EXTENSIBLE LATTICE SEQUENCES FOR QUASI-MONTE CARLO QUADRATURE

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Abstract. Integration lattices are one of the main types of low discrepancy sets used in quasi-Monte Carlo methods. However, they have the disadvantage of being of fixed size. This article describes the construction of an infinite sequence of points, the first b^m of which form a lattice for any non-negative integer m. Thus, if the quadrature error using an initial lattice is too large, the lattice can be extended without discarding the original points. Generating vectors for extensible lattices are found by minimizing a loss function based on some measure of discrepancy, or non-uniformity of the lattice. The spectral test used for finding pseudo-random number generators is one important example of such a discrepancy. The performance of the extensible lattices proposed here is compared to that of other methods for some practical quadrature problems.

Key words. Discrepancy, good lattice point sets, multidimensional, spectral test

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1. Introduction.

Multidimensional integrals appear in a wide variety of applications in finance [4, 48, 50], physics and engineering [29, 42, 49, 58], and statistics [8, 12, 13]. The integration domain may often be assumed, after some appropriate transformation, to be the unit cube, in which case the integral takes the form:

$$I(f) \equiv \int_{[0,1)^s} f(x)\,dx$$

for some known integrand, f.

Adaptive methods, such as [2], have been developed for approximating multidimensional integrals, but their performance deteriorates as the dimension increases. For finance problems the dimension can be in the hundreds or even thousands. An alternative to adaptive quadrature is Monte Carlo methods, where the integral is approximated by the sample mean of the integrand evaluated on a set, P, of N independent random points drawn from a uniform distribution on $[0,1)^s$:

$$Q(f) \equiv \frac{1}{N}\sum_{z\in P} f(z). \tag{1.1}$$

The quadrature error for Monte Carlo methods is typically $\mathrm{O}(N^{-1/2})$. One reason for this relatively low accuracy is that the points in P are chosen independently of each other. Thus, some parts of the integration domain contain clumps of points while other parts are empty of points.

To obtain greater accuracy one may replace the random set P by a carefully chosen deterministic set that is more uniformly distributed on $[0,1)^s$. As is explained in Section 3, one may define a **discrepancy** that measures how much the empirical distribution function of P differs from the continuous uniform distribution. Then

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one chooses P in quadrature rule (1.1) to have as small a discrepancy as possible. The quadrature methods based on low discrepancy sets are called quasi-Monte Carlo methods. They are discussed in several review articles [3, 16, 40, 59] and monographs [27, 44, 53].

Two important families of low discrepancy sets are:

i. integration lattices [44, Chap. 5] and [53], and

ii. digital nets and sequences [44, Chap. 4].

These two families are introduced in Section 2. One advantage of the second family is that any number of consecutive points from a good digital sequence has low discrepancy. If one needs more points, one may use additional terms from the digital sequence without discarding the original ones. On the other hand, until now, the number of points in an integration lattice has had to be specified in advance. So far, there has been no systematic way of adding points to an integration lattice while still retaining its lattice structure.

The purpose of this article is to provide a method for constructing *infinite lattice sequences*, thereby eliminating the need to know N, the number of points, in advance. Although the emphasis is on rank-1 lattices, the method may be applied to integration lattices of arbitrary rank. Given an infinite lattice sequence one may approximate a multidimensional integrand with a quadrature rule of the form (1.1) for moderate number of points N_0. If the error estimate is unacceptably high, then one may choose an additional $N_1 - N_0$ points from the lattice sequence to obtain a quadrature rule with N_1 points, and so on.

The following section describes the new method for obtaining infinite lattice sequences. Section 3 briefly reviews some results on discrepancy and quadrature error analysis for quasi-Monte Carlo methods. These are used to find the generating vectors for the new lattice sequences in Section 4. The issue of error estimation is addressed in Section 5. Two practical examples are explored in Section 6, where the new lattice sequences are compared with existing quadrature methods. The last section contains some concluding remarks.

2. Integration Lattices and Digital Sequences. This section begins by introducing integration lattices. Next, digital sequences and (t,s)-sequences are described. Finally, the idea underlying digital sequences is used to produce infinite lattice sequences.

2.1. Integration Lattices. Rank-1 lattices, also known as good lattice point (glp) sets, were introduced by Korobov [31] and have been widely studied since then (see [27, 44, 53] and the references therein). The formula for a shifted rank-1 lattice set is simply

$$P = \{\{ih/N + \Delta\} : i = 0, \dots, N-1\}, \tag{2.1}$$

where N is the number of points, h is an s-dimensional generating vector of integers (a good lattice point) that depends on N, Δ is an s-dimensional shift vector in $[0,1)^s$, and $\{x\}$ denotes the fractional part of a vector x, i.e. $\{x\} = x \mod 1$. Sloan [52, 54] later generalized glp sets by introducing more than one generating vector. A shifted integration lattice with $N = N_1 \cdots N_p$ points based on generating vectors $h^{(1)}, \dots, h^{(p)}$ is:

$$P = \left\{ \{i_1 h^{(1)}/N_1 + \cdots + i_p h^{(p)}/N_p + \Delta\} : i_k = 0, \dots, N_k - 1,\ k = 1, \dots, p \right\}.$$

Integration lattices and their use for quadrature are discussed in the monograph [53].

For a given N there is the problem of choosing good generating vectors. Although theoretical constructions exist for $s = 1$ and 2, in higher dimensions one typically finds generating vectors by minimizing a discrepancy or measure of non-uniformity of the lattice. Several examples of discrepancies are given in Section 3.

2.2. Digital Nets and Sequences. Digital nets and sequences are another method of constructing low discrepancy sets (see [32] and [44, Chapter 4]). Let b denote a positive integer greater than one. For any non-negative integer one may extract the digits of its base b representation, $i_1, i_2, \ldots \in \{0, \ldots, b-1\}$, only finitely many of which are nonzero:

$$i = \ldots i_3 i_2 i_1 \text{ (base } b) = i_1 + i_2 b + i_3 b^2 + \cdots . \tag{2.2a}$$

The i^{th} term of a digital net or sequence is given by

$$z^{(i)} = (z_1^{(i)}, \ldots, z_s^{(i)}), \tag{2.2b}$$

$$z_j^{(i)} = 0.\zeta_{j1}^{(i)} \zeta_{j2}^{(i)} \ldots \text{(base } b) = \zeta_{j1}^{(i)} b^{-1} + \zeta_{j2}^{(i)} b^{-2} + \cdots \tag{2.2c}$$

where

$$\begin{pmatrix} \zeta_{j1}^{(i)} \\ \zeta_{j2}^{(i)} \\ \vdots \end{pmatrix} = \mathbf{C}_j \begin{pmatrix} i_1 \\ i_2 \\ \vdots \end{pmatrix} \quad \text{mod } b, \quad j = 1, \ldots, s. \tag{2.2d}$$

If the generating matrices $\mathbf{C}_1, \ldots, \mathbf{C}_s$ are $m \times m$, then this construction yields a digital net $\{z^{(i)} : i = 0, \ldots, b^m - 1\}$ with b^m points. If the generating matrices are $\infty \times \infty$, i.e. each $\mathbf{C}_j$ has entries c_{jkl} defined for $k, l = 1, 2 \ldots$, then one has a digital sequence $\{z^{(i)} : i = 0, 1, \ldots\}$.

The prototype digital sequence is the one-dimensional Van der Corput sequence, $\{\phi_b(i) : i = 0, 1, \ldots\}$. This is defined by taking $s = 1$ and $\mathbf{C}_1$ equal to the identity matrix:

$$\phi_b(i) = 0.i_1 i_2 \ldots \text{ (base } b) = i_1 b^{-1} + i_2 b^{-2} + \ldots . \tag{2.3}$$

In essence, the Van der Corput sequence, takes the b-ary representation of an integer and reflects it about the decimal point.

