Worst-case error for unshifted lattice rules without randomisation

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Abstract An existence result is presented for the worst-case error of lattice rules for high dimensional integration over the unit cube, in an unanchored weighted space of functions with square-integrable mixed first derivatives. Existing studies rely on random shifting of the lattice to simplify the analysis, whereas in this paper neither shifting nor any other form of randomisation is considered. Given that a certain number-theoretic conjecture holds, it is shown that there exists an N-point rank-one lattice rule which gives a worst-case error of order $1/\sqrt{N}$ up to a (dimension-independent) logarithmic factor. Numerical results suggest that the conjecture is plausible.

1 Introduction

This paper is concerned with an error estimate for a numerical integration rule for functions defined on high-dimensional hypercube $[0,1)^s$, $s \in \mathbb{N}$,

$$\int_{[0,1)^s} f(x)\,\mathrm{d}x. \tag{1}$$

More specifically, we consider the worst-case error for rank-one lattice rules. The main contribution of this paper is the analysis of unshifted lattice rules without randomisation; we allow neither shifting nor any other form of randomisation. Given the truth of a certain conjecture with a number-theoretic flavour (Conjecture 1), our results show the existence of a deterministic cubature point set that attains the worst-

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case error of the order $1/\sqrt{N}$, up to a logarithmic factor, where N is the number of cubature points, with a dimension-independent constant (Corollary 1).

An N-point rank-one lattice rule in s-dimension is an equal-weight cubature rule for approximating the integral (1) — a quasi-Monte Carlo rule — of the form

$$\frac{1}{N}\sum_{k=0}^{N-1} f(t_k), \tag{2}$$

with cubature points

$$t_k = \left\{\frac{kz}{N}\right\}, \quad k = 0,\ldots,N-1, \tag{3}$$

for some $z \in \{1,\ldots,N-1\}^s$, where $\{x\} \in [0,1)^s$ for $x = (x_1,\ldots,x_s) \in [0,\infty)^s$ denotes the vector consisting of the fractional part of each component of x. The choice of z, known as the *generating vector*, completely determines the cubature points, and thus the quality of the cubature rule. Our interest in this paper lies in proving the existence of a good generating vector $z \in \{1,\ldots,N-1\}^s$. The figure of merit we consider is the so-called worst-case error, defined by

$$e(N,z) := e(N,(\{kz/N\})_k) := \sup_{f\in H_{s,\gamma},\, \|f\|_{H_{s,\gamma}}\le 1} \left| \int_{[0,1)^s} f(x)\,\mathrm{d}x - \frac{1}{N}\sum_{k=0}^{N-1} f(\{kz/N\}) \right|,$$

where $H_{s,\gamma}$ is a suitable normed space consisting of non-periodic functions over $[0,1)^s$, specified below. As is standard nowadays, we will assume that the norm incorporates certain parameters $\gamma_{\mathfrak{u}}$, one for each subset $\mathfrak{u} \subseteq \{1,2,\ldots,s\}$, since without weights integration problems are often intractable, see [1, 9] for more details.

It is natural to seek a generating vector z that makes the worst-case error small. If $H_{s,\gamma}$ is a reproducing kernel Hilbert space then the worst-case error $e(N,z)$ can be computed for any value of z (see below), but there is no known formula that gives a good value of z for general s. The strategy we take in this paper is to prove an existence result, by considering the average of $e^2(N,z)$ over all possible generating vectors $z \in Z_N^s$, with $Z_N := \{1,2,\ldots,N-1\}$, i.e. we compute

$$\overline{e}^2(N) := \frac{1}{(N-1)^s}\sum_{z\in Z_N^s} e^2(N,z); \tag{4}$$

and then use the well known principle that there must exist one choice of z that is as good as average. With the support of a certain number-theoretic conjecture (Conjecture 1), which does not depend on the choice of z, we will show that

$$\overline{e}^2(N) \le \frac{C\,(\ln N)^{\alpha}}{N},$$

with C independent of N, where $\alpha > 0$ is an exponent appearing in the conjecture that depends on neither s nor N. Moreover, C is independent of s for suitable weights

$\gamma_{\mathfrak{u}}$. It follows that there exists a generating vector z^* for which the worst-case error $e(N,z^*)$ is bounded by $\sqrt{C}(\ln N)^{\alpha/2}/\sqrt{N}$ (Corollary 1).

For periodic function spaces, error estimates for rank-one lattice rules are well known; see [1, 4, 7, 8] and references therein. For non-periodic functions, with the aid of *shifting*—changing the cubature points from $\{kz/N\}$ to $\{kz/N+\Delta\}$ with elements $\Delta \in [0,1)^s$—good results have been obtained for shift-averaged worst-case errors; see [1] and references therein for more details. In the present paper, however, the function space is not periodic, and the worst-case error we consider is not shift-averaged. Approaches to estimating the error for lattice rules for non-periodic functions without randomisation include [2, 3], where a mapping called the tent transform was applied to the lattice rule. In this paper, however, no transformation of the lattice points is considered.

The shift-averaged worst-case error mentioned above is the expected worst-case error for *randomly shifted* lattice rules, see [1]. The present paper is a first step in our project to "*derandomise*" randomly shifted lattice rules—that is, to produce explicit shifts (for an untransformed rule) that gives worst-case errors that lose no accuracy compared to the shift-averaged worst-case errors. While randomly shifted lattice rules have the advantages of providing us with an online error estimator and of being simple to analyse and construct, they are less efficient than a good deterministic rule, because of the need in practice to repeat the calculations of integrals with fixed z for some number (say 30) of random shifts. In this first step in this programme, we study the case of zero shifts. (Experience suggests that this is a poor choice—perhaps the worst!)

There are related works in [5, 6] where a quantity called 'R', which is connected to the so-called (weighted) star discrepancy, was considered as the error criterion. In the weighted setting in [6], lattice rules can be constructed to achieve $O(n^{-1+\delta})$ convergence rate for any $\delta > 0$, with the implied constant independent of s and N for suitable weights.

After establishing the setting in Section 2, the conjecture and the main results are stated in Section 3. Section 4 provides numerical evidence relating to the conjecture. Finally in Section 5 we give concluding remarks.

