{0})$ coincides with the integral $I_s(f)$. As a class of periodic functions, we consider the following weighted Korobov space.
- DEFINITION 2.2 (weighted Korobov space). Let $\alpha > 1/2$ and $\gamma = \{\gamma_u\}_{u \subseteq \{1,...,s\}}$ be a set of positive weights with $\gamma_0 = 1$. For a non-empty subset $u \subseteq \{1,...,s\}$ and a vector $\mathbf{k}_u \in (\mathbb{Z} \setminus \{0\})^{|u|}$, we denote by $(\mathbf{k}_u, \mathbf{0})$ the vector $\mathbf{h} \in \mathbb{Z}^s$ such that $h_j = k_j$ if $j \in u$ and $h_j = 0$ otherwise, and define

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$$r_{\alpha,\gamma}(\boldsymbol{k}_{u},\boldsymbol{0}) := \gamma_{u} \prod_{j \in u} \frac{1}{|k_{j}|^{\alpha}},$$

and set $r_{\alpha,\gamma}(\mathbf{0}) = 1$. The weighted Korobov space, denoted by $\mathcal{F}_{s,\alpha,\gamma}^{\text{kor}}$, is a reproducing kernel Hilbert space with reproducing kernel

$$K_{s,\alpha,oldsymbol{\gamma}}^{\mathrm{kor}}(oldsymbol{x},oldsymbol{y}) = \sum_{oldsymbol{k} \in \mathbb{Z}^s} (r_{lpha,oldsymbol{\gamma}}(oldsymbol{k})^2 \exp\left(2\pi i oldsymbol{k} \cdot (oldsymbol{x} - oldsymbol{y})
ight),$$

159 and inner product

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$$\langle f, g \rangle_{s, \alpha, \gamma}^{\text{kor}} = \sum_{\mathbf{k} \in \mathbb{Z}^s} \frac{\hat{f}(\mathbf{k}) \overline{\hat{g}(\mathbf{k})}}{(r_{\alpha, \gamma}(\mathbf{k}))^2}.$$

161 We denote the induced norm by $||f||_{s,\alpha,\gamma}^{\text{kor}} := \sqrt{\langle f, f \rangle_{s,\alpha,\gamma}^{\text{kor}}}$

One wishes to have a good generating vector z such that the worst-case error of the corresponding lattice rule for $\mathcal{F}_{s,\alpha,\gamma}^{\mathrm{kor}}$, defined by

$$e^{\operatorname{wor}}(Q_{P_{N,s,z}}; \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}}) := \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \leq 1}} |Q_{P_{N,s,z}}(f) - I_{s}(f)|,$$

- is small. No good explicit construction scheme for such a z is known for $s \ge 3$, so that we usually resort to a computer search algorithm as mentioned earlier. By restricting each z_i to be in the set
- 168 $\mathbb{U}_N := \{ 1 \le z \le N 1 \mid \gcd(z, N) = 1 \},$
- we ensure that each projection of $P_{N,s,z}$ on a single coordinate contains the N distinct values $\{0, 1/N, \dots, (N-1)/N\}$ (no superposed points). The CBC construction algorithm for a good generating vector z starts with $z_1 = 1$, then for $j = 2, \dots, s$ it searches for the best component z_j from the set \mathbb{U}_N while keeping the earlier compo-
- searches for the best component z_j from the set \mathbb{U}_N while keeping the earlier components z_1, \ldots, z_{j-1} unchanged.
- For our median QMC rank-1 lattice rule for weighted Korobov spaces, we select an independent random sample z_1, \ldots, z_r from the set \mathbb{U}_N^s , and we approximate $I_s(f)$ by the median

$$M_{N,s,r}(f) := \operatorname{median}\left(Q_{P_{N,s,z_1}}(f), \dots, Q_{P_{N,s,z_r}}(f)\right).$$

- Note that, for given z_1, \ldots, z_r , the index ℓ for which z_ℓ gives the median $M_{N,s,r}(f)$
- generally depends on f. The worst-case error in this case is the random variable

180 (2.1)
$$e^{\operatorname{wor}}(M_{N,s,r}; \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}}) := \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \le 1}} |M_{N,s,r}(f) - I_s(f)|.$$

- In this random expression, we assume that z_1, \ldots, z_r are first picked randomly, then f is taken as the worst-case function for the median, for these given z_1, \ldots, z_r .
- 2.2. Our main results on lattice rules for Korobov spaces. To prove our main result, we need a few more definitions.
- DEFINITION 2.3 (dual lattice). For $N \geq 2$ and $z \in \mathbb{U}_N^s$, the set

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$$P_{N,s,\boldsymbol{z}}^{\perp} := \{ \boldsymbol{k} \in \mathbb{Z}^s \mid \boldsymbol{k} \cdot \boldsymbol{z} \equiv 0 \pmod{N} \}$$

- is called the dual lattice of the rank-1 lattice point set $P_{N,s,z}$.
- The following character property of the rank-1 lattice rule is well-known, see for instance [5, Lemmas 4.2 and 4.3].
- LEMMA 2.4 (character property). For $N \geq 2$, $z \in \mathbb{U}_N^s$ and $k \in \mathbb{Z}^s$, we have

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$$\frac{1}{N} \sum_{\boldsymbol{x} \in P_{N,s,\boldsymbol{z}}} \exp\left(2\pi i \boldsymbol{k} \cdot \boldsymbol{x}\right) = \begin{cases} 1 & \text{if } \boldsymbol{k} \in P_{N,s,\boldsymbol{z}}^{\perp}, \\ 0 & \text{otherwise.} \end{cases}$$

As our first main result, we prove a probabilistic upper bound on the worst-case error of our median rank-1 lattice rule for weighted Korobov spaces.

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THEOREM 2.5. Let $N \geq 2$ be an integer, r > 0 be an odd integer, and z_1, \ldots, z_r be chosen independently and randomly from the set \mathbb{U}_N^s (with replacement). Then, for any $\alpha > 1/2$ and γ , the worst-case error of the median rule obeys the following bound:

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$$e^{\text{wor}}(M_{N,s,r}; \mathcal{F}_{s,\alpha,\boldsymbol{\gamma}}^{\text{kor}}) \leq \inf_{1/(2\alpha) < \lambda < 1} \left(\frac{1}{\eta \varphi(N)} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_u^{2\lambda} (2\zeta(2\alpha\lambda))^{|u|} \right)^{1/(2\lambda)}$$

199 with a probability of at least

$$1 - \binom{r}{(r+1)/2} \eta^{(r+1)/2},$$

for any $0 < \eta < 1$, where φ and ζ denote the Euler totient function and the Riemann zeta function, respectively.

We note that the result for r = 1, i.e., the case without taking the median, can be found, for instance, in [11, Theorem 2], and has been used together with a random choice of N in [20] to prove an improved rate of convergence of the randomized error.

The following inequality on medians is a key ingredient in the proof of the theorem. Although it can be regarded as a special case of Jensen's inequality on medians proven in [32], we give a short direct proof to make the paper more self-contained.

LEMMA 2.6. For any odd integer r and real numbers a_1, \ldots, a_r , it holds that

$$|\operatorname{median}(a_1,\ldots,a_r)| \leq \operatorname{median}(|a_1|,\ldots,|a_r|).$$

211 Proof. Let $a_m = \text{median}(a_1, \dots, a_r)$. If $a_m \ge 0$, then $|a_m| = a_m \le \text{median}(|a_1|, \dots, |a_r|)$. If $a_m < 0$, there is at least (r-1)/2 other a_ℓ 's for which $a_\ell \le a_m < 0$, so 213 $|a_\ell| \ge |a_m| > 0$. Then, $|\text{median}(a_1, \dots, a_r)| = |a_m| \le \text{median}(|a_1|, \dots, |a_r|)$.

We now prove our main result.

215 Proof of Theorem 2.5. Since any $f \in \mathcal{F}_{s,\alpha,\gamma}^{\text{kor}}$ has an absolutely convergent Fourier 216 series, by applying Lemma 2.4, Lemma 2.6 and the Cauchy–Schwarz inequality, it 217 holds for given z_1, \ldots, z_r that

$$e^{\operatorname{wor}}(M_{N,s,r}; \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}})$$

$$= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\operatorname{median}} \frac{1}{N} \sum_{\boldsymbol{x} \in P_{N,s,\boldsymbol{z}_{\ell}}} f(\boldsymbol{x}) - I(f) \right|$$

$$= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\operatorname{median}} \frac{1}{N} \sum_{\boldsymbol{x} \in P_{N,s,\boldsymbol{z}_{\ell}}} \sum_{\boldsymbol{k} \in \mathbb{Z}^{s}} \hat{f}(\boldsymbol{k}) \exp\left(2\pi i \boldsymbol{k} \cdot \boldsymbol{x}\right) - \hat{f}(\boldsymbol{0}) \right|$$

$$= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\operatorname{median}} \sum_{\boldsymbol{k} \in P_{N,s,\boldsymbol{z}_{\ell}}^{\perp} \setminus \{\boldsymbol{0}\}} \hat{f}(\boldsymbol{k}) \right|$$

$$= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\operatorname{median}} \sum_{\boldsymbol{k} \in P_{N,s,\boldsymbol{z}_{\ell}}^{\perp} \setminus \{\boldsymbol{0}\}} |\hat{f}(\boldsymbol{k})| \right|$$

$$= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\operatorname{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\operatorname{kor}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\operatorname{median}} \sum_{\boldsymbol{k} \in P_{N,s,\boldsymbol{z}_{\ell}}^{\perp} \setminus \{\boldsymbol{0}\}} |\hat{f}(\boldsymbol{k})| \right|$$

$$= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\text{kor}} \\ \|f\|_{s,\alpha,\gamma}^{\text{kor}} \le 1}} \operatorname{median}_{1 \le \ell \le r} \sum_{\mathbf{k} \in P_{N,s,\mathbf{z}_{\ell}}^{\perp} \setminus \{\mathbf{0}\}} \frac{|\hat{f}(\mathbf{k})|}{r_{\alpha,\gamma}(\mathbf{k})} r_{\alpha,\gamma}(\mathbf{k})$$

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$$\leq \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma}^{\text{kor}} \\ \|f\|^{\text{kor}} \\ \dots < 1}} \operatorname{median}_{1 \leq \ell \leq r} \left(\sum_{\boldsymbol{k} \in P_{N,s,\boldsymbol{z}_{\ell}}^{\perp} \setminus \{\boldsymbol{0}\}} \frac{|\hat{f}(\boldsymbol{k})|^{2}}{(r_{\alpha,\gamma}(\boldsymbol{k}))^{2}} \right)^{1/2}$$