2.3. (t, m, s)-Nets and (t, s)-Sequences. Similarly to integration lattices one has the problem of how to choose the generating matrices $\mathbf{C}_j$ in (2.2). Usually this is done to optimize the quality factor of the net or sequence. For any non-negative s-vector k, and for a base b consider the following set of disjoint boxes, whose union is the unit cube:

$$\mathcal{B}_k = \{[n_1 b^{-k_1}, (n_1+1) b^{-k_1}) \times \cdots \times [n_s b^{-k_s}, (n_s+1) b^{-k_s}) \\ : n_j = 0, \ldots, b^{k_j} - 1\}. \tag{2.4}$$

Each such box in $\mathcal{B}_k$ has volume $b^{-k_1 - \cdots - k_s}$. A (t, m, s)-net in base b is a set of $N = b^m$ points in $[0, 1)^s$, such that every box in $\mathcal{B}_k$ contains $b^{m - k_1 - \cdots - k_s}$ of these points for any k satisfying $m - k_1 - \cdots - k_s \geq t$. Thus, any function that is piecewise constant on the boxes in $\mathcal{B}_k$ will be integrated exactly according to quadrature rule (1.1) if

$$k_1 + \cdots + k_s \le m - t. \tag{2.5}$$

The integer parameter t is called the quality parameter of the net and it takes values between 0 and m. A smaller value of t means a better net.

A (t,s)-sequence is an infinite sequence of points in $[0,1)^s$ such that the b^m points numbered lb^m to $(l+1)b^m - 1$ always form a (t,m,s)-net for any non-negative integer l. By using a (t,s)-sequence to do quasi-Monte Carlo calculations, one need not know the number of points required in advance. If the first b^{m_1} points do not give sufficient accuracy, then one may add the next $b^{m_2} - b^{m_1}$ points in the sequence to get a net with b^{m_2} points, without throwing away the first b^{m_1} points.

There is a connection between digital nets and sequences as defined above and (t,m,s)-nets and (t,s)-sequences [32]. Let $c_{ji\bullet}^{(m)}$ denote the vector containing the first m elements of the i^{th} row of the the generating matrix $\mathbf{C}_j$. Given a non-negative integer s-vector k, let $\mathcal{C}(m,k)$ be the following set of the first k_j rows of the j^{th} generating matrix for $j = 1, \ldots, s$:

$$\mathcal{C}(m,k) = \left\{ \mathbf{c}_{ji\bullet}^{(m)} : i = 1, \ldots, k_j, \right\}.$$

Furthermore, let

$$\begin{aligned} T(m,s) &= \min_t \{t : \mathcal{C}(m,k) \text{ is a linearly independent set of vectors} \\ &\qquad\qquad \text{for all } k \text{ with } k_1 + \cdots + k_s = m - t\}, \\ T(s) &= \max_m T(m,s). \end{aligned}$$

The following theorem (see [32]) gives the condition for which a digital net is a (t,m,s)-net and a digital sequence is a (t,s)-sequence.

THEOREM 2.1. *For prime bases b the digital net defined above in* (2.2) *is a $(T(m,s),m,s)$-net. If, in addition, $T(s)$ is finite, then the digital sequence defined in* (2.2) *is a $(T(s),s)$-sequence.*

Finding good generating matrices for digital nets and sequences is an active area of research. Virtually all generators found so far have been based on number theoretic arguments. Early sequences include those of Sobol' [56], Faure [9] and Niederreiter [43]. Algorithms for these sequences can be found in the ACM Transactions on Mathematical Software collection. The FINDER software developed at Columbia University by Traub and Papageorgiou implements generalized Sobol' and generalized Faure sequences. New constructions with smaller t values are given by Niederreiter and Xing [47].

2.4. Infinite Lattice Sequences. The idea underlying digital sequences may be extended to integration lattices to obtain infinite lattice sequences. The i^{th} term of a rank-1 lattice, which is $\{ih/N\}$, depends inherently on the number of points, N. Thus, the formula for a lattice must be rewritten in a way that does not involve N explicitly. A way to do this was first suggested in [24].

Suppose that the number of points, N, is some integer power of a base $b \ge 2$, that is, $N = b^m$. This is the same assumption as for a digital or (t,m,s)-net. The first N values of the Van der Corput sequence, defined in (2.3) are

$$\frac{0}{b^m}, \ldots, \frac{b^m - 1}{b^m},$$

although in a different order. Therefore, the term $i/N = i/b^m, i = 0, \dots, N-1$, that appears in the definition of the rank-1 lattice may be replaced by $\phi_b(i)$, a term that does not depend on N.

The s-dimensional generating vector h in (2.1) typically depends on N also. It may be expressed in b-ary form as:

$$h = (h_{1m} \dots h_{11},\ h_{2m} \dots h_{21},\ \dots,\ h_{sm} \dots h_{s1}) \quad (\text{base } b),$$

where $h_{jk} \in \{0, \dots, b-1\}$ are digits. For $k > m$ the digits h_{jk} do not affect the definition of the rank-1 lattice set with $N = b^m$ points since they only contribute integers to the product $\phi_b(i)h$. Therefore, each component of h may be written (in principle) as an infinite string of digits:

$$h = (\dots h_{12}h_{11},\ \dots h_{22}h_{21},\ \dots,\ \dots h_{s2}h_{s1}) \quad (\text{base } b). \tag{2.6}$$

This single "infinite" generating vector may serve for all possible values of m.

The preceding paragraphs provide the basis for defining an infinite rank-1 lattice sequence. Altering the original definition in (2.1) leads to the following:

Definition 2.2. *An infinite rank-1 lattice sequence in base b with generating vector h of the form* (2.6) *and shift Δ is defined as:*

$$\{\{\phi_b(i)h + \Delta\} : i = 0, 1, 2, \dots\}. \tag{2.7}$$

The first b^m terms of the infinite rank-1 lattice sequence (2.7) are a rank-1 lattice. Moreover, just as certain subsets of a (t, s)-sequence are (t, m, s)-nets, so subsets of an infinite rank-1 lattice sequence are shifted rank-1 lattices.

Theorem 2.3. *Suppose that P is the set consisting of the $l + 1^{st}$ run of b^m terms of the infinite lattice rank-1 sequence defined in* (2.7)*:*

$$P = \{\{\phi_b(lb^m + i)h + \Delta\} : i = 0, \dots, b^m - 1\}, \quad l = 0, 1, \dots.$$

Then, P is a rank-1 lattice with shift $\phi_b(l)b^{-m}h + \Delta$, that is,

$$P = \left\{\{\phi_b(i)h + \phi_b(l)b^{-m}h + \Delta\} : i = 0, \dots, b^m - 1\right\}.$$

Proof. The proof follows directly from the definition of the Van der Corput sequence. For all $i = 0, \dots, b^m - 1$, note that

$$\phi_b(lb^m + i) = \phi_b(i) + \phi_b(lb^m) = \phi_b(i) + \phi_b(l)b^{-m}.$$

Substituting the right hand side into the definition of P completes the proof. □

The definition of an infinite rank-1 lattice sequence may be extended to integration lattices of arbitrary rank.

Definition 2.4. *An infinite lattice sequence (of arbitrary rank) with bases $b_1, \dots, b_p$ and generating vectors $h^{(1)}, \dots, h^{(p)}$ of the form* (2.6) *is defined as:*

$$\left\{\{\phi_{b_1}(i_1)h^{(1)} + \dots + \phi_{b_p}(i_p)h^{(p)} + \Delta\} : i_1, \dots, i_p = 0, 1, 2, \dots\right\} \tag{2.8}$$

A practical complication for an integration lattice of rank greater than 1 is that there are multiple indices, i_k, each of which may or may not tend to infinity, and each at its own rate. Because of this complication we will focus on rank-1 lattices in the sections that follow. Theorem 2.3 also has a natural extension to infinite lattice sequences of arbitrary rank, and its proof is similar.

3. Discrepancy. Unlike (t,s)-nets for which there exist explicit constructions of the generating matrices $\mathbf{C}_j$, there are no such explicit constructions of generating vectors h for rank-1 lattices for arbitrary s. Tables of generating vectors for lattices that do exist (see [8, 14, 27]) are usually obtained by minimizing some measure of non-uniformity, or discrepancy, of the lattice. This section describes several useful discrepancy measures.