2 Preliminaries

In this section, we introduce the setting and recall some facts on lattice rules that will be needed later. Throughout this paper, we assume that N, the number of cubature points, is a prime number. Let us start with a general reproducing kernel Hilbert space (RKHS) H_s with a reproducing kernel $K\colon [0,1]^s \times [0,1]^s \to \mathbb{R}$ that satisfies

$$\int_{[0,1]^s}\int_{[0,1]^s} K(x,y)\,\mathrm{d}x\,\mathrm{d}y < \infty.$$

It is well known that for a general quasi-Monte Carlo (QMC) rule (2), the square of the worst-case error in H_s,

$$e(N,(t_k)_k) := \sup_{f\in H_s,\, \|f\|_{H_s}\le 1} \left| \int_{[0,1)^s} f(x)\,\mathrm{d}x - \frac{1}{N}\sum_{k=0}^{N-1} f(t_k) \right|,$$

is given by

$$\begin{aligned} &e^2(N,(t_k)_k) \\ &= \int_{[0,1]^s}\int_{[0,1]^s} K(x,y)\,\mathrm{d}x\,\mathrm{d}y - \frac{2}{N}\sum_{k=0}^{N-1}\int_{[0,1]^s} K(t_k,x)\,\mathrm{d}x + \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{k'=0}^{N-1} K(t_k,t_{k'}), \end{aligned}$$

see for example [1, Theorem 3.5]. We specialise to the case

$$\int_{[0,1]^s} K(x,y)\,\mathrm{d}x = 1 \qquad \text{for any } y\in[0,1]^s,$$

to obtain

$$e^2(N,(t_k)_k) = \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{k'=0}^{N-1} K(t_k,t_{k'}) - 1. \tag{5}$$

In particular, for the QMC rule we here take an unshifted lattice rule with cubature points given by (3) for some $z\in Z_N^s$. Then, we have

$$e^2(N,z) = \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{k'=0}^{N-1} K\left(\left\{\frac{kz}{N}\right\},\left\{\frac{k'z}{N}\right\}\right) - 1. \tag{6}$$

Now we further specialise the RKHS to $H_{s,\gamma}$ with kernel

$$K_{s,\gamma}(x,y) = \sum_{\mathfrak{u}\subseteq\{1:s\}} \gamma_{\mathfrak{u}} \prod_{j\in\mathfrak{u}} \eta(x_j,y_j), \tag{7}$$

where

$$\eta(x,y) := \frac{1}{2}B_2(|x-y|) + \left(x-\frac{1}{2}\right)\left(y-\frac{1}{2}\right), \qquad x,y\in[0,1].$$

Here $B_2(t) = t^2 - t + 1/6$, $t\in\mathbb{R}$ is the Bernoulli polynomial of degree 2, $\{1:s\}$ is a shorthand notation for $\{1,2,...,s\}$, and the sum in (7) is over all subsets $\mathfrak{u}\subseteq\{1:s\}$, including the empty set; and $\gamma = \{\gamma_{\mathfrak{u}}\}_{\mathfrak{u}\subset\mathbb{N}}$ is an arbitrary collection of positive numbers called *weights* with $\gamma_\emptyset = 1$. The choice of weights plays an important role in deriving a dimension-independent error estimate, see Corollary 1. This space, discussed fully in [1], is an "unanchored" space of functions on the unit cube with square integrable mixed first derivatives. We again refer the readers to [1] for more details. For this space it follows from (5) that

$$e^2(N,z) = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}\, e_{\mathfrak{u}}^2(N, z_{\mathfrak{u}}), \tag{8}$$

where for $\mathfrak{u} \subseteq \{1:s\}$ and $z_{\mathfrak{u}} = (z_j)_{j\in\mathfrak{u}}$, from (5) and (7)

$$e_{\mathfrak{u}}^2(N,z_{\mathfrak{u}}) := \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{k'=0}^{N-1}\prod_{j\in\mathfrak{u}}\left[\frac{1}{2}B_2\left(\left|\left\{\frac{kz_j}{N}\right\}-\left\{\frac{k'z_j}{N}\right\}\right|\right)+\left(\left\{\frac{kz_j}{N}\right\}-\frac{1}{2}\right)\left(\left\{\frac{k'z_j}{N}\right\}-\frac{1}{2}\right)\right]. \tag{9}$$

Thus the quantity $e_{\mathfrak{u}}^2(N,z_{\mathfrak{u}})$ is a key to deriving an estimate for $e^2(N,z)$.

3 Existence result for worst-case error

In this section, we derive an existence result for the worst-case error. We first note the following property.

Proposition 1. *Let g be a function that satisfies $g(t) = g(1-t)$ for $t \in [0,1]$. Then for $a, b \geq 0$ we have*

$$g(|\{a\}-\{b\}|) = g(\{a-b\}),$$

where, as before, the braces indicate that we take the fractional part of the real number.

Proof. Note first that $\{a\},\{b\} \in [0,1)$ and therefore $\{a\}-\{b\} \in (-1,1)$. It is clear that $\{a\}-\{b\}$ differs from $\{a-b\}$ by 1 or 0. If $\{a\}=\{b\}$, then $\{a-b\}=0$ and the result is trivial. If $\{a\}>\{b\}$, then $\{a\}-\{b\} \in (0,1)$, and so $\{a\}-\{b\}=\{a-b\}$. Thus, again the result is trivial. If $\{a\}<\{b\}$, then $|\{a\}-\{b\}| = \{b\}-\{a\} \in (0,1)$ and so $|\{a\}-\{b\}| = \{b-a\}$. Thus, using $g(t)=g(1-t)$, $t\in[0,1]$ we have

$$g(|\{a\}-\{b\}|) = g(\{b\}-\{a\}) = g(\{b-a\}) = g(1-\{b-a\}) = g(\{a-b\}),$$

where in the last step we used the identity $\{t\}+\{-t\}=1$ for $t \notin \mathbb{Z}$. □

In particular, Proposition 1 applies to the function $B_2(\cdot)$ so we can rewrite (9) as

$$e_{\mathfrak{u}}^2(N,z_{\mathfrak{u}}) = \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{k'=0}^{N-1}\prod_{j\in\mathfrak{u}}\left[\frac{1}{2}B_2\left(\left\{\frac{(k-k')z_j}{N}\right\}\right)+\left(\left\{\frac{kz_j}{N}\right\}-\frac{1}{2}\right)\left(\left\{\frac{k'z_j}{N}\right\}-\frac{1}{2}\right)\right]. \tag{10}$$

Now we obtain the average over $z \in Z_N^s$. From (4) and (8) we have

$$\overline{e}^2(N) = \sum_{\emptyset \neq \mathfrak{u} \subseteq \{1:s\}} \gamma_{\mathfrak{u}}\, \overline{e}_{\mathfrak{u}}^2(N), \tag{11}$$

where

$$\overline{e}^2_{\mathfrak{u}}(N) := \frac{1}{(N-1)^s} \sum_{z \in Z_N^s} e^2_{\mathfrak{u}}(N, z_{\mathfrak{u}}) = \frac{1}{(N-1)^{|\mathfrak{u}|}} \sum_{z_{\mathfrak{u}} \in Z_N^{|\mathfrak{u}|}} e^2_{\mathfrak{u}}(N, z_{\mathfrak{u}})$$
$$= \frac{1}{N^2} \sum_{k=0}^{N-1} \sum_{k'=0}^{N-1} (X_{N;k,k'} + J_{N;k,k'})^{|\mathfrak{u}|}, \qquad (12)$$

with

$$X_{N;k,k'} := \frac{1}{2(N-1)} \sum_{z=1}^{N-1} B_2\left(\left\{\frac{(k-k')z}{N}\right\}\right), \qquad (13)$$

and

$$J_{N;k,k'} := \frac{1}{N-1} \sum_{z=1}^{N-1} \left(\left\{\frac{kz}{N}\right\} - \frac{1}{2}\right)\left(\left\{\frac{k'z}{N}\right\} - \frac{1}{2}\right). \qquad (14)$$