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$$\times \left(\sum_{\boldsymbol{k} \in P_{N,s,\boldsymbol{z}_{\ell}} \setminus \{\boldsymbol{0}\}} (r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{k}))^{2}\right)^{1/2}$$

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$$\leq \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\boldsymbol{\gamma}}^{\text{kor}} \\ \|f\|_{s,\alpha,\boldsymbol{\gamma}}^{\text{kor}} \leq 1}} \left(\sum_{\boldsymbol{k} \in \mathbb{Z}^s \setminus \{\boldsymbol{0}\}} \frac{|\hat{f}(\boldsymbol{k})|^2}{(r_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{k}))^2} \right)^{1/2} \underset{1 \leq \ell \leq r}{\operatorname{median}} \mathcal{S}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}_{\ell})$$

227 (2.2)
$$\leq \underset{1 \leq \ell \leq r}{\operatorname{median}} S_{\alpha, \gamma}(z_{\ell}),$$

229 in which

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$$\mathcal{S}_{\alpha, \gamma}(\boldsymbol{z}) := \left(\sum_{\boldsymbol{k} \in P_{N, s, \boldsymbol{z}}^{\perp} \setminus \{\boldsymbol{0}\}} (r_{\alpha, \gamma}(\boldsymbol{k}))^2\right)^{1/2}.$$

For $1/(2\alpha) < \lambda \le 1$, by using the subadditivity

232 (2.3)
$$\left(\sum_{i} a_{i}\right)^{\lambda} \leq \sum_{i} a_{i}^{\lambda},$$

which holds for non-negative reals $a_1, a_2, \ldots > 0$, see [5, Theorem 2.2], and noting

that the cardinality of \mathbb{U}_N is equal to $\varphi(N)$, we have

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$$\frac{1}{(\varphi(N))^{s}} \sum_{\boldsymbol{z} \in \mathbb{U}_{N}^{s}} (S_{\alpha, \gamma}(\boldsymbol{z}))^{2\lambda}$$
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$$= \frac{1}{(\varphi(N))^{s}} \sum_{\boldsymbol{z} \in \mathbb{U}_{N}^{s}} \left(\sum_{\boldsymbol{k} \in P_{N, s, \boldsymbol{z}}^{\perp} \setminus \{\boldsymbol{0}\}} (r_{\alpha, \gamma}(\boldsymbol{k}))^{2} \right)^{\lambda}$$
238
$$\leq \frac{1}{(\varphi(N))^{s}} \sum_{\boldsymbol{z} \in \mathbb{U}_{N}^{s}} \sum_{\boldsymbol{k} \in P_{N, s, \boldsymbol{z}}^{\perp} \setminus \{\boldsymbol{0}\}} (r_{\alpha, \gamma}(\boldsymbol{k}))^{2\lambda}$$
239
$$= \sum_{\boldsymbol{k} \in \mathbb{Z}^{s} \setminus \{\boldsymbol{0}\}} (r_{\alpha, \gamma}(\boldsymbol{k}))^{2\lambda} \frac{1}{(\varphi(N))^{s}} \sum_{\boldsymbol{z} \in \mathbb{U}_{N}^{s}} \frac{1}{N} \sum_{\boldsymbol{x} \in P_{N, s, \boldsymbol{z}}} \exp(2\pi i \boldsymbol{k} \cdot \boldsymbol{x})$$

$$= \sum_{\boldsymbol{k} \in \mathbb{Z}^s \setminus \{\boldsymbol{0}\}} (r_{\alpha, \gamma}(\boldsymbol{k}))^{2\lambda} \frac{1}{(\varphi(N))^s} \sum_{\boldsymbol{z} \in \mathbb{U}_N^s} \frac{1}{N} \sum_{n=0}^{N-1} \exp(2\pi i n \boldsymbol{k} \cdot \boldsymbol{z}/N)$$

$$241 \qquad = \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_u^{2\lambda} \sum_{\mathbf{k}_u \in (\mathbb{Z} \setminus \{0\})^{|u|}} \frac{1}{(\varphi(N))^s} \sum_{\mathbf{z} \in \mathbb{U}_N^s} \frac{1}{N} \sum_{n=0}^{N-1} \prod_{j \in u} \frac{\exp(2\pi i n k_j z_j/N)}{|k_j|^{2\alpha\lambda}}$$

$$= \frac{1}{N} \sum_{n=0}^{N-1} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \frac{\gamma_u^{2\lambda}}{(\varphi(N))^{|u|}} \sum_{\boldsymbol{z}_u \in \mathbb{U}_N^{|u|}} \sum_{\boldsymbol{k}_u \in (\mathbb{Z} \setminus \{0\})^{|u|}} \prod_{j \in u} \frac{\exp(2\pi i n k_j z_j/N)}{|k_j|^{2\alpha\lambda}}$$

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$$= \frac{1}{N} \sum_{n=0}^{N-1} \sum_{\emptyset \neq u \subseteq \{1,...,s\}} \gamma_u^{2\lambda} (T_{2\alpha\lambda}(n,N))^{|u|},$$

245 where we write

$$T_{2\alpha\lambda}(n,N) := \frac{1}{\varphi(N)} \sum_{z \in \mathbb{U}_N} \sum_{k \in \mathbb{Z} \setminus \{0\}} \frac{\exp(2\pi i nkz/N)}{|k|^{2\alpha\lambda}}.$$

Since it follows from [22, Lemmas 2.1 & 2.2] that, for any positive integer d

$$\frac{1}{N} \sum_{n=0}^{N-1} (T_{2\alpha\lambda}(n,N))^d \le \frac{(2\zeta(2\alpha\lambda))^d}{\varphi(N)},$$

249 we obtain

$$\frac{1}{(\varphi(N))^{s}} \sum_{\boldsymbol{z} \in \mathbb{U}_{N}^{s}} (\mathcal{S}_{\alpha, \boldsymbol{\gamma}}(\boldsymbol{z}))^{2\lambda} \leq \sum_{\emptyset \neq u \subseteq \{1, \dots, s\}} \gamma_{u}^{2\lambda} \frac{1}{N} \sum_{n=0}^{N-1} (T_{2\alpha\lambda}(n, N))^{|u|}$$

$$\leq \frac{1}{\varphi(N)} \sum_{\emptyset \neq u \subseteq \{1, \dots, s\}} \gamma_{u}^{2\lambda} (2\zeta(2\alpha\lambda))^{|u|}.$$

This gives an upper bound on the average of $(S_{\alpha,\gamma}(z))^{2\lambda}$ over all of the admissible $z \in \mathbb{U}_N^s$, which holds for any $1/(2\alpha) < \lambda \leq 1$.

Then, Markov's inequality ensures that for any $0 < \eta < 1$, the probability of having

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$$\mathcal{S}_{\alpha,\gamma}(z) > \inf_{1/(2\alpha) < \lambda < 1} \left(\frac{1}{\eta \varphi(N)} \sum_{\emptyset \neq u \subseteq \{1, \dots, s\}} \gamma_u^{2\lambda} (2\zeta(2\alpha\lambda))^{|u|} \right)^{1/(2\lambda)} =: B(\alpha, \gamma)$$

258 is at most η for a random choice of $z \in \mathbb{U}_N^s$. For the median estimator $M_{N,s,r}$ to be

larger than this bound $B(\alpha, \gamma)$, we must have $S_{\alpha, \gamma}(z_{\ell}) > B(\alpha, \gamma)$ for at least (r+1)/2

vectors among z_1, \ldots, z_r . Taking the union bound on possible sets of (r+1)/2 vectors

with $S_{\alpha,\gamma}(z_{\ell}) > B(\alpha,\gamma)$, the probability that this happens is bounded above by

$$\binom{r}{(r+1)/2}\eta^{(r+1)/2}.$$

263 Combining this with the bound shown in (2.2) completes the proof.

Remark 2.7. One can easily prove by induction on k that $\binom{2k-1}{k} < 4^{k-1}$ for $k \ge 2$. Indeed, this is true for k = 2, and for $k \ge 2$, one has

$$\binom{2k+1}{k+1} = \frac{2(2k+1)}{(k+1)} \binom{2k-1}{k} < 4 \binom{2k-1}{k} < 4^k.$$

Then, for any odd r > 3, we have

268 (2.4)
$$\binom{r}{(r+1)/2} \eta^{(r+1)/2} < (4\eta)^{(r+1)/2}/4.$$

Thus, the probability given in Theorem 2.5 must be larger than $1 - (4\eta)^{(r+1)/2}/4$,

which converges to 1 exponentially fast as a function of r for $0 < \eta < 1/4$.

By taking $1/(2\lambda) = \alpha - \epsilon$ and $\rho = 4\eta$ and using the previous remark, we obtain 271 272 the following corollary as a simplified version of Theorem 2.5.

COROLLARY 2.8. For any odd $r \geq 3$, $\epsilon > 0$, and $0 < \rho < 1$, there is a constant 273 $c_1 = c_1(\alpha, \gamma, \epsilon) > 0$ (which depends on α , the γ_u 's and ϵ) such that 274

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$$\mathbb{P}\left[e^{\mathrm{wor}}(M_{N,s,r};\mathcal{F}_{s,\alpha,\boldsymbol{\gamma}}^{\mathrm{kor}}) \leq \frac{c_1(\alpha,\boldsymbol{\gamma},\epsilon)}{(\rho N)^{\alpha-\epsilon}}\right] \geq 1 - \rho^{(r+1)/2}/4.$$

Proof. For prime N, we have $\varphi(N) = N - 1$ and the corollary follows from 276 Theorem 2.5 and the bound (2.4) in Remark 2.7. For a general N, we know from [41, 277 278 Theorem 15] that

$$\frac{1}{\varphi(N)} \le \frac{1}{N} \left[e^C \log \log N + \frac{2.50637}{\log \log N} \right]$$

for any $N \geq 3$, where C = 0.57721... is the Euler's constant. From this, the proba-280 bilistic bound follows.

Remark 2.9. Under some additional conditions on the weights γ , this bound depends only polynomially on the dimension s, and can even be independent on the dimension s. We refer to [11, Theorem 3] for the case of general weights and [11, Theorem 4] for the case of product weights.