Let $\mathrm{Err}(f;P)$ denote the quadrature error for a rule of the form (1.1) for an arbitrary set P. Worst case error analysis of the quadrature error leads to a Koksma-Hlawka-type inequality of the form [23]:

$$|\mathrm{Err}(f;P)| \equiv |I(f) - Q(f)| \le D(P)V(f), \tag{3.1}$$

where $D(P)$ is the discrepancy or measure of nonuniformity of the point set defining the quadrature rule, and $V(f)$ is the variation or fluctuation of the integrand, f. The precise definitions of the discrepancy and the variation depend on the particular space of integrands.

In the traditional Koksma-Hlawka inequality (see [26] and [44, Theorem 2.11]), the variation is the variation in the sense of Hardy and Krause, and the discrepancy is the $\mathcal{L}_\infty$-star discrepancy:

$$D^*(P) = \|F_{\mathrm{unif}}(x) - F_P(x)\|_\infty = \left\| x_1 \ldots x_s - \frac{|P \cap [0,x]|}{N} \right\|_\infty . \tag{3.2}$$

Here F_{unif} is the uniform distribution on the unit cube, F_P is the empirical distribution function for the sample P, and $|\cdot|$ denotes the number of points in a set. The notation $\|\cdot\|_p$ denotes the $\mathcal{L}_p$-norm or the ℓ_p-norm, depending on the context. Error bounds of the form (3.1) involving the $\mathcal{L}_p$-star discrepancy have been derived by [57, 62]. Error bounds involving generalizations of the star discrepancy appear in [21, 22, 23, 55].

When the integrands belong to a reproducing kernel Hilbert space, the error bound (3.1) may be easily obtained [21, 23]. The discrepancy may be written in terms of the reproducing kernel

$$\begin{aligned} D(P) &= \left\{ \int_{[0,1)^{2s}} K(x,y)\ d(F_{\mathrm{unif}} - F_P)(x)\ d(F_{\mathrm{unif}} - F_P)(y) \right\}^{1/2} \qquad (3.3)\\ &= \left\{ \int_{[0,1)^{2s}} K(x,y)\ dx\ dy - \frac{2}{N}\sum_{z\in P}\int_{[0,1)^s} K(z,y)\ dy + \frac{1}{N^2}\sum_{z,t\in P} K(z,t) \right\}^{1/2} . \end{aligned}$$

For example, the $\mathcal{L}_2$-star discrepancy, whose formula was originally derived in [60], is a special case of the above formula with $K(x,y) = \prod_{j=1}^s [1 - \max(x,y)]$. An advantage of considering reproducing kernel Hilbert spaces of integrands is that the computational complexity of the discrepancy is relatively small (at worst $\mathrm{O}(N^2)$ operations). By contrast the $\mathcal{L}_\infty$-star discrepancy requires $\mathrm{O}(N^s)$ operations to evaluate.

The discrepancy of type (3.3) can also be interpreted as an average-case quadrature error [25, 41, 61]. Suppose that the integrand is a random function lying in the sample space $\mathcal{A}$, and suppose that the integrand has zero mean and covariance kernel, $K(x,y)$, that is,

$$E_{f\in\mathcal{A}}[f(x)] = 0 \text{ and } E_{f\in\mathcal{A}}[f(x)f(y)] = K(x,y) \quad \forall x,y \in [0,1)^s.$$

Then the root mean square quadrature error over $\mathcal{A}$ is the discrepancy as defined in (3.3):

$$\sqrt{E_{f\in\mathcal{A}}[\mathrm{Err}(f;P)]^2} = \sqrt{E_{f\in\mathcal{A}}\left|I(f)-Q(f)\right|^2} = D(P). \tag{3.4}$$

If P is a simple random sample, then the mean square discrepancy is [25]:

$$E_P\{[D(P)]^2\} = \frac{1}{N}\left\{\int_{[0,1)^s} K(x,x)\ dx - \int_{[0,1)^s\times[0,1)^s} K(x,y)\ dy\ dx\right\} \tag{3.5}$$

This formula serves as a benchmark for other (presumably superior) low discrepancy sets. Since the mean square discrepancy is $\mathrm{O}(N^{-1})$, the discrepancy itself is typically $\mathrm{O}(N^{-1/2})$ for a simple random sample. The variance of a function, f, may be defined as

$$\mathrm{Var}(f) \equiv \int_{[0,1)^s} f^2\ dx - \left(\int_{[0,1)^s} f\ dx\right)^2.$$

The mean value of the variance over the space of average-case integrands can be shown to be [25]:

$$E_{f\in\mathcal{A}}[\mathrm{Var}(f)] = \int_{[0,1)^s} K(x,x)\ dx - \int_{[0,1)^{2s}} K(x,y)\ dy\ dx, \tag{3.6}$$

which is just the term in braces in (3.5).

It may seem odd at first that the discrepancy can serve both as an average-case and worst-case quadrature error. The explanation is that the space of integrands, $\mathcal{A}$, in the average-case analysis is much larger than the space of integrands, $\mathcal{W}$, in the worst-case analysis. See [21, 25] and the references therein for the proofs of the above results as well as further details.

There are some known asymptotic results for the discrepancies of (t,m,s)-nets. The $\mathcal{L}_\infty$-star discrepancy of any (t,m,s)-net is $\mathrm{O}(N^{-1}[\log N]^{s-1})$ [44, Theorem 4.10]. Moreover, the typical (in the sense of an average taken over all possible nets) $\mathcal{L}_2$-star discrepancy of $(0,m,s)$-nets is $\mathrm{O}(N^{-1}[\log N]^{(s-1)/2})$ [19] — the best possible for any set. For discrepancies of the form (3.3) with sufficiently smooth kernels, typical $(0,m,s)$-nets have $\mathrm{O}(N^{-3/2}[\log N]^{(s-1)/2})$ discrepancy [25].

Lattice rules, the topic of this article, are known to be particularly effective for integrating periodic functions. Suppose that the integrand has an absolutely convergent Fourier series with Fourier coefficients $\hat{f}(k)$:

$$f(x) = \sum_{k\in\mathbf{Z}^s} \hat{f}(k)e^{2\pi i k'x}, \qquad \hat{f}(k) = \int_{[0,1)^s} f(x)e^{-2\pi i k'x}\ dx. \tag{3.7}$$

Here $k'x$ denotes the dot product of the s-dimensional wavenumber vector k with x.

The quadrature error for a particular integrand with an absolutely convergent Fourier series is simply the sum of the quadrature errors of each term:

$$\mathrm{Err}(f;P) = -\sum_{\substack{k\in\mathbf{Z}^s\\ k\neq 0}} \hat{f}(k)\left[\frac{1}{N}\sum_{z\in P} \mathrm{e}^{2\pi i k'z}\right],$$

where the term corresponding to $k = 0$ does not enter because constants are integrated exactly. One can multiply and divide by arbitrary weights $w(k)$ inside this sum. Then by applying Hölder's inequality one has the following error bound of the form (3.1) [23]:

$$|\mathrm{Err}(f;P)| \le D_{\mathcal{F},p}(P) V_{\mathcal{F},q}(f), \quad \frac{1}{p} + \frac{1}{q} = 1, \tag{3.8a}$$

$$D_{\mathcal{F},p}(P) = \left\| \left(\frac{1_{\{k \neq 0\}}}{w(k)} \left[\frac{1}{N} \sum_{z \in P} e^{2\pi i k' z} \right] \right)_{k \in \mathbf{Z}^s} \right\|_p, \tag{3.8b}$$

$$V_{\mathcal{F},q}(f) = \left\| \left(1_{\{k \neq 0\}} w(k) \hat{f}(k) \right)_{k \in \mathbf{Z}^s} \right\|_q. \tag{3.8c}$$