Further, the binomial theorem gives

$$\overline{e}^2_{\mathfrak{u}}(N) = \frac{1}{N^2} \sum_{k=0}^{N-1} \sum_{k'=0}^{N-1} \sum_{\mathfrak{v} \subseteq \mathfrak{u}} (X_{N;k,k'})^{|\mathfrak{u} \setminus \mathfrak{v}|} (J_{N;k,k'})^{|\mathfrak{v}|}. \qquad (15)$$

In seeking an error estimate for the generating-vector-averaged worst-case error $\overline{e}^2(N)$, we take the point of view that estimates of order $1/N$ or higher are relatively harmless, so we are concentrating on isolating terms that are more slowly converging.

In the following two subsections, we derive estimates for $X_{N;k,k'}$ and $J_{N;k,k'}$. It turns out that, roughly speaking, the terms $(X_{N;k,k'})^{|\mathfrak{u}\setminus\mathfrak{v}|}$ yield the order $1/N$. The terms $(J_{N;k,k'})^{|\mathfrak{v}|}$ seem to converge more slowly, and require more detailed analysis.

3.1 Estimates for $X_{N;k,k'}$

We have the following expression for $X_{N;k,k'}$.

Lemma 1. *For N prime and $k, k' \in \{0, 1, \ldots, N-1\}$, the quantity $X_{N;k,k'}$ defined in* (13) *satisfies*

$$X_{N;k,k'} = \begin{cases} \dfrac{1}{12} & \text{if } k = k', \\ -\dfrac{1}{12N} & \text{if } k \neq k'. \end{cases} \qquad (16)$$

Proof. For $k = k'$, we have $X_{N;k,k} = \frac{1}{2}B_2(0) = \frac{1}{12}$. For $k \neq k'$, recalling the (absolutely convergent) series representation

$$B_2(x) = \frac{1}{2\pi^2} \sum_{h \neq 0} \frac{\exp(2\pi \mathrm{i} h x)}{h^2}, \qquad x \in [0,1],$$

we have

$$X_{N;k,k'} = \frac{1}{4\pi^2(N-1)} \sum_{h\neq 0} \frac{1}{h^2} \sum_{z=1}^{N-1} \exp(2\pi \mathrm{i} h(k-k')z/N)$$
$$= \frac{1}{4\pi^2(N-1)} \sum_{h\neq 0} \frac{1}{h^2} \left(\sum_{z=0}^{N-1} \exp(2\pi \mathrm{i} z h(k-k')/N) - 1 \right),$$

with

$$\sum_{z=0}^{N-1} \exp(2\pi \mathrm{i} z h(k-k')/N) = \begin{cases} N & \text{if } h(k-k') \equiv_N 0, \\ 0 & \text{if } h(k-k') \not\equiv_N 0. \end{cases}$$

Throughout this paper, the notation $a \equiv_N b$ means that $a \equiv b \pmod N$, and similarly $a \not\equiv_N b$ means that $a \not\equiv b \pmod N$. Since N is prime and $k \neq k'$, we conclude that all possible values of $k-k'$, namely, $\pm 1, \pm 2, \ldots, \pm(N-1)$, are relatively prime to N, and so $h(k-k') \equiv_N 0 \iff h \equiv_N 0$. Thus

$$X_{N;k,k'} = \frac{1}{4\pi^2(N-1)} \left(N \sum_{\substack{h\neq 0\\ h\equiv_N 0}} \frac{1}{h^2} - \sum_{h\neq 0} \frac{1}{h^2} \right)$$
$$= \frac{1}{4\pi^2(N-1)} \left(N \sum_{\ell \neq 0} \frac{1}{(\ell N)^2} - \frac{\pi^2}{3} \right) = \frac{1}{4\pi^2(N-1)} \left(\frac{N}{N^2}\frac{\pi^2}{3} - \frac{\pi^2}{3} \right) = -\frac{1}{12N},$$

which completes the proof. □

We deduce the following estimate for $\overline{e}^2_{\mathfrak{u}}(N)$.

Proposition 2. *For N prime, the quantity $\overline{e}^2_{\mathfrak{u}}(N)$ defined in* (15) *satisfies*

$$\overline{e}^2_{\mathfrak{u}}(N) \le c_{\mathfrak{u}} \frac{1}{N} + \frac{1}{N^2} \sum_{k=1}^{N-1} \sum_{k'=1}^{N-1} (J_{N;k,k'})^{|\mathfrak{u}|}, \qquad \text{with} \quad c_{\mathfrak{u}} := \frac{2}{3^{|\mathfrak{u}|}} + \frac{1}{4^{|\mathfrak{u}|}}.$$

Proof. On separating out the diagonal terms of (15), we have

$$\overline{e}^2_{\mathfrak{u}}(N) = \frac{1}{N^2} \sum_{k=0}^{N-1} (X_{N;k,k} + J_{N;k,k})^{|\mathfrak{u}|} + \frac{1}{N^2} \sum_{k=0}^{N-1} \sum_{\substack{k'=0\\ k'\neq k}}^{N-1} \sum_{\mathfrak{v}\subseteq \mathfrak{u}} (X_{N;k,k'})^{|\mathfrak{u}\setminus\mathfrak{v}|} (J_{N;k,k'})^{|\mathfrak{v}|}. \quad (17)$$

From $X_{N;k,k} = \frac{1}{12}$ and $0 \le J_{N;k,k} \le \frac{1}{N-1} \sum_{z=1}^{N-1} \frac{1}{4} = \frac{1}{4}$, the first term in (17) can be bounded by

$$\frac{1}{N^2} \sum_{k=0}^{N-1} (X_{N;k,k} + J_{N;k,k})^{|\mathfrak{u}|} \le \frac{1}{3^{|\mathfrak{u}|} N}.$$

For the second term in (17), noting $|J_{N;k,k'}| \le \frac{1}{4}$, from Lemma 1 we have for any $\mathfrak{v} \subseteq \mathfrak{u}$

$$\left| (X_{N;k,k'})^{|\mathfrak{u}\setminus\mathfrak{v}|} (J_{N;k,k'})^{|\mathfrak{v}|} \right| \le \frac{1}{(12N)^{|\mathfrak{u}\setminus\mathfrak{v}|}\, 4^{|\mathfrak{v}|}},$$

and thus summing over $\mathfrak{v} \subsetneq \mathfrak{u}$ and estimating $N^{-|\mathfrak{u}\setminus\mathfrak{v}|}$ by N^{-1} we obtain

$$\sum_{\mathfrak{v}\subsetneq\mathfrak{u}} \left|(X_{N;k,k'})^{|\mathfrak{u}\setminus\mathfrak{v}|}(J_{N;k,k'})^{|\mathfrak{v}|}\right| \le \frac{1}{N}\sum_{\mathfrak{v}\subsetneq\mathfrak{u}} \frac{1}{12^{|\mathfrak{u}\setminus\mathfrak{v}|}\,4^{|\mathfrak{v}|}}.$$