Remark 2.10. As mentioned in Section 1, our median rank-1 lattice rule is motivated by the observation that most of the possible generating vectors $z \in \mathbb{U}_N^s$ are a good choice, but the remaining ones are bad. To show this, let us first point out that $S_{\alpha,\gamma}(z)$ coincides with the worst-case error of the rank-1 lattice rule with the given z, see [7, Theorem 5.12]. As already seen in the proof of Theorem 2.5, a proportion of the generating vectors z which satisfy the bound of order $N^{-\alpha+\epsilon}$, i.e.,

$$\mathcal{S}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{z}) \leq \inf_{1/(2\alpha) < \lambda < 1} \left(\frac{1}{\eta \varphi(N)} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_u^{2\lambda} (2\zeta(2\alpha\lambda))^{|u|} \right)^{1/(2\lambda)},$$

is greater than or equal to $1-\eta$, for any $0<\eta<1$. On the other hand, the averaging argument in the proof of Theorem 2.5 with $\lambda = 1$ gives

$$\frac{1}{(\varphi(N))^s} \sum_{\boldsymbol{z} \in \mathbb{U}_N^s} (\mathcal{S}_{\alpha, \boldsymbol{\gamma}}(\boldsymbol{z}))^2 \leq \frac{1}{\varphi(N)} \sum_{\emptyset \neq u \subset \{1, \dots, s\}} \gamma_u^2 (2\zeta(2\alpha))^{|u|}.$$

This implies that, for each N, there exists a small, distinct set of "bad" generating 296 vectors whose $S_{\alpha,\gamma}(z)$ values are quite large so that the average of the squared worst-297 case error over all the possible generating vectors is merely of order N^{-1} . Such bad 298 vectors may include those with all components being the same. 299

Remark 2.11. Theorem 2.5 (or its corollary) gives a probabilistic error bound on the worst-case error (2.1), together with a lower bound on the probability that this error bound holds. The exact value of this probability depends on the probability distribution of $Q_{P_{N,s,z}}(f)$ when z is drawn uniformly from \mathbb{U}_N^s , and on the choices of r and of the other parameters in the error bound. To get some insight on how it behaves, we will simplify the setting slightly and look at a one-side error bound for a fixed f: we want to estimate the probability that the median $M_{N,s,r}(f)$ does not exceed some arbitrary constant y larger than the mean $I_s(f)$. Suppose that this 308 y is the q-quantile y_q of the distribution of $Q_{P_{N,s,z}}(f)$ for some $q \in (3/4, 1)$, i.e., 309 $q = \mathbb{P}[Q_{P_{N,s,z}}(f) \leq y_q]$. Then the median $M_{N,s,r}(f)$ is larger than y_q if and only if at 310 least (r+1)/2 values are larger than y_q , and the probability that this happens is

311 (2.5)
$$p_{+}(r,q) = \sum_{i=(r+1)/2}^{r} {r \choose i} (1-q)^{i} q^{r-i}.$$

Figure 1 plots $\log_{10} p_+(r,q)$ as a function of $r \in \{3,5,\ldots,49\}$ for q=0.5, q=0.75 and 313 q=0.9, respectively. We see that $p_+(r,0.5)=0.5$ for any r and that $p_+(r,q)\approx 10^{-\gamma r}$ where $\gamma \approx 0.071$ for q = 0.75 and $\gamma \approx 0.231$ for q = 0.9. These plots provide some 315 insight on the choice of r. In particular, for fixed q > 0.5, doubling r squares the probability $p_+(r,q)$. Suppose for example that we want $p_+(r,q) \leq 10^{-4}$, to have a 317 reasonable assurance that $M_{N,s,r}(f) \leq y_q$. The plot shows that the minimal value of 318 r for this is about r=13 for q=0.9, and about r=49 for q=0.75. For a given 319 $f \in \mathcal{F}_{s,\alpha,\gamma}^{\mathrm{kor}}$ and fixed N, a larger q means a larger y_q , but for a fixed q we can reduce y_q and bring it close to $I_s(f)$ by increasing N. From Theorem 2.5 with r=1 and 322 $\eta = 1 - q < 1/4$ (or its corollary with $\rho = 4(1 - q) < 1$), we have that $|y_q - I_s(f)|$ is $\mathcal{O}(N^{-\alpha+\epsilon})$. In summary, for a fixed q>3/4, we can decrease the error bound 323 by increasing N and increase the probability that the bound holds by increasing r. 324 We can also increase both q and N in a way y_q remains about the same; then the 325 same $p_+(r,q)$ can be obtained with a reduced r. What we just said is for the upper 326 bound $M_{N,s,r}(f) \leq y_q$, but essentially the same discussion can be made concerning the assurance that $M_{N,s,r}(f) > y_{1-q}$. In applications, the values of y_q and y_{1-q} are 328 unknown, but our reasoning suggests that a moderate value of r, say no more than 330 25, should be sufficient in practice, together with a large N (as large as the computing budget allows). The results of our numerical experiments support this. 331

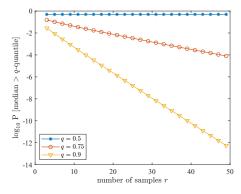


Fig. 1. Probability $p_+(r,q)$ (on a \log_{10} scale) as a function of r for q=0.5 (blue), q=0.75 (red) and q=0.9 (yellow).

Remark 2.12. It is known that rank-1 lattice rules also work for non-periodic functions by applying the tent transformation

$$\pi(x) = 1 - |2x - 1|$$

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component-wise to every point in the set $P_{N,s,z}$ [18, 8, 2, 16]. The same probabilistic upper bound, shown in Theorem 2.5, holds for the worst-case error of the median rule

built up of the tent-transformed rank-1 lattice rules in the so-called weighted halfperiod cosine spaces with any parameter α and weights γ . As shown in [8, Lemma 1], the half-period cosine space coincides with an unanchored Sobolev space with smoothness 1 when $\alpha = 1$.

3. High-order polynomial lattice rules for Sobolev spaces. We now consider high-order polynomial lattice point sets as defined in [9]. These point sets are well suited for performing numerical integration of smooth non-periodic functions. In what follows let b be a prime, and \mathbb{F}_b be the finite field of order b, which we identify with the set $\{0, 1, \ldots, b-1\}$. Let \mathbb{N} be the set of positive integers and $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$. For $k \in \mathbb{N}_0$ having the b-adic finite expansion $k = \kappa_0 + \kappa_1 b + \cdots$, we write $k(x) = \kappa_0 + \kappa_1 x + \cdots \in \mathbb{F}_b[x]$. With these ingredients, we have the following definition from [9].

DEFINITION 3.1 (high-order polynomial lattice point sets). Let $m, n \in \mathbb{N}$ with $m \leq n, p \in \mathbb{F}_b[x]$ with $\deg(p) = n$ and $\mathbf{q} = (q_1, \dots, q_s) \in (\mathbb{F}_b[x])^s$ with $\deg(q_j) < n$.

The high-order polynomial lattice point set defined by m, n, p and \mathbf{q} consists of $N = b^m$ points and is given by

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$$P_{m,n,s,p,q} = \left\{ \left(\nu_n \left(\frac{h(x)q_1(x)}{p(x)} \right), \dots, \nu_n \left(\frac{h(x)q_s(x)}{p(x)} \right) \right) \in [0,1)^s \mid h = 0, \dots, b^m - 1 \right\},$$

354 where $\nu_n : \mathbb{F}_b((x^{-1})) \to [0,1)$ is defined by

$$\nu_n\left(\sum_{i=w}^{\infty} \frac{a_i}{x^i}\right) := \sum_{i=\max(1,w)}^{n} \frac{a_i}{b^i}.$$

The QMC algorithm using $P_{m,n,s,p,q}$ as a point set is called the high-order polynomial lattice rule with modulus p and generating vector \mathbf{q} . The order of this rule is defined as $\lfloor n/m \rfloor$.

Typically, n will be a multiple of m. When n=m, this gives the digital net construction introduced in [34] and called polynomial lattice rule in [10]. Note that [25, 30] introduced the term "polynomial lattice rule" with a slightly different definition, in which the coordinates of the points have an infinite periodic expansion and the modulus p has degree m. The construction in Definition 3.1 essentially builds a polynomial lattice point set with p0 points and uses only the first p1 points.

Instead of the weighted Korobov space $\mathcal{F}_{s,\alpha,\gamma}^{\mathrm{kor}}$, we consider the following Sobolev-type Banach space as our target space for high-order polynomial lattice rules.

DEFINITION 3.2 (weighted Sobolev space). Let $\alpha \in \mathbb{N}$, $\alpha \geq 2$, $1 \leq q \leq \infty$ and let $\gamma = \{\gamma_u\}_{u \subseteq \{1,...,s\}}$ be a set of positive weights with $\gamma_{\emptyset} = 1$. The weighted Sobolev space, denoted by $\mathcal{F}_{s,\alpha,\gamma,q}^{\mathrm{sob}}$, is a Banach space consisting of non-periodic (in the sense of not necessarily periodic) smooth functions with the norm

$$||f||_{s,\alpha,\boldsymbol{\gamma},q}^{\text{sob}} :=$$

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$$\sup_{u \subseteq \{1,...,s\}} \gamma_u^{-1} \left(\sum_{v \subseteq u} \sum_{\tau_{u \setminus v} \in \{1,...,\alpha\}^{|u \setminus v|}} \int_{[0,1)^{|v|}} \left| \int_{[0,1)^{s-|v|}} f^{(\tau_{u \setminus v}, \boldsymbol{\alpha}_v, \boldsymbol{0})}(\boldsymbol{x}) \, \mathrm{d}\boldsymbol{x}_{-v} \right|^q \, \mathrm{d}\boldsymbol{x}_v \right)^{1/q},$$

where $(\boldsymbol{\tau}_{u\setminus v}, \boldsymbol{\alpha}_v, \mathbf{0})$ denotes the vector $\boldsymbol{h} \in \mathbb{N}_0^s$ such that $h_j = \tau_j$ if $j \in u \setminus v$, $h_j = \alpha$ if $j \in v$, and $h_j = 0$ otherwise, and $f^{(\boldsymbol{\tau}_{u\setminus v}, \boldsymbol{\alpha}_v, \mathbf{0})}(\boldsymbol{x})$ denotes the mixed derivative of order $(\boldsymbol{\tau}_{u\setminus v}, \boldsymbol{\alpha}_v, \mathbf{0})$ of f. Moreover, we write $\boldsymbol{x}_v = (x_j)_{j \in v}$ and $\boldsymbol{x}_{-v} = (x_j)_{j \in \{1, \dots, s\}\setminus v}$.