Here $1_{\{\cdot\}}$ denotes the indicator function. In order to insure that the discrepancy is finite we assume that the weights increase sufficiently fast as k tends to infinity:

$$\left\| \left(\frac{1}{w(k)} \right)_{k \in \mathbf{Z}^s} \right\|_p < \infty.$$

If P is the node set of an integration lattice, then it is known that trigonometric polynomials are integrated exactly for all nonzero wavenumbers *not* in the dual lattice, $L^\perp$, (see [53, Lemma 2.7]):

$$\frac{1}{N} \sum_{z \in P} e^{2\pi i k' z} = 1_{\{k \in L^\perp\}}.$$

The dual lattice is the set of all k satisfying $k'z = 0 \pmod 1$ $\forall z \in P$. Thus, for node sets of lattices the definition of discrepancy above may be simplified to

$$D_{\mathcal{F},p}(P) = \left\| \left(\frac{1_{\{0 \neq k \in L^\perp\}}}{w(k)} \right)_{k \in \mathbf{Z}^s} \right\|_p.$$

Certain explicit choices of $w(k)$ have appeared in the literature. For example, one may choose

$$w(k) = \left[\overline{(\beta_1^{-1} k_1)} \cdots \overline{(\beta_s^{-1} k_s)} \right]^\alpha, \quad \alpha > 0, \tag{3.9}$$

where the over-bar notation is defined as

$$\bar{k}_j = \begin{cases} |k_j| & \text{for } k_j \neq 0, \\ 1 & \text{for } k_j = 0, \end{cases} \tag{3.10}$$

$\beta_1, \ldots, \beta_s$ are arbitrary positive weights, and α is a measure of the assumed smoothness of the integrand. If $\beta_1 = \cdots = \beta_s = 1$ and P is the node set of a lattice, then $D_{\mathcal{F},p}(P) = [P_{\alpha p}(L)]^{1/p}$ for $1 \le p < \infty$, where $P_\gamma(L)$ is a traditional figure of merit for lattices [53]. Furthermore, for $p = \infty$ the discrepancy is $D_{\mathcal{F},\infty}(P) = [\rho(L)]^{-\alpha}$, where $\rho(L)$ is the **Zaremba figure of merit** for lattice rules [44, Def. 5.31]. The more general case of P not a lattice is considered in [20], and the case of unequal weights β_j is discussed in [22].

If the weight function $w(k)$ takes the form (3.9) for *positive integer* α, then for $p = q = 2$ the infinite sum defining the discrepancy in (3.8b) may be written as a finite sum:

$$D_{\mathcal{F},2}(P) = \left\{ -1 + \frac{1}{N^2} \sum_{z,t \in P} \prod_{j=1}^{s} \left[1 - \frac{(-4\pi^2\beta_j^2)^\alpha}{(2\alpha)!} B_{2\alpha}(\{z_j - t_j\}) \right] \right\}^{1/2}, \quad (3.11a)$$

for general sets P, where $B_{2\alpha}$ denotes the Bernoulli polynomial of degree 2α [1, Chap. 23]. When P is the node set of an integration lattice, the double sum can be simplified to a single sum:

$$D_{\mathcal{F},2}(P) = \left\{ -1 + \frac{1}{N} \sum_{z \in P} \prod_{j=1}^{s} \left[1 - \frac{(-4\pi^2\beta_j^2)^\alpha}{(2\alpha)!} B_{2\alpha}(z_j) \right] \right\}^{1/2}. \quad (3.11b)$$

Another choice for $w(k)$ is a weighted ℓ_r-norm of the vector k to some power:

$$w(k) = \left[\left(\frac{k_1}{\beta_1}\right)^r + \cdots + \left(\frac{k_s}{\beta_s}\right)^r \right]^{\alpha/r}, \quad \alpha > 0,$$

again for arbitrary positive weights $\beta_1, \ldots, \beta_s$. When these weights are unity, P is the node set of a lattice, and $p = \infty$, then

$$D_{\mathcal{F},\infty}(P) = \max_{0 \neq k \in L^\perp} \|k\|_r^{-\alpha} = \left\{ \min_{0 \neq k \in L^\perp} \|k\|_r \right\}^{-\alpha}. \quad (3.12)$$

For $r = 2$ this discrepancy is equivalent to the **spectral test**, commonly employed to measure the quality of linear congruential pseudo-random number generators [30, 33]. The spectral test has been used to select lattices for quasi-Monte Carlo quadrature in [7, 34, 35, 36]. The case $r = 1$, which one might call an ℓ_1-spectral test is also interesting. We will return to these two cases in the next section.

4. Good Generating Vectors for Lattice Sequences. As mentioned at the beginning of the previous section, finding good generating vectors for lattices typically requires optimizing some discrepancy measure. In this subsection we propose some loss functions and optimization algorithms for choosing good generating vectors for extensible rank-1 lattice sequences.

In principle one would like to have an $s \times \infty$ array of digits h_{jk}, according to (2.6). However, in practice it is only necessary to have an $s_{\max} \times m_{\max}$ array of digits h_{jk}, where $N_{\max} = b^{m_{\max}}$ is the maximum number of points and $s_{\max}$ is the maximum dimension to be considered. In finance calculations, for example, the necessity of timely forecasts may constrain one to a budget of $10^3 - 10^4$ points (Anargyros Papageorgiou, private communication).

For simplicity we consider generating vectors h that are of the form originally proposed by Korobov, that is,

$$h = (1, \eta, \eta^2, \ldots, \eta^{s-1}). \quad (4.1)$$

This means that only the digits $\eta_1, \eta_2, \ldots, \eta_{m_{\max}}$ need to be chosen, for which there are $b^{m_{\max}} = N_{\max}$ choices. The generating vector is tested for dimensions up to $s_{\max}$, but in fact it can be extended to any dimension.

The number η defining the generating vector is chosen by minimizing a loss function, G, of the form

$$G(\eta) = \max_{m,s} \tilde{G}(\eta, m, s). \tag{4.2}$$

Here the function $\tilde{G}(\eta, m, s)$ is related to one of the measures of discrepancy introduced in Section 3, and the maximum over some range of values of m and s insures that the resulting generating vector is good for a range of numbers of points and dimensions. However, since the discrepancy itself depends significantly on the number of points and the dimension, it must be appropriately scaled to arrive at the function $\tilde{G}$. The details of this scaling are given below.

4.1. Generating Vectors Based on Minimizing P_α. The discrepancy defined in (3.11), which is a generalization of the P_α figure of merit for lattice rules, has the advantage of requiring only $\mathrm{O}(sN)$ operations to evaluate for lattices. To remove some of the dimension dependence of this discrepancy it is divided by the square root of right hand side of (3.6). The root mean square of this scaled discrepancy for a random sample is then $N^{-1/2}$, independent of s. The formula for the scaled discrepancy of the node set of a lattice with $\alpha = 1$ and $4\pi^2\beta_j^2 = 6$ is

$$D(P) = \left[\left(\frac{3}{2}\right)^s - 1\right]^{-1/2} \left\{-1 + \frac{1}{N}\sum_{z\in P}\prod_{j=1}^{s}[1 + 3B_2(z_j)]\right\}^{1/2}.$$

The specific choice of the value of β_j here is not crucial, but seems to give good results.