Further, from the binomial theorem we have $\sum_{\mathfrak{v}\subsetneq\mathfrak{u}} \frac{1}{12^{|\mathfrak{u}\setminus\mathfrak{v}|}4^{|\mathfrak{v}|}} = \left(\frac{1}{12}+\frac{1}{4}\right)^{|\mathfrak{u}|} - \frac{1}{4^{|\mathfrak{u}|}} = \frac{1}{3^{|\mathfrak{u}|}} - \frac{1}{4^{|\mathfrak{u}|}}$. Using this, together with the case $\mathfrak{v}=\mathfrak{u}$, we obtain

$$\bar{e}^2_{\mathfrak{u}}(N) \le \left(\frac{2}{3^{|\mathfrak{u}|}} - \frac{1}{4^{|\mathfrak{u}|}}\right)\frac{1}{N} + \frac{1}{N^2}\sum_{k=0}^{N-1}\sum_{\substack{k'=0\\k'\neq k}}^{N-1}(J_{N;k,k'})^{|\mathfrak{u}|}.$$

Using again $|J_{N;k,k'}| \le 1/4$, we can separate out the contributions for $k=0$ or $k'=0$, to obtain

$$\frac{1}{N^2}\sum_{k'=1}^{N-1}|J_{N;0,k'}|^{|\mathfrak{u}|} \le \frac{N-1}{4^{|\mathfrak{u}|}N^2} \le \frac{1}{4^{|\mathfrak{u}|}N} \qquad \text{and} \qquad \frac{1}{N^2}\sum_{k=1}^{N-1}|J_{N;k,0}| \le \frac{1}{4^{|\mathfrak{u}|}N}.$$

Finally noting $(J_{N;k,k})^{|\mathfrak{u}|} \ge 0$ yields the desired result. □

3.2 Estimates for $J_{N;k,k'}$

In this subsection, we derive estimates for $J_{N;k,k'}$ for $k,k' \ge 1$. In the following we will make use of the Fourier series for the real 1-periodic sawtooth function, defined on $[0,1)$ by

$$b(x) := \begin{cases} x - 1/2 & \text{if } x \in (0,1), \\ 0 & \text{if } x = 0, \end{cases}$$

and then extended to the whole of $\mathbb{R}$ by $b(x) = b(x+1)$ for all $x \in \mathbb{R}$. Thus $b(x)$ is the periodic version of the first-degree Bernoulli polynomial $B_1(x) = x - 1/2$. It is well known (following, for example, from the Dini criterion) that the symmetric partial sums in its Fourier series converge to $b(x)$ pointwise for all $x \in \mathbb{R}$, that is

$$b(x) = \lim_{M\to\infty}\frac{\mathrm{i}}{2\pi}\sum_{\substack{h=-M\\h\neq 0}}^{M}\frac{\exp(2\pi \mathrm{i} hx)}{h}, \quad x \in \mathbb{R}.$$

For notational simplicity we shall often omit the limit, writing simply

$$b(x) = \frac{\mathrm{i}}{2\pi}\sum_{h\neq 0}\frac{\exp(2\pi \mathrm{i} hx)}{h}, \quad x \in \mathbb{R},$$

but this is always to be understood as the limit of the symmetric partial sum.

We have the following expression for $J_{N;k,k'}$, $k,k' \in \{1,\ldots,N-1\}$.

Lemma 2. *For N prime and $k,k' \in \{1,\ldots,N-1\}$, the quantity $J_{N;k,k'}$ defined in* (14) *satisfies*

$$J_{N;k,k'} = \frac{1}{4\pi^2}\frac{N}{N-1}\sum_{h\neq 0}\sum_{\substack{h'\neq 0\\ h'k'\equiv_N hk}} \frac{1}{hh'}, \tag{18}$$

where the double sum is to be interpreted as the double limit

$$\sum_{h\neq 0}\sum_{\substack{h'\neq 0\\ h'k'\equiv_N hk}} \frac{1}{hh'} := \lim_{M\to\infty}\lim_{M'\to\infty}\sum_{h\in\{-M,\ldots,M\}\setminus\{0\}}\sum_{\substack{h'\in\{-M',\ldots,M'\}\setminus\{0\}\\ h'k'\equiv_N hk}} \frac{1}{hh'}.$$

Proof. For $(x,y)\in(0,1)^2$ we have

$$\begin{aligned} B_1(x)B_1(y) &= \frac{1}{4\pi^2}\sum_{h\neq 0}\sum_{h'\neq 0}\frac{e^{2\pi i h x}}{h}\frac{e^{-2\pi i h' y}}{h'} \\ &:= \lim_{M\to\infty}\lim_{M'\to\infty}\frac{1}{4\pi^2}\sum_{h\in\{-M,\ldots,M\}\setminus\{0\}}\sum_{h'\in\{-M',\ldots,M'\}\setminus\{0\}}\frac{e^{2\pi i h x}}{h}\frac{e^{-2\pi i h' y}}{h'}. \end{aligned}$$

Thus for any $k,k' = 1,\ldots,N-1$ we have, noting that the finite sum over z may be interchanged with the implied limits,

$$\begin{aligned} &J_{N;k,k'} \\ &= \frac{1}{4\pi^2(N-1)}\sum_{h\neq 0}\sum_{h'\neq 0}\frac{1}{hh'}\sum_{z=1}^{N-1}\exp\left(2\pi i\left(\frac{hk-h'k'}{N}\right)z\right) \\ &= -\frac{1}{4\pi^2(N-1)}\sum_{h\neq 0}\sum_{h'\neq 0}\frac{1}{hh'} + \frac{1}{4\pi^2(N-1)}\sum_{h\neq 0}\sum_{h'\neq 0}\frac{1}{hh'}\sum_{z=0}^{N-1}\exp\left(2\pi i\left(\frac{hk-h'k'}{N}\right)z\right). \end{aligned}$$

The first term vanishes because it has as a factor the limit of the product of symmetric partial sums of the odd function $1/h$. For the second term we use

$$\sum_{z=0}^{N-1}\exp(2\pi i z(hk-h'k')/N) = \begin{cases} N & \text{if } hk-h'k' \equiv_N 0, \\ 0 & \text{if } hk-h'k' \not\equiv_N 0, \end{cases}$$

which leads to the desired formula. □

We now want to estimate $J_{N;k,k'}$ for $k,k' \geq 1$ using (18). It turns out that it suffices to consider $J_{N;\kappa,1}$, for $\kappa = 1,\ldots,N-1$.