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This Sobolev space was introduced by [6] in the context of partial differential equations with random coefficients. (The original function space in [6] contains the additional parameter $r \in [1, \infty]$, and the definition of the norm has been corrected in https://arxiv.org/abs/1309.4624. In this paper we choose $r = \infty$, which makes the norm smallest over $r \in [1, \infty]$.) The parameter α determines the differentiability of the non-periodic functions. As for the rank-1 lattice rules for the weighted Korobov spaces, it is desirable to have good modulus p and generating vector q such that the worst-case error of the corresponding high-order polynomial lattice rule for $\mathcal{F}_{s,\alpha,\gamma}^{\text{sob}}$ is small. Originally in [6], interlaced polynomial lattice rules [13, 15] were used instead of high-order polynomial lattice rules, and it was shown that the worst-case error bound of order $N^{-\alpha+\epsilon}$ with arbitrarily small $\epsilon>0$ can be achieved by the CBC algorithm applied to interlaced polynomial lattice rules. The major advantage of interlaced polynomial lattice rules over high-order polynomial lattice rules lies in the construction cost for the CBC algorithm: for the product weights, constructing an interlaced rule requires $\mathcal{O}(\alpha s N \log N)$ operations with $\mathcal{O}(N)$ memory [13], whereas constructing a high-order rule require $\mathcal{O}(sN^{\alpha}\log N)$ operations with $\mathcal{O}(N^{\alpha})$ memory

However, interlaced polynomial lattice rules are not necessarily a better choice than high-order polynomial lattice rules. To construct an interlaced polynomial lattice rule, which relies on the digit interlacing method due to Dick [3], we must select an integer interlacing factor d, the construction cost increases linearly with d, and the resulting rule cannot exploit the smoothness of functions beyond d. This means that if $\alpha > d$, the worst-case error bound is only of order $N^{-d+\epsilon}$. High-order polynomial lattice rules do not explicitly require such a factor. We only need to specify the maximum precision n of the points. This n can be set as large as possible, for instance, with b=2, we can take n=53 for the double-precision floating-point format. This way, high-order polynomial lattice rules can be possibly made adaptive to the smoothness α of functions, addressing the drawback of interlaced polynomial lattice rules. Since we do not apply CBC in this paper, we prefer high-order rules over the interlaced ones.

In what follows, we assume that the polynomial p is irreducible and we write

$$G_n := \{ q \in \mathbb{F}_b[x] \mid q \neq 0 \quad \text{and} \quad \deg(q) < n \}.$$

Analogously to the rank-1 lattice case in Section 2, we consider the following median high-order polynomial lattice rule for weighted Sobolev spaces. For an odd integer r, we draw q_1, \ldots, q_r randomly and independently from the set G_n^s , and we approximate $I_s(f)$ by

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$$M_{m,n,s,p,r}(f) := \text{median} (Q_{P_{m,n,s,p,q_1}}(f), \dots, Q_{P_{m,n,s,p,q_r}}(f)).$$

413 The worst-case error is the random variable

414
$$e^{\operatorname{wor}}(M_{m,n,s,p,r}; \mathcal{F}_{s,\alpha,\gamma,q}^{\operatorname{sob}}) := \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\operatorname{sob}} \\ \|f\|_{s,\alpha,\gamma,q} \le 1}} |M_{m,n,s,p,r}(f) - I_s(f)|.$$

3.1. Main results for polynomial lattice point sets in Sobolev spaces. We first need a few definitions and lemmas.

Definition 3.3 (dual polynomial lattice). Let $m, n \in \mathbb{N}$ with $m \leq n, p \in \mathbb{F}_b[x]$ 418 with $\deg(p) = n$ and $q \in G_n^s$. For $k \in \mathbb{N}_0$ with the b-adic finite expansion k = 1 419 $\kappa_0 + \kappa_1 b + \cdots$, we define

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$$\operatorname{tr}_{n}(k) = \sum_{i=0}^{n-1} \kappa_{i} x^{i} \in G_{n} \cup \{0\}.$$

421 This operator is applied component-wise to a vector. Then the set

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$$P_{m,n,s,p,q}^{\perp} = \{ \mathbf{k} \in \mathbb{N}_0^s \mid \operatorname{tr}_n(\mathbf{k}) \cdot \mathbf{q} \equiv a \pmod{p} \quad \text{with } \deg(a) < n - m \},$$

- 423 is called the dual net of the high-order polynomial lattice point set $P_{m,n,s,p,q}$.
- DEFINITION 3.4 (Walsh functions). Let us write $\omega_b := \exp(2\pi i/b)$. For $k \in \mathbb{N}_0$,
- 425 we denote the b-adic expansion of k by $k = \kappa_0 + \kappa_1 b + \cdots$. The k-th Walsh function
- 426 $\operatorname{wal}_k \colon [0,1) \to \mathbb{C}$ is defined by

$$wal_k(x) := \omega_b^{\kappa_0 \xi_1 + \kappa_1 \xi_2 + \cdots},$$

- where the b-adic expansion of $x \in [0,1)$ is denoted by $x = \xi_1/b + \xi_2/b^2 + \cdots$, which is
- understood to be unique in the sense that infinitely many of the ξ_i are different from
- 430 b-1.

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- For $s \geq 2$ and $\mathbf{k} = (k_1, \dots, k_s) \in \mathbb{N}_0^s$, the s-dimensional \mathbf{k} -th Walsh function
- 432 wal_k: $[0,1)^s \to \mathbb{C}$ is defined by

$$\operatorname{wal}_{\boldsymbol{k}}(\boldsymbol{x}) := \prod_{j=1}^{s} \operatorname{wal}_{k_{j}}(x_{j}).$$

- 434 It is well-known that the system of Walsh functions is a complete orthogonal system in
- 435 $L_2([0,1)^s)$, see [10, Appendix A]. The following character property of the high-order
- polynomial lattice point set is analogous to what is stated in Lemma 2.4.
- LEMMA 3.5 (character property). For $m, n \in \mathbb{N}$ with $m \leq n$, $p \in \mathbb{F}_b[x]$ with
- 438 $\deg(p) = n \text{ and } \mathbf{q} \in G_n^s$, we have

$$\frac{1}{b^m} \sum_{\boldsymbol{x} \in P_{m,n,s,p,q}} \operatorname{wal}_{\boldsymbol{k}}(\boldsymbol{x}) = \begin{cases} 1 & \text{if } \boldsymbol{k} \in P_{m,n,s,p,q}^{\perp}, \\ 0 & \text{otherwise.} \end{cases}$$

For any $f \in \mathcal{F}^{\text{sob}}_{s,\alpha,\boldsymbol{\gamma},q}$, we have the following absolutely convergent Walsh series

$$f(\boldsymbol{x}) = \sum_{\boldsymbol{k} \in \mathbb{N}_0^s} \tilde{f}(\boldsymbol{k}) \operatorname{wal}_{\boldsymbol{k}}(\boldsymbol{x}),$$

where $\tilde{f}(\mathbf{k})$ denotes the \mathbf{k} -th Walsh coefficient of f:

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$$\tilde{f}(\mathbf{k}) := \int_{[0,1)^s} f(\mathbf{x}) \overline{\operatorname{wal}_{\mathbf{k}}(\mathbf{x})} \, \mathrm{d}\mathbf{x}.$$

- Note that $\tilde{f}(\mathbf{0})$ coincides with the integral $I_s(f)$. The following result on the decay of
- Walsh coefficients for $f \in \mathcal{F}^{\text{sob}}_{s,\alpha,\boldsymbol{\gamma},q}$ was shown in [6, Theorem 3.5].
- Lemma 3.6 (decay of Walsh coefficients). Let $\alpha \in \mathbb{N}$, $\alpha \geq 2$, $1 \leq q \leq \infty$ and
- 447 $\gamma = \{\gamma_u\}_{u \subset \{1,...,s\}}$ be a set of positive weights with $\gamma_\emptyset = 1$. For any $f \in \mathcal{F}^{\text{sob}}_{s,\alpha,\gamma,g}$, a
- 448 non-empty subset $u \subseteq \{1, ..., s\}$ and $\mathbf{k}_u \in \mathbb{N}^{|u|}$, it holds that

$$|\tilde{f}(\mathbf{k}_u, \mathbf{0})| \le ||f||_{s,\alpha,\gamma,q}^{\text{sob}} \gamma_u C_{\alpha}^{|u|} b^{-\mu_{\alpha}(\mathbf{k}_u)}$$

450 where

$$451 \quad C_{\alpha} := \left(1 + \frac{1}{b} + \frac{1}{b(b+1)}\right)^{\alpha - 2} \left(3 + \frac{2}{b} + \frac{2b+1}{b-1}\right) \max\left(\frac{2}{(2\sin\frac{\pi}{b})^{\alpha}}, \max_{1 \le \tau < \alpha} \frac{1}{(2\sin\frac{\pi}{b})^{\tau}}\right)$$

452 and $\mu_{\alpha}(\mathbf{k}_u) := \sum_{j \in u} \mu_{\alpha}(k_j)$, with

$$\mu_{\alpha}(k) = \sum_{i=1}^{\min(\alpha,c)} a_i$$

- 454 for $k \in \mathbb{N}$ whose b-adic expansion is given by $k = \kappa_1 b^{a_1-1} + \kappa_2 b^{a_2-1} + \cdots + \kappa_c b^{a_c-1}$
- 455 such that $c \geq 1, \kappa_1, \ldots, \kappa_c \in \{1, \ldots, b-1\}$ and $a_1 > \cdots > a_c$.
- As the second main result of this paper, we show a probabilistic upper bound on the worst-case error of our median high-order polynomial lattice rule for weighted Sobolev spaces.
- Theorem 3.7. Let $m, n \in \mathbb{N}$ with $m \leq n, p \in \mathbb{F}_b[x]$ be irreducible with $\deg(p) = 1$
- 460 n, r be odd and q_1, \ldots, q_r be chosen independently and randomly from the set G_n^s
- 461 Then, for any integer $\alpha \geq 2$ and γ , the worst-case error is bounded above by

$$462 \qquad e^{\text{wor}}(M_{m,n,s,p,r}; \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}}) \leq \inf_{1/\alpha < \lambda < 1} \left(\frac{2}{\eta(b^{\min(m,\lambda n)} - 1)} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_u^{\lambda} C_{\alpha}^{\lambda|u|} A_{\alpha,\lambda}^{|u|} \right)^{1/\lambda}$$

463 with a probability of at least

$$1 - \binom{r}{(r+1)/2} \eta^{(r+1)/2},$$

465 for any $0 < \eta < 1$, where we write

466 (3.1)
$$A_{\alpha,\lambda} = \sum_{\tau=1}^{\alpha-1} \prod_{i=1}^{\tau} \frac{b-1}{b^{\lambda i}-1} + \frac{b^{\lambda \alpha}-1}{b^{\lambda \alpha}-b} \prod_{i=1}^{\alpha} \frac{b-1}{b^{\lambda i}-1}.$$