For one-dimensional lattices, i.e. evenly spaced points on the interval $[0, 1)$, this discrepancy is N^{-1}, and one would expect that as the dimension increases this scaled discrepancy would tend to (or at least do no worse than) $N^{-1/2}$. Therefore, to remove this remaining dimension dependence the above scaled discrepancy is divided by the function:

$$D_{\text{asy}}(m, s) = b^{-m}\left(1 + \frac{m\log b}{s-1}\right)^{(s-1)/2} = N^{-1}\left(1 + \frac{\log N}{s-1}\right)^{(s-1)/2}.$$

For a fixed s, D_{asy}(m,s) is asymptotically $\mathrm{O}(b^{-m}m^{(s-1)/2}) = \mathrm{O}(N^{-1}[\log N]^{(s-1)/2})$ as N tends to infinity. This is the asymptotic order for $(0, m, s)$-nets [25], and what we hope to achieve for lattice sequences. Furthermore, $N^{-1} = b^{-m} \leq D_{\text{asy}}(m, s) \leq b^{-m/2} = N^{-1/2}$ for any m and s. In summary, the resulting loss function is

$$\begin{aligned}\tilde{G}_1(\eta, m, s) = \frac{D(P)}{D_{\text{asy}}(m, s)} &= b^m\left(1 + \frac{m\log b}{s-1}\right)^{-(s-1)/2}\left[\left(\frac{3}{2}\right)^s - 1\right]^{-1/2} \\ &\times \left\{-1 + \frac{1}{b^m}\sum_{i=0}^{b^m-1}\prod_{j=1}^{s}\left[1 + 3B_2(\{\phi_b(i)\eta^{j-1}\})\right]\right\}^{1/2}\end{aligned} \tag{4.3}$$

The optimal values of η found by minimizing $G_1(\eta)$ for $b = 2$ and for different ranges of m and s are given in Table 4.1. The algorithm for optimizing $G_1(\eta)$ may be described as an intelligent exhaustive search. One need not compute $G_1(\eta)$ for all possible values of η. Suppose at any stage of the optimization η_* is the best known value of η, and one finds that $\tilde{G}_1(\tilde{\eta}, m, s) > G_1(\eta_*)$ for some $\tilde{\eta}$. Since $\tilde{G}_1(\eta, m, s)$ depends only on the first $m-1$ digits of η, one can immediately eliminate from consideration all η that have the same first $m-1$ digits as $\tilde{\eta}$. This same search strategy is also used for the other loss functions described below.

4.2. Generating Vectors Based on the Spectral Test. The use of the spectral test to analyze the lattice structure of linear congruential generators is described in [30] and tables of good integration lattices are given in [34]. The difference here is that nearly all smaller lattices imbedded in the largest lattice considered must have low discrepancy. In [34], only the full lattice was examined.

The length of the shortest non-zero vector in the dual lattice $L^{\perp}$ is

$$d_2(\eta, m, s) = \min\{\|k\|_2 : k \neq 0,\ k'(1, \eta, \dots, \eta^{s-1}) = 0 \mod b^m\}, \tag{4.4}$$

which is related to the discrepancy (3.12) with $r = 2$. This length has the absolute upper bound

$$d_2^*(m, s) = \begin{cases} \gamma_s b^{m/s} & 1 \leq s \leq 8 \\ \rho_s b^{m/s} & 8 < s \end{cases} \tag{4.5}$$

where the constants γ_s and ρ_s depend only on s (see [34] and the references therein). The bound for $s \leq 8$ is the least upper bound for a general s-dimensional lattice with real-valued coordinates, and with b^{-m} points per unit of volume. The bound for $s > 8$ is not the least upper bound, but it is still reasonably tight, as our numerical results will show. We define the normalized ℓ_2-spectral test discrepancy as

$$\tilde{G}_2(\eta, m, s) = \frac{d_2^*(m, s)}{d_2(\eta, m, s)}, \tag{4.6}$$

which is larger than 1 and is the inverse of the quantity S_t defined in [34]. (The different notation here is to be consistent with the rest of this article). The loss function to be minimized is of the form (4.2) with $\tilde{G} = \tilde{G}_2$.

We note that $1/d_2(\eta, m, s)$ can be interpreted as the (Euclidean) distance between the successive hyperplanes that contain all the points of the *primal* lattice L, for the family of hyperplanes for which this distance is the largest. The problem of computing a shortest vector in (4.4) can be formulated as a quadratic optimization problem with s integer decision variables, because k can be written as a linear combination of the s vectors of a basis of the dual lattice, with integer coefficients. The decision variables are these coefficients. (See [30] for details.) We solved this problem by using the branch-and-bound algorithm of Fincke and Pohst [10], with a few heuristic modifications to improve the speed. The *worst-case* time complexity of this algorithm is exponential in $d_2(\eta, m, s)$, and polynomial in s for $d_2(\eta, m, s)$ fixed [10]. In practice, it (typically) works nicely even when $d_2(\eta, m, s)$ is large. For example, one can compute $d_2(\eta, 30, s)$ for $b = 2$, an arbitrary η and $s = 2, \dots, 30$ in less than 1 second on a Pentium-II computer.

4.3. Generating Vectors Based on the ℓ_1-spectral Test. With the ℓ_1 norm, the length of the shortest non-zero vector in $L^{\perp}$ is

$$d_1(\eta, m, s) = \min\{\|k\|_1 : k \neq 0,\ k'(1, \eta, \dots, \eta^{s-1}) = 0 \mod b^m\}, \tag{4.7}$$

which is related to the discrepancy (3.12) with $r = 1$. One has the upper bound

$$d_1(\eta, m, s) \leq d_1^*(m, s) \stackrel{\text{def}}{=} (s! b^m)^{1/s},$$

which was established by Marsaglia [37] by applying the general convex body theorem of Minkowski. This suggests the normalized ℓ_1-spectral test quantity:

$$\tilde{G}_3(\eta, m, s) = \frac{d_1^*(m, s)}{d_1(\eta, m, s)}. \tag{4.8}$$

Here, we want to minimize the loss function (4.2) with $\tilde{G} = \tilde{G}_3$.

One can interpret $d_1(\eta, m, s)$ (or $d_1(\eta, m, s) - 1$ in certain cases; see [30]) as the minimal number of hyperplanes that cover all the points of P. We computed $d_1(\eta, m, s)$ via the algorithm of Dieter [6], which works fine for s up to about 10 (independently of m), but becomes very slow for larger s (the time is exponential in s).

The ℓ_1-spectral test quantity in (4.8) has an interpretation similar that the quality parameter t for (t, m, s)-nets. Define

$$T(\eta, m, s) = \log_b(\tilde{G}_3(\eta, m, s)) = \frac{m + \log_b(s!)}{s} - \log_b(d_1(\eta, m, s)).$$

Since $\tilde{G}_3 \geq 1$ and $d_1(\eta, m, s) \geq 1$, it follows that $0 \leq T(\eta, m, s) \leq [m + \log_b(s!)]/s$. Thus, the rank-1 lattice defined by η integrates exactly all trigonometric polynomials of wavenumber k when

$$\log(|k_1| + \cdots + |k_s|) \leq \frac{m + \log_b(s!)}{s} - T(\eta, m, s).$$

If one considers $T(\eta, m, s)$ as the quality parameter of the lattice, then this condition is similar to that in (2.5). There, t determines the resolution at which piecewise constant functions that are exactly integrated by a net. Here, $T(\eta, m, s)$ determines the resolution at which trigonometric polynomials are integrated exactly by a lattice.

The discrepancy for the node set of this lattice as defined in (3.12) with $r = 1$ is

$$D_{\mathcal{F},\infty}(P) = d_1(\eta, m, s)^{-\alpha} = (s!)^{-\alpha/s} b^{\alpha T(\eta, m, s)} N^{-\alpha/s}.$$

If one can construct an infinite sequence of digits, η, for which

$$T(\eta, s) = \max_m T(\eta, m, s) < \infty,$$

then the above discrepancy decays like $N^{-\alpha/s}$. Again, the parameter α indicates the assumed smoothness of the integrands.

4.4. Tables of Coefficients. We made computer searches to find the best η's, based on minimizing the worst-case loss function

$$G_i(\eta, m_0, m_1, s_1) = \max_{\substack{m_0 \leq m \leq m_1 \\ 1 \leq s \leq s_1}} \tilde{G}_i(\eta, m, s) \tag{4.9}$$

for $i = 1, 2, 3$, and selected values of m_0, m_1, and s_1. The bounds m_0, m_1, and s_1 define a range of number of points in the lattice, and maximal number of dimensions, that we are interested in. Selecting different parameters η for different ranges of values of m and s is a convenient compromise between the extreme cases of choosing a different η for each pair (m, s), and choosing the same η for all pairs (m, s). In practice one typically has a general idea of how many points one is going to take. By selecting an η specialized for that range, one can obtain a lattice with a better figure of merit for this particular range.