Proposition 3. *For N prime, the quantity $\overline{e}_{\mathrm{u}}^2(N)$ defined in* (15) *satisfies*

$$\bar{e}^2_{\mathfrak{u}}(N) \le c_{\mathfrak{u}} \frac{1}{N} + \frac{1}{N} \sum_{\kappa=1}^{N-1} |J_{N;\kappa,1}|^{|\mathfrak{u}|}.$$

Proof. Because N is prime, for each $k' \in \{1,\dots,N-1\}$ there is a unique inverse ${k'}^{-1} \in \{1,\dots,N-1\}$ such that $k'{k'}^{-1} \equiv_N 1$, and therefore

$$h'k' \equiv_N hk \quad \Leftrightarrow \quad h' \equiv_N h(k{k'}^{-1}).$$

It follows from (18) that

$$J_{N;k,k'} = J_{N;\kappa,1}, \qquad \text{with} \qquad \kappa := k{k'}^{-1} \mod N,$$

and since κ runs over all of $\{1,\dots,N-1\}$ as k' runs over $\{1,\dots,N-1\}$, we have

$$\frac{1}{N^2} \sum_{k=1}^{N-1} \sum_{k'=1}^{N-1} (J_{N;k,k'})^{|\mathfrak{u}|} = \frac{N-1}{N^2} \sum_{\kappa=1}^{N-1} (J_{N;\kappa,1})^{|\mathfrak{u}|} \le \frac{1}{N} \sum_{\kappa=1}^{N-1} |J_{N;\kappa,1}|^{|\mathfrak{u}|}.$$

Applying this to Proposition 2 yields the desired result. □

From Lemma 2 we have

$$J_{N;\kappa,1} = \frac{1}{4\pi^2} \frac{N}{N-1} \sum_{h \ne 0} \sum_{\substack{h' \ne 0 \\ h' \equiv_N h\kappa}} \frac{1}{hh'} = \frac{1}{4\pi^2} \frac{N}{N-1} \lim_{M\to\infty} \lim_{M'\to\infty} S(M,M'), \tag{19}$$

where

$$S(M,M') := \sum_{h \in \{-M,\dots,M\}\setminus\{0\}} \sum_{\substack{h' \in \{-M',\dots,M'\}\setminus\{0\} \\ h' \equiv_N h\kappa}} \frac{1}{hh'}. \tag{20}$$

To further simplify $J_{N;\kappa,1}$, we note that for h,h' satisfying $h' \equiv_N h\kappa$ with $\kappa \in \{1,\dots,N-1\}$ we have

$$h \equiv_N 0 \quad \Leftrightarrow \quad h\kappa \equiv_N 0 \quad \Leftrightarrow \quad h' \equiv_N 0.$$

Hence, for the $h \equiv_N 0$ contribution to the double sum (20) we have

$$\sum_{\substack{h \in \{-M,\dots,M\}\setminus\{0\} \\ h \equiv_N 0}} \frac{1}{h} \sum_{\substack{h' \in \{-M',\dots,M'\}\setminus\{0\} \\ h' \equiv_N 0}} \frac{1}{h'} = 0.$$

Thus, we can restrict the double sum (20) to $h \not\equiv_N 0$ so that

$$S(M,M') = \sum_{\substack{h \in \{-M,\dots,M\}\setminus\{0\} \\ h \not\equiv_N 0}} \sum_{\substack{h' \in \{-M',\dots,M'\}\setminus\{0\} \\ h' \equiv_N h\kappa}} \frac{1}{hh'}. \tag{21}$$

We now assume $N \geq 3$ so that $N-1$ is even for N prime. We can write $h \not\equiv_N 0$ as

$$h = \ell N + q, \quad \text{with} \quad \ell \in \mathbb{Z} \quad \text{and} \quad q \in \left\{-\tfrac{N-1}{2}, \ldots, \tfrac{N-1}{2}\right\} \setminus \{0\} =: R_N. \tag{22}$$

Then, we can write $h' \equiv_N h\kappa$ with $h \not\equiv_N 0$ as

$$h' = \ell' N + r(q\kappa, N), \quad \text{with} \quad \ell' \in \mathbb{Z},$$

where $r(j,N)$ is the unique integer congruent to $j \bmod N$ with the smallest magnitude. More precisely, the function $r(\cdot,N)\colon \mathbb{Z} \to R_N \cup \{0\}$ is defined for $j \geq 0$ by

$$r(j,N) := \begin{cases} j \bmod N & \text{if} \quad j \bmod N \leq \frac{N-1}{2}, \\ j \bmod N - N & \text{if} \quad j \bmod N > \frac{N-1}{2}, \end{cases} \tag{23}$$

and extended to all integers j by $r(j,N) = r(j+N,N)$. It follows that for $j > 0$ we have $r(-j,N) = r(N-j \bmod N, N) = -r(j,N)$. Hence the function is both N-periodic and odd. If N divides j, then we have $r(j,N) = 0$, but otherwise $r(j,N) \in R_N$.

Using these representations of h and h', the double limit in $J_{N;\kappa,1}$ as in (19) can be rewritten as follows.

Lemma 3. *For $N \geq 3$ prime and $\kappa \in \{1,\ldots,N-1\}$, the quantity $J_{N;\kappa,1}$ given by* (19) *satisfies*

$$J_{N;\kappa,1} \tag{24}$$
$$= \frac{1}{2\pi^2}\frac{N}{N-1}\sum_{q=1}^{(N-1)/2}\left(\frac{1}{q} - \sum_{\ell=1}^{\infty}\frac{2q}{(\ell N)^2 - q^2}\right)\left(\frac{1}{r(q\kappa,N)} - \sum_{\ell'=1}^{\infty}\frac{2\,r(q\kappa,N)}{(\ell' N)^2 - r(q\kappa,N)^2}\right), \tag{25}$$

where $r(\cdot,N)$ is defined as in (23).

Proof. We begin with the expression (19) for $J_{N;\kappa,1}$. Writing $M = LN + Q$ and $M' = L'N + Q'$ with $L, L' \in \mathbb{N}$ and $Q, Q' \in R_N \cup \{0\}$, the double sum (21) can be rewritten as

$$\begin{aligned} S(M,M') &= \sum_{\substack{\ell\in\mathbb{Z},\, q\in R_N \\ |\ell N+q|\leq LN+Q}} \; \sum_{\substack{\ell'\in\mathbb{Z},\, q'\in R_N \\ |\ell' N+q'|\leq L'N+Q' \\ q'\equiv_N q\kappa}} \frac{1}{\ell N+q}\,\frac{1}{\ell' N+q'} \\ &= \sum_{\substack{q,q'\in R_N \\ q'\equiv_N q\kappa}} \left(\sum_{\substack{\ell=-L \\ |\ell N+q|\leq LN+Q}}^{L} \frac{1}{\ell N+q}\right)\left(\sum_{\substack{\ell'=-L' \\ |\ell' N+q'|\leq L'N+Q'}}^{L'} \frac{1}{\ell' N+q'}\right), \end{aligned} \tag{26}$$

where we used the fact that the inequalities in the summation conditions cannot hold if $|\ell| > L$ or $|\ell'| > L'$.