468 *Proof.* Throughout this proof, we write

$$\tilde{r}_{\alpha,\gamma}(\boldsymbol{k}_u,\boldsymbol{0}) = \gamma_u C_{\alpha}^{|u|} b^{-\mu_{\alpha}(\boldsymbol{k}_u)},$$

- 470 for a non-empty subset $u \subseteq \{1, \ldots, s\}$ and $k_u \in \mathbb{N}^{|u|}$. Since any $f \in \mathcal{F}^{\text{sob}}_{s,\alpha,\boldsymbol{\gamma},q}$ has
- an absolutely convergent Walsh series, by applying Lemma 3.5, Lemma 2.6, Hölder's
- 472 inequality and Lemma 3.6 in this order, it holds that

$$\begin{aligned}
&e^{\text{wor}}(M_{m,n,s,p,r}; \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}}) \\
&= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}}, \\ \|f\|_{s,\alpha,\gamma,q}^{\text{sob}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\text{median}} \frac{1}{b^m} \sum_{\boldsymbol{x} \in P_{m,n,s,p,q_{\ell}}} f(\boldsymbol{x}) - I(f) \right| \\
&= \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}}, \\ \|f\|_{s,\alpha,\gamma,q}^{\text{sob}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\text{median}} \frac{1}{b^m} \sum_{\boldsymbol{x} \in P_{m,n,s,p,q_{\ell}}} \sum_{\boldsymbol{k} \in \mathbb{N}_0^s} \tilde{f}(\boldsymbol{k}) \operatorname{wal}_{\boldsymbol{k}}(\boldsymbol{x}) - \tilde{f}(\boldsymbol{0}) \right| \end{aligned}$$

$$476 = \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}} \\ \|f\|_{s,\alpha,\gamma,q}^{\text{sob}} \leq 1}} \left| \underset{1 \leq \ell \leq r}{\operatorname{median}} \sum_{\mathbf{k} \in P_{m,n,s,p,q_{\ell}}^{\perp} \setminus \{\mathbf{0}\}} \tilde{f}(\mathbf{k}) \right| \\
477 \leq \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}} \\ \|f\|_{s,\alpha,\gamma,q}^{\text{sob}} \leq 1}} \max_{1 \leq \ell \leq r} \sum_{\mathbf{k} \in P_{m,n,s,p,q_{\ell}}^{\perp} \setminus \{\mathbf{0}\}} \frac{|\tilde{f}(\mathbf{k})|}{\tilde{r}_{\alpha,\gamma}(\mathbf{k})} \tilde{r}_{\alpha,\gamma}(\mathbf{k}) \\
478 \leq \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}} \\ \|f\|_{s,\alpha,\gamma,q}^{\text{sob}} \leq 1}} \max_{1 \leq \ell \leq r} \left(\sup_{\mathbf{k} \in P_{m,n,s,p,q_{\ell}}^{\perp} \setminus \{\mathbf{0}\}} \frac{|\tilde{f}(\mathbf{k})|}{\tilde{r}_{\alpha,\gamma}(\mathbf{k})} \right) \left(\sum_{\mathbf{k} \in P_{m,n,s,p,q_{\ell}}^{\perp} \setminus \{\mathbf{0}\}} \tilde{r}_{\alpha,\gamma}(\mathbf{k}) \right) \\
479 \leq \sup_{\substack{f \in \mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}} \\ \|f\|_{s,\alpha,\gamma,q}^{\text{sob}} \leq 1}} \left(\sup_{\mathbf{k} \in \mathbb{N}_{0}^{s} \setminus \{\mathbf{0}\}} \frac{|\tilde{f}(\mathbf{k})|}{\tilde{r}_{\alpha,\gamma}(\mathbf{k})} \right) \max_{1 \leq \ell \leq r} \tilde{S}_{\alpha,\gamma,p}(q_{\ell}) \\
480 (3.2) \leq \underset{1 \leq \ell \leq r}{\operatorname{median}} \tilde{S}_{\alpha,\gamma,p}(q_{\ell}),$$

482 where

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$$\tilde{\mathcal{S}}_{\alpha,\gamma,p}(q) = \sum_{\boldsymbol{k} \in P_{m,n,s,p,q}^{\perp} \setminus \{\boldsymbol{0}\}} \tilde{r}_{\alpha,\gamma}(\boldsymbol{k}).$$

484 For $1/(\alpha) < \lambda \le 1$, by using the subadditivity (2.3), we have

485
$$\frac{1}{|G_n|^s} \sum_{\boldsymbol{q} \in G_n^s} (\tilde{S}_{\alpha,\boldsymbol{\gamma},p}(\boldsymbol{q}))^{\lambda} = \frac{1}{(b^n - 1)^s} \sum_{\boldsymbol{q} \in G_n^s} \left(\sum_{\boldsymbol{k} \in P_{m,n,s,p,\boldsymbol{q}_{\ell}}^{\perp} \setminus \{\boldsymbol{0}\}} \tilde{r}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{k}) \right)^{\lambda}$$

$$\leq \frac{1}{(b^n - 1)^s} \sum_{\boldsymbol{q} \in G_n^s} \sum_{\boldsymbol{k} \in P_{m,n,s,p,\boldsymbol{q}_{\ell}}^{\perp} \setminus \{\boldsymbol{0}\}} (\tilde{r}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{k}))^{\lambda}$$

$$= \sum_{\boldsymbol{k} \in \mathbb{N}_0^s \setminus \{\boldsymbol{0}\}} (\tilde{r}_{\alpha,\boldsymbol{\gamma}}(\boldsymbol{k}))^{\lambda} \frac{1}{(b^n - 1)^s} \sum_{\substack{\boldsymbol{q} \in G_n^s \\ \text{tr}_n(\boldsymbol{k}) \cdot \boldsymbol{q} \equiv a \pmod{p} \\ \text{deg}(a) < n - m}} 1.$$

489 If $p \mid \operatorname{tr}_n(\mathbf{k})$, the condition $\operatorname{tr}_n(\mathbf{k}) \cdot \mathbf{q} \equiv a \pmod{p}$ trivially holds with a = 0 for all 490 $\mathbf{q} \in G_n^s$. Otherwise if $p \nmid \operatorname{tr}_n(\mathbf{k})$, i.e., if there exists a non-empty subset $u \subseteq \{1, \ldots, s\}$ 491 such that $p \nmid \operatorname{tr}_n(\mathbf{k}_j)$ for all $j \in u$ and $p \mid \operatorname{tr}_n(\mathbf{k}_j)$ for $j \not\in u$, the condition $\operatorname{tr}_n(\mathbf{k}) \cdot \mathbf{q} \equiv a$ 492 (mod p) is equivalent to $\operatorname{tr}_n(\mathbf{k}_u) \cdot \mathbf{q}_u \equiv a \pmod{p}$, which itself is equivalent to

$$\operatorname{tr}_n(k_j)q_j \equiv a - \operatorname{tr}_n(\boldsymbol{k}_{u\setminus\{j\}}) \cdot \boldsymbol{q}_{u\setminus\{j\}} \pmod{p},$$

for any $j \in u$. As we have $p \nmid \operatorname{tr}_n(k_j)$ and we assume that p is irreducible, there exists at most one $q_j \in G_n$ which satisfies the above equality for each $a \in \mathbb{F}_b[x]$ with $\deg(a) < n - m$ and $q_{u \setminus \{j\}} \in G_n^{|u|-1}$. Therefore, the number of $\mathbf{q} \in G_n^s$ which satisfy $p \nmid \operatorname{tr}_n(\mathbf{k})$ and $\operatorname{tr}_n(\mathbf{k}) \cdot \mathbf{q} \equiv a \pmod{p}$ with $\deg(a) < n - m$ is bounded above by the product of the number of possible choices for $a \in \mathbb{F}_b[x]$, which is b^{n-m} , and the number of possible choices for $q_{\{1,\ldots,s\}\setminus\{j\}}$, which is $(b^n-1)^{s-1}$. Thus it follows that

$$500 \qquad \frac{1}{|G_n|^s} \sum_{\boldsymbol{q} \in G_s^s} (\tilde{\mathcal{S}}_{\alpha, \boldsymbol{\gamma}, p}(\boldsymbol{q}))^{\lambda}$$

$$501 \qquad \leq \sum_{\substack{\mathbf{k} \in \mathbb{N}_{0}^{s} \setminus \{\mathbf{0}\}\\p \mid \operatorname{tr}_{n}(\mathbf{k})}} (\tilde{r}_{\alpha,\gamma}(\mathbf{k}))^{\lambda} + \sum_{\substack{\mathbf{k} \in \mathbb{N}_{0}^{s} \setminus \{\mathbf{0}\}\\p \nmid \operatorname{tr}_{n}(\mathbf{k})}} (\tilde{r}_{\alpha,\gamma}(\mathbf{k}))^{\lambda} \frac{b^{n-m}(b^{n}-1)^{s-1}}{(b^{n}-1)^{s}}$$

$$502 \qquad \leq \sum_{\substack{\mathbf{k} \in \mathbb{N}_{0}^{s} \setminus \{\mathbf{0}\}\\p \nmid \operatorname{tr}_{n}(\mathbf{k})}} (\tilde{r}_{\alpha,\gamma}(b^{n}\mathbf{k}))^{\lambda} + \frac{1}{b^{m}-1} \sum_{\substack{\mathbf{k} \in \mathbb{N}_{0}^{s} \setminus \{\mathbf{0}\}\\p \nmid \operatorname{tr}_{n}(\mathbf{k})}} (\tilde{r}_{\alpha,\gamma}(b^{n}\mathbf{k}_{u},\mathbf{0}))^{\lambda} + \frac{1}{b^{m}-1} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \sum_{\substack{\mathbf{k}_{u} \in \mathbb{N}^{|u|}\\p \mid u \mid}} (\tilde{r}_{\alpha,\gamma}(\mathbf{k}_{u},\mathbf{0}))^{\lambda}$$

$$504 \qquad = \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_{u}^{\lambda} C_{\alpha}^{\lambda|u|} \left(\sum_{k \in \mathbb{N}} b^{-\lambda\mu_{\alpha}(b^{n}k)}\right)^{|u|}$$

$$505 \qquad + \frac{1}{b^{m}-1} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_{u}^{\lambda} C_{\alpha}^{\lambda|u|} \left(\sum_{k \in \mathbb{N}} b^{-\lambda\mu_{\alpha}(k)}\right)^{|u|}$$

$$506 \qquad \leq \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_{u}^{\lambda} \frac{C_{\alpha}^{\lambda|u|} A_{\alpha,\lambda}^{|u|}}{b^{\lambda n|u|}} + \frac{1}{b^{m}-1} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_{u}^{\lambda} C_{\alpha}^{\lambda|u|} A_{\alpha,\lambda}^{|u|}$$

 $\begin{array}{ll}
507 & \leq \frac{2}{b^{\min(m,\lambda n)} - 1} \sum_{\emptyset \neq u \subseteq \{1,\dots,s\}} \gamma_u^{\lambda} C_{\alpha}^{\lambda |u|} A_{\alpha,\lambda}^{|u|}, \\
508 & \end{array}$

where we have used the results of [14, Lemma 7] on the sums of $b^{-\lambda\mu_{\alpha}(k)}$ and $b^{-\lambda\mu_{\alpha}(b^n k)}$ in the third inequality, which involve $A_{\alpha,\lambda}$ given in (3.1). This gives a bound on the average of $(\tilde{\mathcal{S}}_{\alpha,\gamma,p}(q))^{\lambda}$ which holds for any $1/\alpha < \lambda \leq 1$.