Table 4.1 gives the optimal η's and the corresponding figures of merit (4.9) for $i = 1, 2, 3$ and certain triples (m_0, m_1, s_1). Because of computational efficiency constraints, for the searches, we limited ourselves to $m_1 \leq 20$ for $i = 1$ and to $s_1 \leq 10$ for $i = 3$. Then, for the best η that we found, we verified the performance when m_0 was reduced or when m_1 or s_1 was increased, and retained the smallest m_0 and largest m_1 and s_1 for which G_i was unchanged. The table also gives the value of $G_{i,\min}(\eta, m_0, m_1, s_1)$, defined by replacing max by min in (4.9). This best-case figure tells us the range of values taken by $\tilde{G}_i(\eta, m, s)$ over the given region. We also made exhaustive searches with $s_1 = 15$ for all the entries where $i = 1$ or 2 in the table, and obtained the same values of η and $G_i(\eta, m_0, m_1, s_1)$ in all cases.

TABLE 4.1
Values of η defining generating vectors of the form (4.1) *for rank-1 lattice sequences with base $b = 2$, and minimizing* (4.9).

i	m_0	m_1	s_1	η	$G_i(\eta, m_0, m_1, s_1)$	$G_{i,\min}(\eta, m_0, m_1, s_1)$
1	0	17	32	17797	4.11	0.78
1	0	12	32	203	2.33	0.78
1	0	16	32	17797	3.57	0.78
1	13	20	32	407641	5.86	0.97
2	0	17	25	1267	2.05	1.00
2	1	16	34	12915	1.90	1.00
2	6	12	33	1571	1.88	1.10
2	8	17	32	11335	1.83	1.03
2	14	20	37	156487	1.76	1.05
2	15	24	32	4450341	1.79	1.07
3	6	16	12	237	2.25	1.07
3	6	12	10	53	2.25	1.14
3	10	16	11	173	2.25	1.15
3	14	21	11	391485	2.00	1.01
3	16	24	10	1459305	2.10	1.11

5. Estimating Quadrature Error. The advantage of an extensible lattice sequence is that N need not be specified in advance. Therefore, in practice one would estimate the quadrature error for an initial lattice, and continue to increase the lattice size until the quadrature error meets the desired tolerance. Although the discrepancy, $D(P)$, is a good measure for the quality of a set P, it cannot be used directly for error estimation. The worst case error bounds (3.1) are often quite conservative, and there is no easy way to estimate the variation of the integrand. The average case error given, (3.4), is sensitive to how one defines the kernel — multiplying the kernel by a factor of c^2 changes the average case error by a factor of c.

Quadrature error estimates for lattice rules have been investigated by [5, 28, 53]. Two different kinds of quadrature rules and error estimates have been proposed. Both involve estimating the error for $Q(f;P)$ in terms of $Q(f;P)$ and $Q(f;P_l)$, $l = 1, \ldots, M$, where the P_l are node sets of lattices and $P = P_1 \cup \cdots \cup P_M$.

The method proposed in [53] takes P to be composed of 2^s shifted copies of a rank-1 lattice. Rather than considering copy rules, we take P_l to be the node sets of shifted lattices of size b^{m_1} imbedded in the extensible lattice described in Section 2.4:

$$P_l = \{\{\phi_b((l-1)b^{m_1} + i)h + \Delta\} : i = 0, \ldots, b^{m_1} - 1\}, \quad l = 1, \ldots, M, \tag{5.1a}$$
$$P = \{\{\phi_b(i)h + \Delta\} : i = 0, \ldots, Mb^{m_1} - 1\}, \tag{5.1b}$$

Another quadrature rule and error estimate takes the P_l to be independent random shifts of a lattice. This can be done by taking:

$$P_l = \{\{\phi_b(i)h + \Delta_l\} : i = 0, \dots, b^{m_1} - 1\}, \quad l = 1, \dots, M, \tag{5.2a}$$
$$P = \{\{\phi_b(i)h + \Delta_l\} : i = 0, \dots, b^{m_1} - 1, \ l = 1, \dots, M\}, \tag{5.2b}$$

where the Δ_l are independent, uniformly distributed random vectors in $[0,1]^s$.

Note that for both (5.1) and (5.2) the set P can be extended in size as necessary by increasing m_1. The theory behind the error estimates for cases (5.1) and (5.2) are given in the following theorem.

THEOREM 5.1. *Suppose that a quadrature rule $Q(\cdot;P)$ based on some arbitrary P, as given in* (1.1), *is the average value of the quadrature rules based on the sets $P_1, \dots, P_M$, that is,*

$$Q(\cdot;P) = \frac{1}{M}\sum_{l=1}^{M} Q(\cdot;P_l). \tag{5.3}$$

First, consider the case where the integrands are random functions from a sample space $\mathcal{A}$ as described in the paragraph preceding (3.4). *Then it follows that*

$$E_{f\in\mathcal{A}}[I(f) - Q(f;P)]^2$$
$$= \left\{-1 + \frac{1}{M}\sum_{l=1}^{M}\left[\frac{D(P_l)}{D(P)}\right]^2\right\}^{-1} \frac{1}{M}\sum_{l=1}^{M} E_{f\in\mathcal{A}}[Q(f;P_l) - Q(f;P)]^2, \tag{5.4}$$

where D is the discrepancy based on the covariance kernel for $\mathcal{A}$.

Secondly, consider the case of a fixed integrand, f, but where the P_l are random shifts of a set P_0, that is,

$$P = P_1 \cup \dots \cup P_M, \qquad P_l = \{\{z + \Delta_l\} : z \in P_0\}, \tag{5.5}$$

for independent, uniformly distributed $\Delta_1, \dots, \Delta_M$. Then

$$E_{\Delta_l}\{[I(f) - Q(f;P)]^2\} = \frac{1}{M(M-1)}\sum_{l=1}^{M} E_{\Delta_l}[Q(f;P_l) - Q(f;P)]^2. \tag{5.6}$$

Proof. Assuming that the quadrature rules satisfy (5.3), it follows that the mean square deviation of the $Q(f;P_l)$ from $Q(f;P)$ may be written as

$$\frac{1}{M}\sum_{l=1}^{M}[Q(f;P_l) - Q(f;P)]^2 = \frac{1}{M}\sum_{l=1}^{M}\{[I(f) - Q(f;P)] - [I(f) - Q(f;P_l)]\}^2$$
$$= -[I(f) - Q(f;P)]^2 + \frac{1}{M}\sum_{l=1}^{M}[I(f) - Q(f;P_l)]^2. \tag{5.7}$$

If the integrand is a random function from a sample space $\mathcal{A}$ with covariance kernel K, then average case error analysis in (3.4) plus (5.7) leads to the following equations:

$$E_{f\in\mathcal{A}}[I(f) - Q(f;P)]^2 = [D(P)]^2,$$
$$E_{f\in\mathcal{A}}[I(f) - Q(f;P_l)]^2 = [D(P_l)]^2,$$
$$E_{f\in\mathcal{A}}\left\{\frac{1}{M}\sum_{l=1}^{M}[Q(f;P_l) - Q(f;P)]^2\right\} = -[D(P)]^2 + \frac{1}{M}\sum_{l=1}^{M}[D(P_l)]^2.$$

The equations above may be rearranged to give (5.4).