First we consider the sum over ℓ in (26). Since the condition $|\ell N+q| \le LN+Q$ always holds for $|\ell| \le L-1$, we can write

$$\sum_{\substack{\ell=-L \\ |\ell N+q|\le LN+Q}}^{L} \frac{1}{\ell N+q} = \sum_{\ell=-L}^{L} \frac{1}{\ell N+q} - \sum_{\substack{\ell=\pm L \\ |\ell N+q|>LN+Q}} \frac{1}{\ell N+q},$$

where we have

$$\sum_{\ell=-L}^{L} \frac{1}{\ell N+q} = \frac{1}{q} + \sum_{\ell=1}^{L} \left(\frac{1}{\ell N+q} + \frac{1}{-\ell N+q} \right) = \frac{1}{q} - \sum_{\ell=1}^{L} \frac{2q}{(\ell N)^2 - q^2}$$

and

$$\left| \sum_{\substack{\ell=\pm L \\ |\ell N+q|>LN+Q}} \frac{1}{\ell N+q} \right| \le \frac{2}{LN+Q} \le \frac{2}{LN-N/2} \to 0 \qquad \text{as} \qquad L \to \infty.$$

Thus we conclude that

$$\lim_{L\to\infty} \sum_{\substack{\ell=-L \\ |\ell N+q|\le LN+Q}}^{L} \frac{1}{\ell N+q} = \frac{1}{q} - \lim_{L\to\infty} \sum_{\ell=1}^{L} \frac{2q}{(\ell N)^2 - q^2} = \frac{1}{q} - \sum_{\ell=1}^{\infty} \frac{2q}{(\ell N)^2 - q^2} =: P_N(q).$$

The sum over ℓ' in (26) is similar.

Now since the double limit of $S(M,M')$ exists as $M \to \infty$ and $M' \to \infty$, it must equal the double limit of the last expression in (26) as $L \to \infty$ and $L' \to \infty$, with arbitrary Q and Q'. (This is because for a particular pair (Q,Q'), the last expression in (26), when interpreted as a sequence in the double index (L,L'), can be considered as a subsequence of the convergent sequence $S(M,M')$ with double index (M,M').) Hence we obtain

$$\lim_{M\to\infty} \lim_{M'\to\infty} S(M,M') = \sum_{\substack{q,q'\in R_N \\ q'\equiv_N q\kappa}} P_N(q) P_N(q') = \sum_{q\in R_N} P_N(q) P_N(r(q\kappa,N)),$$

where we used the fact that for a given $q \in R_N$, the only value of $q' \in R_N$ that satisfies $q' \equiv_N q\kappa$ is $q' = r(q\kappa,N)$.

Finally, we observe that $P_N(-q) = -P_N(q)$, and $P_N(r(-q\kappa,N)) = -P_N(r(q\kappa,N))$ since $r(-q\kappa,N) = -r(q\kappa,N)$. Thus the contributions of q and $-q$ to the sum are the same, and so we only need to sum over the positive values of q and then double the result. Applying the result in (19) completes the proof. □

Now we estimate the magnitude of $J_{N;\kappa,1}$.

Lemma 4. *For $N \ge 3$ prime and $\kappa \in \{1,\dots,N-1\}$, the quantity $J_{N;\kappa,1}$ from* (25) *satisfies*

$$|J_{N;\kappa,1}| \le \frac{1}{2\pi^2}\frac{N}{N-1}\left(T_N(\kappa)+\frac{10\pi^2\ln N}{9N}\right),$$

where

$$T_N(\kappa) := \sum_{q=1}^{(N-1)/2} \frac{1}{q\,|r(q\kappa,N)|} < \frac{\pi^2}{6}. \tag{27}$$

Proof. We expand the two factors in the sum over q in (25) and then apply the triangle inequality to obtain

$$|J_{N;\kappa,1}| \le \frac{1}{2\pi^2}\frac{N}{N-1}\big(T_N(\kappa)+A_1+A_2+A_3\big),$$

with

$$\begin{aligned}
A_1 &:= \sum_{q=1}^{(N-1)/2} \frac{1}{|r(q\kappa,N)|}\left(\sum_{\ell=1}^{\infty}\frac{2q}{(\ell N)^2-q^2}\right),\\
A_2 &:= \sum_{q=1}^{(N-1)/2} \frac{1}{q}\left(\sum_{\ell'=1}^{\infty}\frac{2\,|r(q\kappa,N)|}{(\ell' N)^2-r(q\kappa,N)^2}\right),\\
A_3 &:= \sum_{q=1}^{(N-1)/2} \left(\sum_{\ell=1}^{\infty}\frac{2q}{(\ell N)^2-q^2}\right)\left(\sum_{\ell'=1}^{\infty}\frac{2\,|r(q\kappa,N)|}{(\ell' N)^2-r(q\kappa,N)^2}\right).
\end{aligned}$$

Since $q \le N/2 \le \ell N/2$ and $|r(q\kappa,N)| \le N/2 \le \ell' N/2$, we have

$$\sum_{\ell=1}^{\infty}\frac{2q}{(\ell N)^2-q^2} \le \sum_{\ell=1}^{\infty}\frac{N}{(\ell N)^2-(\ell N/2)^2} = \frac{4}{3N}\sum_{\ell=1}^{\infty}\frac{1}{\ell^2} = \frac{2\pi^2}{9N},$$

and

$$\sum_{\ell'=1}^{\infty}\frac{2\,|r(q\kappa,N)|}{(\ell' N)^2-r(q\kappa,N)^2} \le \sum_{\ell'=1}^{\infty}\frac{N}{(\ell' N)^2-(\ell' N/2)^2} = \frac{2\pi^2}{9N}.$$

Moreover, we have

$$\sum_{q=1}^{(N-1)/2}\frac{1}{q} \le 1+\int_1^{(N-1)/2}\frac{1}{t}\,\mathrm{d}t \le 2\ln N \tag{28}$$

and

$$\sum_{q=1}^{(N-1)/2}\frac{1}{|r(q\kappa,N)|} = \sum_{t=1}^{(N-1)/2}\frac{1}{t} \le 2\ln N, \tag{29}$$

where in the penultimate step we used the fact that $|r(q\kappa,N)|$ takes all the values from 1 to $(N-1)/2$ exactly once as q runs from 1 to $(N-1)/2$. These estimates lead to

$$A_1 + A_2 + A_3 \le \frac{4\pi^2 \ln N}{9N} + \frac{4\pi^2 \ln N}{9N} + \frac{N-1}{2}\frac{4\pi^4}{81N^2} \tag{30}$$

$$\le \frac{\pi^2 \ln N}{9N}\left(8 + \frac{2\pi^2}{9\ln 3}\right) \le \frac{10\pi^2 \ln N}{9N}. \tag{31}$$