Then, Markov's inequality ensures that, for any $0 < \eta < 1$, the event

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$$\tilde{\mathcal{S}}_{\alpha,\gamma,p}(\boldsymbol{q}) > \inf_{1/\alpha < \lambda < 1} \left(\frac{2}{\eta(b^{\min(m,\lambda n)} - 1)} \sum_{\emptyset \neq u \subset \{1,\dots,s\}} \gamma_u^{\lambda} C_{\alpha}^{\lambda|u|} A_{\alpha,\lambda}^{|u|} \right)^{1/\lambda} =: \tilde{B}(\alpha, \boldsymbol{\gamma})$$

happens with a probability of at most η under a random choice of $\mathbf{q} \in G_n^s$. For the median estimator $M_{m,n,s,p,r}$ to be larger than this bound $\tilde{B}(\alpha, \gamma)$, we must have $\tilde{S}_{\alpha,\gamma}(\mathbf{q}_{\ell}) > \tilde{B}(\alpha,\gamma)$ for at least (r+1)/2 vectors among $\mathbf{q}_1, \ldots, \mathbf{q}_r$. The probability

that this happens is bounded above by

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$$\binom{r}{(r+1)/2}\eta^{(r+1)/2}.$$

519 Combining this with the bound shown in (3.2) completes the proof.

As pointed out in [6, Section 3.1], $\alpha \geq 2$ is required to ensure the convergence of the infinite sum

$$\sum_{{\bm k}\in P_{m,n,s,p,{\bm q}}^\perp\backslash\{{\bm 0}\}}b^{-\mu_\alpha({\bm k})},$$

523 for any irreducible p and $q \in G_n^s$. Thus, the case $\alpha = 1$ is not covered by our result.

Using Remark 2.7, we obtain the following corollary:

COROLLARY 3.8. Let $\alpha \geq 2$, γ be a set of weights, and $n \geq \alpha m = \alpha \log_b N$. Then for any odd $r \geq 3$, $\epsilon > 0$ and $0 < \rho < 1$, there is a constant $c_1 = c_1(\alpha, \gamma, \epsilon) > 0$ (which depends on α , the γ_u 's and ϵ) such that

$$\mathbb{P}\left[e^{\text{wor}}(M_{m,n,s,p,r}; \mathcal{F}_{s,\alpha,\gamma}^{\text{sob}}) \le \frac{c_1(\alpha, \gamma, \epsilon)}{(\rho N)^{\alpha - \epsilon}}\right] \ge 1 - \rho^{(r+1)/2}/4.$$

Proof. Take $1/\lambda = \alpha - \epsilon$. Under the assumption on n, we have $n \ge \alpha m > m/\lambda$ and then $(b^{\min(m,\lambda n)})^{-1/\lambda} = b^{-\min(m/\lambda,n)} = N^{-1/\lambda} = N^{-\alpha+\epsilon}$. Then the result follows from Theorem 3.7 and the bound (2.4) in Remark 2.7.

Thus, provided that we take n large enough, we get a convergence rate of almost $\mathcal{O}(N^{-\alpha})$ (with high probability) for any $\alpha \geq 2$. In other words, our median high-order polynomial lattice rule exploits the smoothness of functions adaptively. Note that Remark 2.11 also applies here.

4. Numerical experiments. We conclude this paper with numerical experiments both for rank-1 lattice rules and high-order polynomial lattice rules. The goal is to illustrate how the worst-case error for the median rule truly behaves on some concrete examples. In particular, we want to illustrate the fact that most of the possible generating vectors are a good choice, while a small minority are bad.

4.1. Lattice rules for periodic functions.

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EXAMPLE 4.1. For our first example, we consider a weighted Korobov space with integer smoothness parameter $\alpha \geq 1$ and product weights $\gamma_u = \prod_{j \in u} \gamma_j$. The worst-case error of the rank-1 lattice rule with generating vector \boldsymbol{z} for that space has the explicit form

$$S_{\alpha,\gamma}(z) = \left(-1 + \frac{1}{N} \sum_{x \in P_{N,s,z}} \prod_{j=1}^{s} \left[1 + \gamma_j^2 \frac{(-1)^{\alpha+1} (2\pi)^{2\alpha}}{(2\alpha)!} B_{2\alpha}(x_j)\right]\right)^{1/2},$$

where $B_{2\alpha}$ denotes the Bernoulli polynomial of degree 2α ; see [27] and [7, Section 5]. In this artificial simple case, we know the exact optimal weights that must be taken in a CBC search for z, so we can compare the median estimator with the best possible case of a CBC search.

We take two primes N=251 and N=2039, both for s=50 dimensions, with $\alpha = 2$ and $\gamma_j = 1/j^3$. For each of those N, we drew 10^5 generating vectors z randomly and uniformly from $\{1,\ldots,N-1\}^s$, and computed $\mathcal{S}_{\alpha,\gamma}(z)$ for each. The left panels of Figure 2 show a histogram of the 10^5 realizations of $\log_2 S_{\alpha,\gamma}(z)$ for each of these two cases. Each histogram provides a good estimate of the true distribution of $\log_2 S_{\alpha,\gamma}(z)$, which is a discrete distribution because z is drawn from a finite set. Interestingly, the distributions are very asymmetric and are far from smooth on the right side: some rectangles are very high while others are zero in the same area. The largest observed values are -2.4353 for N=251 and -2.4967 for N=2039. We can estimate from this data the q-quantiles y_q of the distribution of $S_{\alpha,\gamma}(z)$, similar to those of the distribution of $Q_{P_{N,s,z}}(f)$ in Remark 2.11. For q=0.75, the corresponding empirical q-quantiles are -8.3907 for N=251 and -12.0306 for N=2039, while, for q = 0.9, they are -7.0975 for N = 251 and -10.3101 for N = 2039. These quantiles are much less than the worst observed values. These empirical results agree with the fact that only a very small proportion of the vectors z are bad. Suppose we draw r random realizations of z and want the median of the r corresponding values of $S_{\alpha,\gamma}(z)$ to be larger than $y=10^{-3}\approx 2^{-10}$ with a probability smaller than 10^{-4} . For N=2039 this y equals y_q for $q\approx 0.9$, and Figure 1 shows that we can achieve approximately the target probability of 10^{-4} with r=13. For a larger N, the required r is even smaller. Note that for N=251, $y_p=2^{-10}$ corresponds to some q<0.5, for which the target probability of 10^{-4} cannot be achieved even for a very large r, as shown in Figure 1.

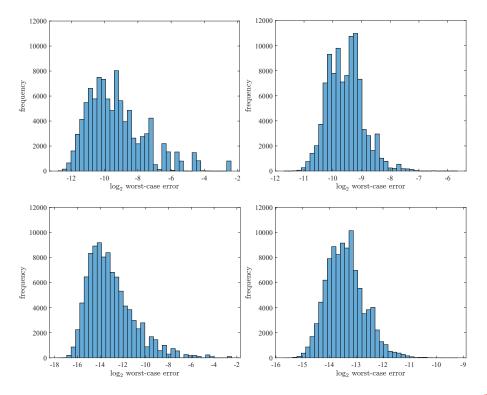


FIG. 2. Histograms of the \log_2 of the worst-case error $S_{\alpha,\gamma}(z)$ with $\alpha=2$ and $\gamma_j=1/j^3$ for rank-1 lattice rules with randomly chosen generating vectors with N=251 (upper panels) and N=2039 (lower panels). The left panels are for a single choice (r=1), while for the right panels we take the median of the worst-case error for rank-1 lattice rules with r=11 randomly chosen generating vectors.

For the remainder of our experiments reported in this paper, we took r=11. The right panels of Figure 2 show histograms of 10^5 independent realizations of $\log_2[\mathrm{median}(\mathcal{S}_{\alpha,\gamma}(z_1),\ldots,\mathcal{S}_{\alpha,\gamma}(z_r))]$ for randomly chosen z_1,\ldots,z_r with r=11, corresponding to the cases N=251 and N=2039. We see that the distributions have much less variance and are more symmetric than for a single random z, confirming the fact that taking the median successfully filters (adaptively) the bad vector generators. Recall that the standard deviation of the empirical median as a function of r generally decreases as $\mathcal{O}(r^{-1/2})$. That is, increasing r decreases the noise rather slowly. For the following examples, we made additional experiments with r=31 to see if it would make the error plots less noisy, and we did not see much visible difference.

EXAMPLE 4.2. For our second example, we perform a numerical integration of the smooth, periodic function

$$f_{\beta, \boldsymbol{\omega}}^{\mathrm{per}}(\boldsymbol{x}) = \prod_{j=1}^{s} \left[1 + \omega_{j} \left(g_{\beta}(x_{j}) - 1\right)\right],$$

with parameters β and ω_i , where the univariate function $g_{\beta}:[0,1]\to\mathbb{R}$ is defined by

$$g_{\beta}(x) = (2\beta + 1) \binom{2\beta}{\beta} x^{\beta} (1 - x)^{\beta}.$$

Note that $I_s(f_{\beta,\omega}^{\text{per}}) = 1$. The function g_{β} has been used for periodization of non-periodic functions, and our test function $f_{\beta,\omega}^{\text{per}}$ belongs to the Korobov space with $\alpha = \beta$ when β is a positive integer, see [7, Section 5.10]. In what follows, we take s = 50 and consider the four cases that correspond to $\beta = 2$ or $\beta = 5$, and $\omega_j = 1/j^{\beta+1}$ or $\omega_j = 1/(s-j+1)^{\beta+1}$. We compare our median lattice rule with r = 11, a QMC rule using non-randomized Sobol' points provided by MATLAB, and the rank-1 lattice rule with generating vector constructed by the fast CBC algorithm with $S_{\alpha,\gamma}(z)$ as a criterion, with $\alpha = 2$ and the product weights $\gamma_j = 1/j^3$. These weights are not optimal, but they are a good heuristic choice when $\omega_j = 1/j^{\beta+1}$. When $\omega_j = 1/(s-j+1)^{\beta+1}$, on the other hand, the weights decrease in the opposite direction as they should: they are very large for the unimportant coordinates and small for the important ones. We do this to show how badly the CBC construction method can work when we have the wrong weights, whereas the median estimator does not need any knowledge about the weights to perform well. We choose N to be a power of 2 for Sobol' points and to be a prime close to a power of 2 for lattice point sets.