The quadrature error for rule $Q(f;P)$ may also be written as:

$$\begin{aligned}[I(f)-Q(f;P)]^2 &= \left\{\frac{1}{M}\sum_{l=1}^{M}[I(f)-Q(f;P_l)]\right\}^2 \\ &= \frac{1}{M^2}\sum_{l=1}^{M}[I(f)-Q(f;P_l)]^2 \\ &\quad + \frac{2}{M^2}\sum_{1\le k<l\le M}[I(f)-Q(f;P_i)][I(f)-Q(f;P_l)].\end{aligned}$$

Substituting the sum of the $[I(f)-Q(f;P_l)]^2$ by equation (5.7) gives:

$$\begin{aligned}[I(f)-Q(f;P)]^2 &= \frac{1}{M(M-1)}\sum_{l=1}^{M}[Q(f;P_l)-Q(f;P)]^2 \\ &\quad + \frac{2}{M(M-1)}\sum_{1\le k<l\le M}[I(f)-Q(f;P_k)][I(f)-Q(f;P_l)]. \qquad (5.8)\end{aligned}$$

If the P_l are random shifts as in (5.5), then the expected value of the term $[I(f) - Q(f;P_k)][I(f)-Q(f;P_l)]$ vanishes for all $k \neq l$ and taking the expected value of (5.8) yields (5.6). □

Some remarks are in order to explain the assumptions and conclusions of the above theorem. These are given below.

Assumption (5.3), and thus conclusion (5.4), holds for both the cases (5.1) and (5.2) above. In fact, this part of the theorem holds for any imbedded rule or any rule where the P_l all contain the same number of points, and their union is P or multiple copies of P. For example, (5.4) would apply to the case where P is a (t,m,s)-net made up of a union of subnets P_l.

Assumption (5.5), and therefore conclusion (5.6) holds for (5.2). There is a difficulty if one tries to derive a result like (5.6) for an imbedded rule of the form (5.1), where Δ is a random shift. The argument leading to (5.6) assumes that the points in different P_l are uncorrelated, which is not true for (5.1). However, if the extensible lattice is a good one, it is expected that the terms $[I(f)-Q(f;P_k)][I(f)-Q(f;P_l)]$ in (5.8) are on average negative. Under this assumption one may then conclude that the right hand side of (5.6) is a conservative (too large) upper bound on the expected square quadrature error.

The factor in (5.4) above involving the discrepancies of P and the P_l does not depend strongly on the particular choice of discrepancy, but only on the asymptotic rate of decay. If, for example, $D(P) \approx CN^{-\alpha}$ for some unknown C, but known α, where N is the number of points in P, then

$$E_{f\in\mathcal{A}}[I(f)-Q(f;P)]^2 \approx \frac{1}{M(M^{2\alpha}-1)}\sum_{l=1}^{M}E_{f\in\mathcal{A}}[Q(f;P_l)-Q(f;P)]^2. \qquad (5.9)$$

Although conclusions (5.6) and (5.9) are derived under different assumptions, they both suggest error estimates of the form

$$[I(f)-Q(f;P)]^2 \lessapprox \frac{c^2}{M(M^{2\alpha}-1)}\sum_{l=1}^{M}[Q(f;P_l)-Q(f;P)]^2, \qquad (5.10)$$

where $\alpha = 1/2$ for (5.6) and α indicates the rate of decay of the discrepancy for (5.9). The factor $c > 1$ depends on how conservative one wishes to be. The Chebyshev inequality implies that the above inequality will hold "at least" $100(1 - c^{-2})\%$ of the time. Error estimate (5.10) leads to the stopping criteria:

$$\frac{c^2}{M(M-1)} \sum_{l=1}^{M} [Q(f;P_l) - Q(f;P)]^2 < \epsilon^2, \tag{5.11}$$

where ϵ is the absolute error tolerance. Note that if the stopping criteria is not met, one would normally increase the *size* of the P_l by increasing m_1, rather than increasing the *number* of the P_l by increasing M.

For some high dimensional problems the discrepancy of a lattice (or other low discrepancy set) may decay as slowly as the Monte Carlo rate of $O(N^{-1/2})$ for small N (see [18, 41]). Therefore, even when using (5.9), it may be advisable to make a conservative choice of $\alpha = 1/2$. This choice makes the approach of error estimate (5.9), based on random integrands, equivalent to that of (5.6), based on randomly shifted P_l.

Sloan and Joe [53, Section 10.3] suggest an error estimate of the form

$$[I(f) - Q(f;P)]^2 \lessapprox \frac{c^2}{s} \sum_{l=1}^{s} [Q(f;P_l) - Q(f;P)]^2,$$

where P is formed from 2^s copies of a rank-1 lattice, and each $Q(f;P_l)$ is an imbedded rule based on half of the points in P. Although this case does not exactly fit Theorem 5.1, the arguments in the proof can be modified to obtain a result similar to to (5.4):

$$\begin{aligned} &E_{f\in\mathcal{A}}[I(f) - Q(f;P)]^2 \\ &\qquad = \left\{ -1 + \frac{1}{s} \sum_{l=1}^{s} \left[\frac{D(P_l)}{D(P)} \right]^2 \right\}^{-1} \frac{1}{s} \sum_{l=1}^{s} E_{f\in\mathcal{A}}[Q(f;P_l) - Q(f;P)]^2. \end{aligned}$$

This would suggest that the error estimation formula of Sloan and Joe is reasonable when $D(P_l) \geq \sqrt{2} D(P)$ on average. The disadvantage of 2^s-copy rules is that they require at least 2^s points, which may be unmanageable for large s.

To summarize, both imbedded lattice rules, (5.1), and independent random shifts of lattices, (5.2), have similar error estimates, (5.10), and stopping criteria, (5.11). The advantage of the independent random shifts approach is that, the theory holds for any integrand, not the average over a space of integrands. One advantage of the imbedded rules approach is that one need only generate a single extensible lattice. Furthermore, the set P for the imbedded rule is the node set of a lattice (if M is a power of b), which is never the case for the independent random shifts approach. Thus, the accuracy of the imbedded rule approach is likely to be better. In the examples in the next section, the imbedded lattice rules based on (5.1) are used.

6. Examples of Multidimensional Quadrature. Two example problems are chosen to demonstrate the performance of the new rank-1 lattice sequences proposed in Section 2.4. The first example is the computation of multivariate normal probabilities and the second is the evaluation of a multidimensional integral arising in physics problems.

6.1. Multivariate Normal Probabilities. Consider the following multivariate normal probability:

$$\frac{1}{\sqrt{|\mathbf{\Sigma}|(2\pi)^s}} \int_{a_1}^{b_1} \cdots \int_{a_s}^{b_s} e^{-\frac{1}{2}\theta' \mathbf{\Sigma}^{-1}\theta} \, d\theta. \tag{6.1a}$$

where, a and b are known s-dimensional vectors, and $\mathbf{\Sigma}$ is a given $s \times s$ positive definite covariance matrix. Some a_j and/or b_j may be infinite.

Unfortunately, the original form is not well-suited for numerical quadrature. Therefore, Alan Genz [12] proposed a transformation of variables that results in an integral over an $s-1$-dimensional unit cube. See [12, 13] for the details of the transformation, and see [13, 15] for comparisons of different methods for calculating multivariate normal probabilities.

The particular test problem is one considered by [13, 24] and may be described as follows:

$$a_1 = \cdots = a_s = -\infty, \tag{6.1b}$$

$$b_j \text{ i.i.d. uniformly on } [0, \sqrt{s}], \tag{6.1c}$$

$$\mathbf{\Sigma} \text{ generated randomly according to [13, 38].} \tag{6.1d}$$

Numerical comparisons were made using three types of algorithms:

i. the adaptive algorithm DCHURE [2],
ii. an older Korobov rank-1 lattice rule with a different generating vector for each N and s — this algorithm is a part of NAG and is used in [5, 12], and
iii. the new rank-1 lattice sequences proposed in Section 2.4 with generating vectors given in Table 4.1

For the second and third algorithms we applied the periodizing transformation $x_j' = |2x_j - 1|$ to the integrand over the unit cube. This appears to increase the accuracy of the lattice rule methods. The computations were carried out in FORTRAN on a Unix work station in double precision. The absolute error tolerance was chosen to be $\epsilon = 10^{-4}$, and this was compared with the actual error E. Since the true value of the integral is unknown for this test problem, the value given by the Korobov algorithm with a tolerance of $\epsilon = 10^{-8}$ was used as the "exact" value for computing the error. For the new rank-1 lattice sequences the stopping criterion (5.11) was used with M between 4 and 7 and $c = 3$.