On the other hand, a crude estimate for $T_N(\kappa)$ follows from the Cauchy-Schwarz inequality:

$$T_N(\kappa) \le \left(\sum_{q=1}^{(N-1)/2} \frac{1}{q^2}\right)^{1/2} \left(\sum_{q=1}^{(N-1)/2} \frac{1}{r(q\kappa,N)^2}\right)^{1/2}$$
$$= \left(\sum_{q=1}^{(N-1)/2} \frac{1}{q^2}\right)^{1/2} \left(\sum_{t=1}^{(N-1)/2} \frac{1}{t^2}\right)^{1/2} < \frac{\pi^2}{6}.$$

This completes the proof. □

Numerical experiments show that the value of $T_N(\kappa)$ is much smaller than the crude bound $\pi^2/6$ for most values of κ, and have led us to the following conjecture. Note that we have $r(q(N-\kappa),N) = r(-q\kappa,N) = -r(q\kappa,N)$, and so $T_N(N-\kappa) = T_N(\kappa)$. Moreover, from (25) we conclude that

$$J_{N;N-\kappa,1} = -J_{N;\kappa,1}.$$

Since we are only interested in the magnitude of $J_{N;\kappa,1}$ (see Proposition 3), it suffices to consider only $\kappa \in R_N^+ := \{1,2,\ldots,(N-1)/2\}$.

Conjecture 1. For $N \ge 3$ prime and $\kappa \in R_N^+$, with $T_N(\kappa)$ as defined in (27), let (κ_j) for $j \in R_N^+$ be an ordering of the elements of R_N^+ such that $(T_N(\kappa_j))$ is non-increasing. The conjecture is that there exist $C_1, C_2 > 0$ and $\alpha \ge 2$ independent of N such that

$$T_N(\kappa_j) \le C_1 \frac{(\ln N)^\alpha}{N} \quad \text{for all} \quad j > C_2 (\ln N)^\alpha. \tag{32}$$

Conjecture 1 together with Lemma 4 lead to an estimate for $|J_{N;\kappa_j,1}|$ of the following form:

$$|J_{N;\kappa_j,1}| \le \begin{cases} C_3 & \text{for } j \le C_2 (\ln N)^\alpha, \\ C_4 \dfrac{(\ln N)^\alpha}{N} & \text{for } j > C_2 (\ln N)^\alpha, \end{cases}$$

where C_3 and C_4 are known numerical constants. We will use this bound in the next subsection to obtain the desired result for the mean of the worst-case error.

3.3 Final results

Now we are ready to state our main results.

Theorem 1. *Suppose that Conjecture 1 holds with some $\alpha \geq 2$. For arbitrary $\mathfrak{u} \subseteq \{1:s\}$ and any prime number $N \geq 3$ such that $(\ln N)^\alpha/N \leq 1$, the quantity $\overline{e}_{\mathfrak{u}}(N)$ defined in* (12) *satisfies*

$$\overline{e}_{\mathfrak{u}}(N) \leq C_{\mathfrak{u}} \frac{(\ln N)^{\alpha/2}}{\sqrt{N}}, \tag{33}$$

where

$$C_{\mathfrak{u}} := \sqrt{c_{\mathfrak{u}} + 2C_2\Big(\frac{23}{24}\Big)^{|\mathfrak{u}|} + \Big(\frac{3C_1}{4\pi^2} + \frac{5}{6}\Big)^{|\mathfrak{u}|}}.$$

Here, the constant $c_{\mathfrak{u}}$ is as in Proposition 2, and C_1, C_2 are as in Conjecture 1.

Proof. From Proposition 3 together with $J_{N;N-\kappa,1} = -J_{N;\kappa,1}$, we have

$$\overline{e}^2_{\mathfrak{u}}(N) \leq c_{\mathfrak{u}} \frac{1}{N} + \frac{2}{N} \sum_{j=1}^{(N-1)/2} |J_{N;\kappa_j,1}|^{|\mathfrak{u}|}. \tag{34}$$

For $j \leq C_2(\ln N)^\alpha$, we use $T_N(\kappa_j) \leq \pi^2/6$, $\ln N/N \leq 1$ and $N/(N-1) \leq 3/2$ in Lemma 4 to obtain

$$|J_{N;\kappa_j,1}| \leq \frac{1}{2\pi^2}\frac{N}{N-1}\left(\frac{\pi^2}{6} + \frac{10\pi^2}{9}\frac{\ln N}{N}\right) \leq \frac{1}{2\pi^2}\frac{3}{2}\left(\frac{\pi^2}{6} + \frac{10\pi^2}{9}\right) = \frac{23}{24}.$$

For $j > C_2(\ln N)^\alpha$, we use $\ln N \geq 1$, $N/(N-1) \leq 3/2$ and Conjecture 1 to obtain

$$|J_{N;\kappa_j,1}| \leq \frac{1}{2\pi^2}\frac{N}{N-1}\left(C_1\frac{(\ln N)^\alpha}{N} + \frac{10\pi^2}{9}\frac{\ln N}{N}\right) \leq \left(\frac{3C_1}{4\pi^2} + \frac{5}{6}\right)\frac{(\ln N)^\alpha}{N}.$$

Combining these and using $(\ln N)^\alpha/N \leq 1$, we obtain

$$\begin{aligned}
&\sum_{j=1}^{(N-1)/2} |J_{N;\kappa_j,1}|^{|\mathfrak{u}|} \\
&\leq \sum_{1\leq j\leq C_2(\ln N)^\alpha} \left(\frac{23}{24}\right)^{|\mathfrak{u}|} + \sum_{C_2(\ln N)^\alpha < j \leq (N-1)/2} \left(\frac{3C_1}{4\pi^2} + \frac{5}{6}\right)^{|\mathfrak{u}|}\left(\frac{(\ln N)^\alpha}{N}\right)^{|\mathfrak{u}|} \\
&\leq C_2(\ln N)^\alpha \left(\frac{23}{24}\right)^{|\mathfrak{u}|} + \frac{N-1}{2}\left(\frac{3C_1}{4\pi^2} + \frac{5}{6}\right)^{|\mathfrak{u}|}\frac{(\ln N)^\alpha}{N} \\
&\leq \left(C_2\left(\frac{23}{24}\right)^{|\mathfrak{u}|} + \frac{1}{2}\left(\frac{3C_1}{4\pi^2} + \frac{5}{6}\right)^{|\mathfrak{u}|}\right)(\ln N)^\alpha.
\end{aligned}$$