The results for the four cases are shown in the corresponding panels of Figure 3. Both our median lattice rule and the rank-1 lattice rule constructed by the CBC algorithm can exploit the periodicity of the integrand and achieve a higher-order rate of convergence than $\mathcal{O}(1/N)$. With a good choice of the weights in the CBC algorithm, the resulting rank-1 lattice rule performs better than our median lattice rule, as shown in the left panels. However, as the right panels clearly depict, if the relative importance of each of individual variables is not correctly specified, the performance of the rank-1 lattice rule with the CBC algorithm can deteriorate and even become inferior to the QMC rule using the Sobol' points when N is not large. In contrast, our median lattice rule performs quite stably regardless of smoothness and weights.

To show that our median lattice rule performs well for functions of non-product forms, let us consider the additional test functions given by

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$$f_{\beta}^{\text{per,cyc}}(\boldsymbol{x}) = \frac{1}{5} \sum_{\ell=1}^{5} \prod_{j=1}^{5/5} g_{\beta}(x_{j+s(\ell-1)/5})$$
 and $f_{\beta}^{\text{per,mod}}(\boldsymbol{x}) = \frac{1}{5} \sum_{\ell=1}^{5} \prod_{j=1}^{s/5} g_{\beta}(x_{\ell+5(j-1)}),$

respectively, with $\beta=5$ and s=20. We have that $I_s(f_{\beta}^{\rm per,cyc})=I_s(f_{\beta}^{\rm per,mod})=1$ and these two integrands belong to the Korobov space with $\alpha=\beta$. The results for the two integrands are shown in the corresponding panels of Figure 4. For large N, both our median lattice rule and the rank-1 lattice rule constructed by the CBC algorithm are superior to the QMC rule using the Sobol' points. Although the difference between $f_{\beta}^{\rm per,cyc}$ and $f_{\beta}^{\rm per,mod}$ lies only in the ordering of variables, the convergence behavior of the rank-1 lattice rule constructed by the CBC algorithm is not consistent for these functions and a strange zig-zag pattern shows up for $f_{\beta}^{\rm per,mod}$. On the contrary, our median lattice rule is not subject to the difference between the ordering of variables and performs almost equivalently.

4.2. High-order polynomial lattice rules for non-periodic functions. Our next examples concern high-order polynomial lattice rules. Here we fix the precision to n = 52 and always use the primitive polynomial $p(x) = x^{52} + x^3 + 1$, found in [17], as the modulus of the polynomial lattice point sets.

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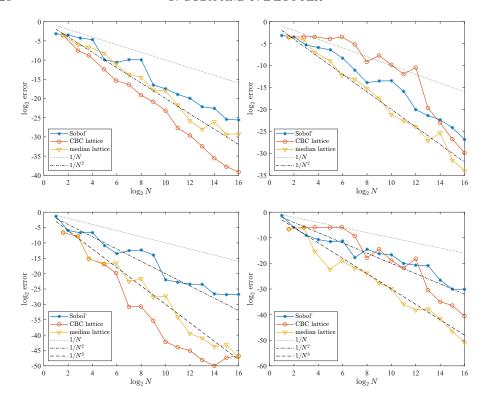


FIG. 3. Comparison of the integration error by our median lattice rule (yellow), QMC rule using Sobol' points (blue), and rank-1 lattice rule with the fast CBC algorithm (orange). The results are shown for the test function $f_{\beta,\omega}^{\rm per}$ with the choices $\beta=2$ and $\omega_j=1/j^3$ (upper left), $\beta=2$ and $\omega_j=1/(s-j+1)^3$ (upper right), $\beta=5$ and $\omega_j=1/j^6$ (lower left), and $\beta=5$ and $\omega_j=1/(s-j+1)^6$ (lower right).

EXAMPLE 4.3. We first consider the two following one-dimensional test functions:

$$f_1^{\text{nonper}}(x) = x^3(1/4 + \log x)$$
 and $f_2^{\text{nonper}}(x) = xe^{x/4}$.

We can see that the third derivative of f_1^{nonper} is in $L_q([0,1))$ for any $1 \leq q < \infty$, whereas the fourth derivative is not in $L_1([0,1))$, implying that $f_1^{\text{nonper}} \in \mathcal{F}_{1,3,\gamma,q}^{\text{sob}}$ but $f_1^{\text{nonper}} \notin \mathcal{F}_{1,4,\gamma,1}^{\text{sob}}$. Thus f_1^{nonper} has a finite smoothness. On the other hand, f_2^{nonper} is obviously infinitely differentiable, so that $f_2^{\text{nonper}} \in \mathcal{F}_{1,\alpha,\gamma,q}^{\text{sob}}$ for any $\alpha \geq 2$ and $1 \leq q \leq \infty$. Note that $I_1(f_1^{\text{nonper}}) = 0$ and $I_1(f_2^{\text{nonper}}) = 16 - 12e^{1/4}$. We compare our median high-order polynomial lattice rule with r = 11 and QMC rules using order 2 and order 3 Sobol' points constructed by the interlacing procedure of [3], with the direction numbers provided in MATLAB. To construct a Sobol' point set of order d by interlacing, we first construct a ds-dimensional Sobol point set with 2^m points (with s = 1 in this case) and then apply the digit interlacing procedure defined in [3] to obtain the digits of the s-dimensional points. This procedure extracts the first m digits of the ds-dimensional points and reorders them in a special way to obtain the first dm digits of the s-dimensional points.

The results for the two one-dimensional functions are shown in Figure 5, respectively. As we can see from the result for f_1^{nonper} , the QMC rule using order 2 Sobol' points cannot fully exploit the smoothness of the function and the error decays at the

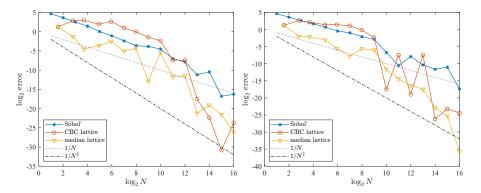


FIG. 4. Comparison of the integration error by our median lattice rule (yellow), QMC rule using Sobol' points (blue), and rank-1 lattice rule with the fast CBC algorithm (orange). The results are shown for the test functions $f_{\beta}^{\text{per,cyc}}$ (left) and $f_{\beta}^{\text{per,mod}}$ (right) with the choices $\beta = 5$ and s = 20.

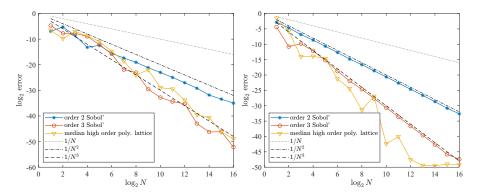


FIG. 5. Comparison of the one-dimensional integration error by our median high-order polynomial lattice rule (yellow), QMC rules using order 2 Sobol' points (blue) and order 3 Sobol' points (orange). The results are shown for the test functions $f_1^{\rm nonper}$ (left) and $f_2^{\rm nonper}$ (right), respectively.

rate of N^{-2} . On the other hand, the QMC rule using order 3 Sobol' points and our median high-order polynomial lattice rule can exploit the smoothness and achieves the convergence rate of N^{-3} . For the infinitely differentiable function f_2^{nonper} , the plot suggests that our median high-order polynomial lattice rule may converge even faster than N^{-3} . These numerical results show the major advantage of our proposed rule in terms of adaptivity in smoothness.

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EXAMPLE 4.4. Finally, we consider the two multivariate non-periodic test functions

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$$f_{3,\boldsymbol{\omega}}^{\text{nonper}}(\boldsymbol{x}) = \exp\left(-\sum_{j=1}^{s} \omega_j x_j\right)$$
 and $f_{3,\boldsymbol{\omega},\text{flip}}^{\text{nonper}}(\boldsymbol{x}) = \exp\left(-\sum_{j=1}^{s} \omega_j x_{s-j+1}\right)$,

with s=10 and $\omega_j=1/(4j^4)$. It is obvious that both $f_{3,\omega}^{\text{nonper}}$ and $f_{3,\omega,\text{flip}}^{\text{nonper}}$ are infinitely differentiable and belong to $\mathcal{F}_{s,\alpha,\gamma,q}^{\text{sob}}$ with arbitrary $\alpha \geq 2$ and $1 \leq q \leq \infty$. Note that $f_{3,\omega,\text{flip}}^{\text{nonper}}$ is defined by reordering the variables of $f_{3,\omega}^{\text{nonper}}$ so that x_j is replaced by

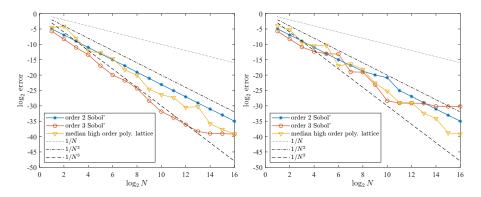


FIG. 6. Comparison of the multi-dimensional integration error by our median high-order polynomial lattice rule (yellow), QMC rules using order 2 Sobol' points (blue) and order 3 Sobol' points (orange). The results are shown for the test functions $f_{3,\omega}^{\text{nonper}}$ (left) and $f_{3,\omega,\text{flip}}^{\text{nonper}}$ (right) with the choice $\omega_i = 1/(4j^4)$.

 x_{s-i+1} , and that we have

$$I_s(f_{3,\boldsymbol{\omega}}^{\text{nonper}}) = I_s(f_{3,\boldsymbol{\omega},\text{flip}}^{\text{nonper}}) = \prod_{j=1}^s \frac{1 - \exp(-\omega_j)}{\omega_j}.$$

The variables are ordered by decreasing order of importance in the first function, and by increasing order in the second one. As our median high-order polynomial lattice rule, based on random choices of generating vectors, does not care about the ordering of variables, it should perform the same for $f_{3,\omega}^{\text{nonper}}$ and $f_{3,\omega,\text{flip}}^{\text{nonper}}$.