For each dimension 50 random test problems were generated and solved by the various quadrature methods. The scaled absolute errors E/ϵ and the computation times in seconds are given in the box and whisker plots of Fig. 6.1. The boxes contain the middle half of the values and the whiskers give the range of most values except the outliers (denoted by $*$).

Ideally, the scaled error should nearly always be less than one, otherwise the error estimate is not conservative enough. On the other hand if the scaled error is too small, then the error estimate is too conservative. Fig. 6.1 shows that the adaptive rule performs well for smaller dimensions, but underestimates the error and is quite slow in higher dimensions. The lattice rules do well even in higher dimensions, and the new rank-1 lattice sequences appear to be faster than the older Korobov-type rule. This is likely due to the fact that the lattice sequences proposed here can re-use the old points when N must be increased.

6.2. A Multidimensional Integral from Physics. Keister [29] considered the following multidimensional integral that has applications in physics:

$$\int_{\mathbf{R}^s} \cos(\|x\|_2) e^{-\|x\|_2^2} \, dx = \pi^{s/2} \int_{[0,1)^s} \cos\left(\sqrt{\sum_{j=1}^{s} \frac{[\Phi^{-1}(y_j)]^2}{2}}\right) \, dy, \tag{6.2}$$

where Φ denotes the standard Gaussian distribution function. Keister gave an exact formula for the answer and compared the quadrature methods of McNamee and Stenger [39] and Genz and Patterson [11, 51] for evaluating this integral. Later, Papageorgiou and Traub [49] applied the generalized Faure sequence from FINDER to this problem.

The results of numerical experiments for the above integral for dimension 25 are shown in Figure 6.2. The exact value of the integral is reported in [49]. To be consistent with the numerical results reported in [29, 49], we did not perform error estimation, but just computed the actual error for each kind of numerical method as a function of N, the number of points. Because $\Phi^{-1}(0) = -\infty$ there is a technical difficulty with using an unshifted lattice rule, so when performing the numerical experiments the lattice sequences were given random shifts (modulo 1). Box and whisker plots show how well the new rank-1 lattice sequences perform for 50 random shifts.

According to Figure 6.2 the generalized Faure sequence (in base 29) and the lattice sequence perform much better than the other two rules. In some cases the lattice sequences perform better than the generalized Faure sequence.

7. Conclusion. Lattice rules are simpler to code than digital nets. Given the construction in Section 2.4, it is now possible to have extensible lattice sequences in the same way that one has (t, s)-sequences. Good generating vectors for these lattice sequences may be found by using the spectral test or minimizing other discrepancy measures, as shown in Section 4. The performance of these lattice rules is in many cases comparable to other multidimensional quadrature rules and in some cases superior.

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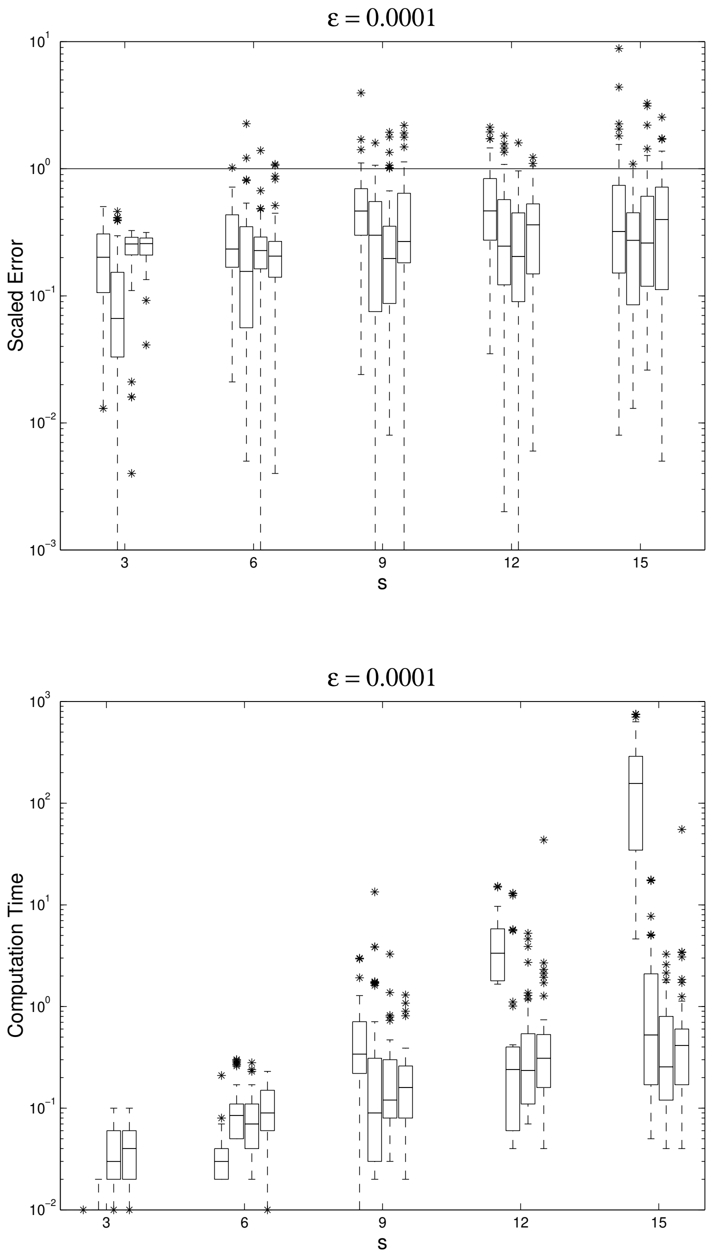

FIG. 6.1. *Box and whisker plots of scaled errors, E/ϵ, and the computation times in seconds for 50 randomly chosen test problems* (6.1). *For each dimension s results from left to right correspond to the DCHURE algorithm, Korobov rank-1 lattice rules used in NAG, and the new, extensible rank-1 lattice rules for $\eta = 17797$ and 1267 from Table 4.1.*

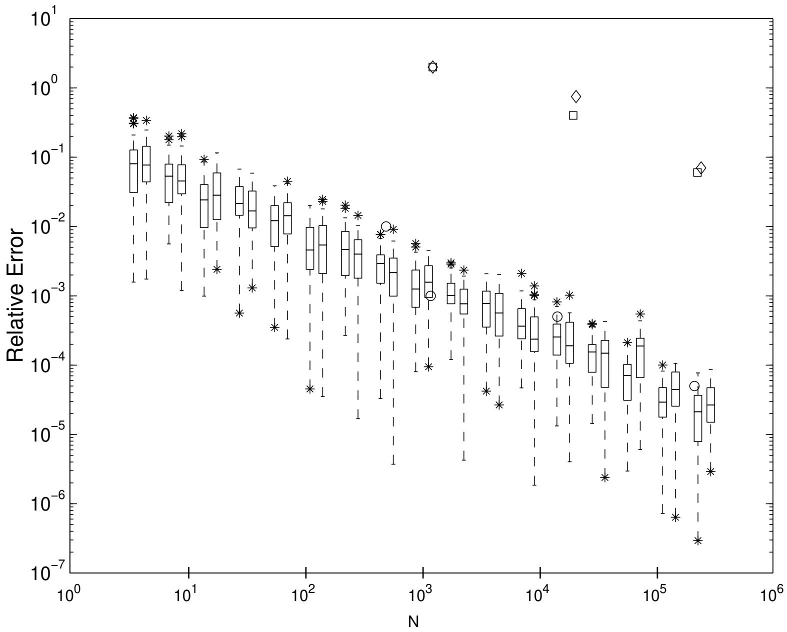

FIG. 6.2. *Plots of the relative error obtained in approximating* (6.2) *for* $s = 25$ *for the McNamee and Stenger* ($\square$) *Genz and Patterson* ($\diamond$), *generalized Faure* ($\circ$) *quadrature rules. The box and whisker plots show the performance of the extensible lattice sequence rules for* $\eta = 17797$ *and 1267 from Table 4.1 for* $N = 4, 8, \ldots, 2^{17}$.