This together with (34) yields the required result. □

Corollary 1. *Suppose that Conjecture 1 holds with some $\alpha \geq 2$. Let $N \geq 3$ be a prime number. Suppose that the weights $\gamma = (\gamma_{\mathfrak{u}})_{\mathfrak{u}}$ satisfy*

$$C := \sum_{|\mathfrak{u}|<\infty} \gamma_{\mathfrak{u}} C_{\mathfrak{u}} < \infty,$$

where C_{u} is the constant as in Theorem 1. Then, the generating-vector-averaged worst-case error $\overline{e}^2(N)$ defined as in (11) *satisfies*

$$\overline{e}^2(N) \le C\frac{(\ln N)^{\alpha}}{N}, \tag{35}$$

with $C > 0$ independent of s and N. As a consequence, there exists a generating vector $z^* \in Z_N^s = \{z \in \mathbb{Z} \mid 1 \le z \le N-1\}^s$ that attains the worst-case error

$$e(N,z^*) \le \sqrt{C}\frac{(\ln N)^{\alpha/2}}{\sqrt{N}}. \tag{36}$$

Proof. From (11) and Theorem 1, we have

$$\overline{e}^2(N) \le \sum_{\emptyset \ne \mathrm{u} \subseteq \{1:s\}} \gamma_{\mathrm{u}} C_{\mathrm{u}} \frac{(\ln N)^{\alpha}}{N} \le C\frac{(\ln N)^{\alpha}}{N}. \tag{37}$$

Now, recall that $\overline{e}^2(N)$ is defined in (11) as the average of $e^2(N,z)$ over all possible z. Thus, there must be at least one z^* such that

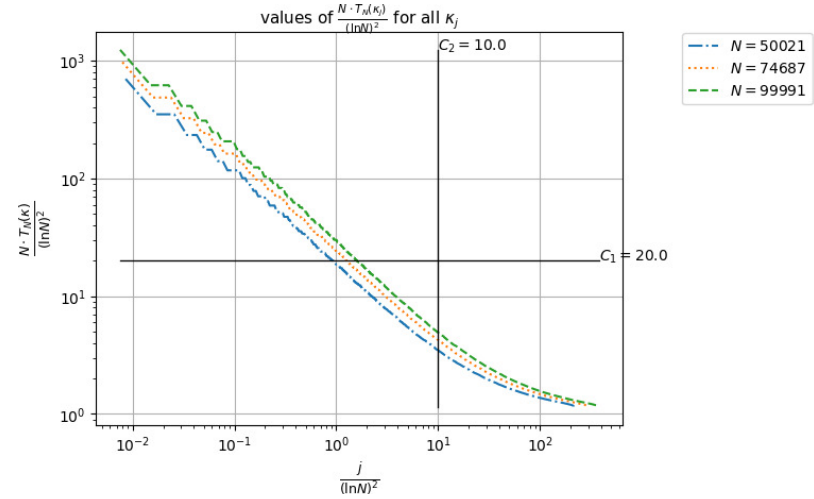
$$e^2(N,z^*) \le C\frac{(\ln N)^{\alpha}}{N},$$

which yields the second statement. □

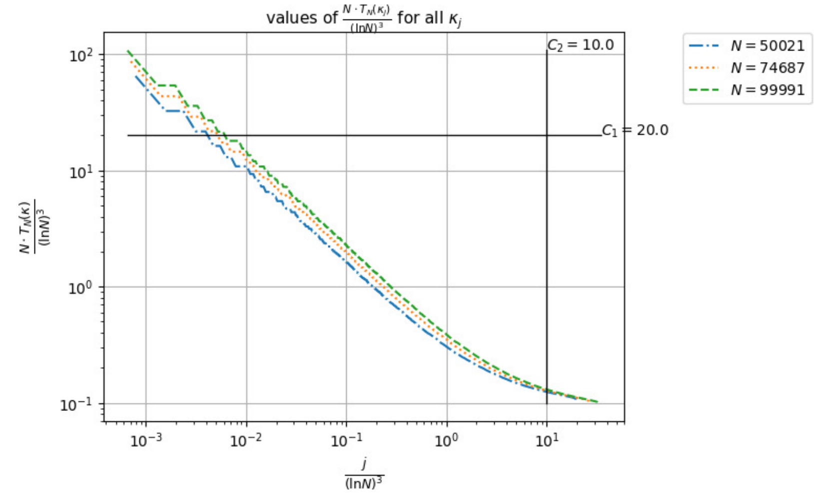
4 Numerical experiments on the conjecture

In this section, we present numerical evidence relating to Conjecture 1. We compute the numbers $\{T_N(\kappa)\}_{\kappa=1}^{(N-1)/2}$, given by (27) for varying N. For each fixed N, we sort these values in non-increasing order, which we write as $(T_N(\kappa_j))_{j=1,\dots,(N-1)/2}$, plot the values, and make a guess of the constants C_1, C_2 in Conjecture 1. We used Julia 0.6.2. for the experiments below.

Figure 1 shows the values of $\frac{N}{(\ln N)^{\alpha}} T_N(\kappa_j)$ against $j/(\ln N)^{\alpha}$ for $j = 1,\dots,(N-1)/2$ with $\alpha = 2,3$, and $N = 50021, 74687, 99991$. We see that for both $\alpha = 2$ and 3 and these values of N we can take constants C_1, C_2 such that for all $j/(\ln N)^{\alpha} > C_2$ with $j = 1,\dots,(N-1)/2$ we have $T_N(\kappa_j)N/(\ln N)^{\alpha} \le C_1$: for example, $C_1 = 20$ and $C_2 = 10$. This is consistent with Conjecture 1, especially for $\alpha = 3$. Of course, we cannot be certain even in this case that the bounds will hold for very large N, with these or any constants. But even if the conjecture fails, the numerical experiments give us confidence, even for $\alpha = 2$, that the bounds in Theorem 1 will hold with $C_1 = 20$ and $C_2 = 10$ for N up to at least a few hundred thousand.



(a)



(b)

Fig. 1: Values of $T_N(\kappa_j)N/(\ln N)^\alpha$, against $j/(\ln N)^\alpha$ for $j = 1,\dots,(N-1)/2$. Top: $\alpha = 2$. Bottom: $\alpha = 3$. We see there exist constants C_1, C_2 such that for all $j/(\ln N)^\alpha > C_2$ we have $T_N(\kappa_j)N/(\ln N)^\alpha \leq C_1$: for example, $C_1 = 20$ and $C_2 = 10$.

5 Concluding remarks

In this paper, we considered the worst-case error for unshifted lattice rules without randomisation. A conjecture to support the error estimate was proposed. Given the conjecture, in Corollary 1 we showed the existence of a generating vector that attains the worst-case error $1/\sqrt{N}$, up to a logarithmic factor. Numerical experiments suggest that the conjecture is plausible.

Corollary 1, which holds if the conjecture is true, shows that some lattice rules work well for non-periodic functions as well. We note that this would not be too surprising: as mentioned in Section 1, Joe [5, 6] has considered CBC constructions for unshifted lattice rules that give good star discrepancy bounds.

In closing, we mention that one difficulty in proving the conjecture is that the ordering of the κ to ensure that $T_N(\kappa_j)$ is non-increasing typically changes completely when N changes.

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