The results are shown in Figure 6. Here again, we compare our median high-order polynomial lattice rule with r=11 and QMC rules using order 2 and order 3 interlaced Sobol' points. For the function $f_{3,\omega}^{\text{nonper}}$, our median high-order polynomial lattice rule can exploit the smoothness better than the QMC rule using order 2 Sobol' points. The QMC rule using order 3 Sobol' points exploits the smoothness of the integrand best and the error decays at the rate of N^{-3} and outperforms our median high-order polynomial lattice rule approximately by a constant factor for small N, but this rate breaks down at around $\log_2 N = 13$ and our median rule catches up at $\log_2 N = 16$.

For $f_{3,\omega,\text{flip}}^{\text{nonper}}$, the situation changes. Our median high-order polynomial lattice rule is now comparable to the QMC rule using order 3 Sobol' points when N is small, and performs better for larger N. The error decays approximately at the rate of $N^{-2.5}$, which the QMC rule using order 2 Sobol' points cannot attain. The slowdown of the convergence for the QMC rule using order 3 Sobol' points might be due to the misspecification of important variables. Although x_s, x_{s-1}, \ldots are the order of the relatively important variables for $f_{3,\omega,\text{flip}}^{\text{nonper}}$, we use the later coordinates of order 3 Sobol' points, whose lower-dimensional projections are not well-distributed compared to the earlier coordinates. In this sense, the median high-order polynomial lattice rule is more robust and adaptive to the integrand at hand.

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691 REFERENCES

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[1] J. Baldeaux, J. Dick, G. Leobacher, D. Nuyens, and F. Pillichshammer. Efficient calculation
 of the worst-case error and (fast) component-by-component construction of higher order
 polynomial lattice rules. Numerical Algorithms, 59(3):403-431, 2012.

- [2] R. Cools, F. Y. Kuo, D. Nuyens, and G. Suryanarayana. Tent-transformed lattice rules for integration and approximation of multivariate non-periodic functions. *Journal of Complexity*, 36:166–181, 2016.
- [3] J. Dick. Walsh spaces containing smooth functions and quasi-Monte Carlo rules of arbitrary high order. SIAM Journal on Numerical Analysis, 46(3):1519-1553, 2008.
- [4] J. Dick and T. Goda. Stability of lattice rules and polynomial lattice rules constructed by the component-by-component algorithm. *Journal of Computational and Applied Mathematics*, 382:113062, 2021.
- [5] J. Dick, A. Hinrichs, and F. Pillichshammer. Proof techniques in quasi-Monte Carlo theory. Journal of Complexity, 31:327–371, 2015.
- [6] J. Dick, F. Y. Kuo, Q. T. Le Gia, D. Nuyens, and C. Schwab. Higher order QMC Petrov-Galerkin discretization for affine parametric operator equations with random field inputs. SIAM Journal on Numerical Analysis, 52(6):2676-2702, 2014.
- [7] J. Dick, F. Y. Kuo, and I. H. Sloan. High-dimensional integration: the quasi-Monte Carlo way. Acta Numerica, 22:133–288, 2013.
- [8] J. Dick, D. Nuyens, and F. Pillichshammer. Lattice rules for nonperiodic smooth integrands. Numerische Mathematik, 126:259-291, 2014.
- [9] J. Dick and F. Pillichshammer. Strong tractability of multivariate integration of arbitrary high order using digitally shifted polynomial lattice rules. *Journal of Complexity*, 23:436–453, 2007.
- [10] J. Dick and F. Pillichshammer. Digital Nets and Sequences: Discrepancy Theory and Quasi-Monte Carlo Integration. Cambridge University Press, Cambridge, 2010.
- [11] J. Dick, I. H. Sloan, X. Wang, and H. Woźniakowski. Good lattice rules in weighted Korobov spaces with general weights. *Numerische Mathematik*, 103(1):63–97, 2006.
- [12] A. Ebert, P. Kritzer, D. Nuyens, and O. Osisiogu. Digit-by-digit and component-by-component constructions of lattice rules for periodic functions with unknown smoothness. *Journal of Complexity*, 66:101555, 2021.
- [13] T. Goda. Good interlaced polynomial lattice rules for numerical integration in weighted Walsh spaces. *Journal of Computational and Applied Mathematics*, 285:279–294, 2015.
- [14] T. Goda. Quasi-Monte Carlo integration using digital nets with antithetics. Journal of Computational and Applied Mathematics, 304:26–42, 2016.
- [15] T. Goda and J. Dick. Construction of interlaced scrambled polynomial lattice rules of arbitrary high order. Foundations of Computational Mathematics, 15(5):1245–1278, 2015.
- [16] T. Goda, K. Suzuki, and T. Yoshiki. Lattice rules in non-periodic subspaces of Sobolev spaces. Numerische Mathematik, 141:399–427, 2019.
- 730 [17] T. Hansen and G. L. Mullen. Primitive polynomials over finite fields. *Mathematics of Computation*, 59:639–643, 1992.
 - [18] F. J. Hickernell. Obtaining $O(n^{-2+\epsilon})$ convergence for lattice quadrature rules. In K.-T. Fang, H. Niederreiter, and F. J. Hickernell, editors, *Monte Carlo and Quasi-Monte Carlo Methods* 2000, pages 274–289, Berlin, 2002. Springer-Verlag.
 - [19] N. M. Korobov. The approximate computation of multiple integrals (in Russian). Doklady Akademii Nauk SSSR, 124:1207—1210, 1959.
 - [20] P. Kritzer, F. Y. Kuo, D. Nuyens, and M. Ullrich. Lattice rules with random n achieve nearly the optimal $\mathcal{O}(n^{-\alpha-1/2})$ error independently of the dimension. *Journal of Approximation Theory*, 240:96–113, 2019.
 - [21] F. Y. Kuo. Component-by-component constructions achieve the optimal rate of convergence for multivariate integration in weighted Korobov and Sobolev spaces. *Journal of Complexity*, 19:301–320, 2003.
 - [22] F. Y. Kuo and S. Joe. Component-by-component construction of good lattice rules with a composite number of points. *Journal of Complexity*, 18:943–976, 2002.
 - [23] F. Y. Kuo, C. Schwab, and I. H. Sloan. Quasi-Monte Carlo finite element methods for a class of elliptic partial differential equations with random coefficients. SIAM Journal on Numerical Analysis, 50:3351–3374, 2012.
 - [24] P. L'Ecuyer. Randomized quasi-Monte Carlo: An introduction for practitioners. In P. W. Glynn and A. B. Owen, editors, Monte Carlo and Quasi-Monte Carlo Methods: MCQMC 2016, pages 29–52, Berlin, 2018. Springer.
 - [25] P. L'Ecuyer and C. Lemieux. Recent advances in randomized quasi-Monte Carlo methods. In

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- M. Dror, P. L'Ecuyer, and F. Szidarovszky, editors, Modeling Uncertainty: An Examination of Stochastic Theory, Methods, and Applications, pages 419–474. Kluwer Academic, Boston, 2002.
- 755 [26] P. L'Ecuyer, P. Marion, M. Godin, and F. Puchhammer. A tool for custom construction of QMC and RQMC point sets, December 2020. arXiv:2012.10263.
 - [27] P. L'Ecuyer and D. Munger. On figures of merit for randomly-shifted lattice rules. In L. Plaskota and H. Woźniakowski, editors, Monte Carlo and Quasi-Monte Carlo Methods 2010, pages 133–159, Berlin, 2012. Springer-Verlag.
 - [28] P. L'Ecuyer and D. Munger. Algorithm 958: Lattice Builder: A general software tool for constructing rank-1 lattice rules. ACM Transactions on Mathematical Software, 42(2):15, 2016.
- 763 [29] C. Lemieux. Monte Carlo and Quasi-Monte Carlo Sampling. Springer, New York, 2009. 764 [30] C. Lemieux and P. L'Ecuver. Randomized polynomial lattice rules for multivariate integr
 - [30] C. Lemieux and P. L'Ecuyer. Randomized polynomial lattice rules for multivariate integration and simulation. SIAM Journal on Scientific Computing, 24(5):1768–1789, 2003.
 - [31] G. Leobacher and F. Pillichshammer. Introduction to Quasi-Monte Carlo Integration and Applications. Birkhäuser, Cham, 2014.
 - [32] M. Merkle. Jensen's inequality for medians. Statistics & Probability Letters, 71(3):277–281, 2005.
 - [33] J. A. Nichols and F. Y. Kuo. Fast CBC construction of randomly shifted lattice rules achieving $O(n^{-1+\delta})$ convergence rate for unbounded integrands over \mathbb{R}^s in weighted spaces with POD weights. *Journal of Complexity*, 30:444–468, 2014.
 - [34] H. Niederreiter. Low-discrepancy point sets obtained by digital constructions over finite fields. Czechoslovak Mathematical Journal, 42:143–166, 1992.
 - [35] H. Niederreiter. Random Number Generation and Quasi-Monte Carlo Methods. SIAM, Philadelphia, 1992.
 - [36] E. Novak and H. Woźniakowski. Tractability of Multivariate Problems. Volume I: Linear Information. EMS, Zürich, 2008.
 - [37] D. Nuyens. The magic point shop, 2020. https://people.cs.kuleuven.be/~dirk.nuyens/qmc-generators/.
 - [38] D. Nuyens and R. Cools. Fast algorithms for component-by-component construction of rank-1 lattice rules in shift-invariant reproducing kernel Hilbert spaces. *Mathematics of Computation*, 75:903–920, 2006.
 - [39] Z. Pan and A. B. Owen. Super-polynomial accuracy of one dimensional randomized nets using the median-of-means, November 2021. arXiv:2111.12676.
 - [40] F. Pillichshammer. Polynomial lattice point sets. In L. Plaskota and H. Woźniakowski, editors, Monte Carlo and Quasi-Monte Carlo Methods 2010, pages 189–210, Berlin, 2012. Springer-Verlag.
 - [41] J. B. Rosser and L. Schoenfeld. Approximate formulas for some functions of prime numbers. Illinois Journal of Mathematics, 6(1):64–94, 1962.
 - [42] I. H. Sloan and S. Joe. Lattice Methods for Multiple Integration. Oxford Science Publications, New York, 1994.
- 793 [43] I. H. Sloan and A. V. Reztsov. Component-by-component construction of good lattice rules.
 794 Mathematics of Computation, 71:263–273, 2002.
- 795 [44] I. H. Sloan and H. Woźniakowski. When are quasi-Monte Carlo algorithms efficient for highdimensional integrals? *Journal of Complexity*, 14:1–33, 1998.