Notes on Lattice Rules[*]

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Abstract

An elementary introduction to lattices, integration lattices and lattice rules is followed by a description of the role of the dual lattice in assessing the trigonometric degree of a lattice rule. The connection with the classical lattice- packing problem is established: Any s-dimensional cubature rule can be associated with an index $\rho = (\delta)^s/s!N$, where δ is the enhanced degree of the rule and N its abscissa count. For lattice rules, this is the packing factor of the associated dual lattice with respect to the unit s-dimensional octahedron.

An individual cubature rule may be represented as a point on a plot of ρ against δ. Two of these plots are presented. They convey a clear idea of the relative cost-effectiveness of various individual rules and sequences of rules.

1   The Integration Lattice and the Lattice Rule

The first two sections contain background material. Much more detailed descriptions of some of this may be found in [Ly89] and [SlJo94].

An s-dimensional lattice (conventionally denoted by Λ) is a set of points $\in R^s$ containing no limit points and satisfying

$$\mathbf{p}, \mathbf{q} \in \Lambda \quad \Longrightarrow \quad \mathbf{p} \pm \mathbf{q} \in \Lambda. \tag{1}$$

Possibly the best-known s-dimensional lattice is the *unit* lattice Λ_0, also termed $\mathbb{Z}^{(s)}$. This is the set of all points $\in R^s$ all of whose components are integers, that is,

$$\mathbf{p} = (p_0, p_1, \ldots, p_s) \in \Lambda_0 \Longleftrightarrow p_j = \text{integer} \ \ j = 1, 2, \ldots, s. \tag{2}$$

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The lattices used in the construction of lattice rules are *integration* lattices, that is, lattices Λ, satisfying

$$\Lambda \supseteq \Lambda_0. \tag{3}$$

There are several conventional ways of specifying lattices. Any s-dimensional lattice may be defined in terms of s appropriately chosen elements of Λ, namely, $\mathbf{a}_1, \mathbf{a}_2, \ldots, \mathbf{a}_s$. These may be assembled to form the rows of a nonsingular matrix

$$A(\Lambda) = A = \begin{pmatrix} \mathbf{a}_1 \\ \mathbf{a}_2 \\ \vdots \\ \mathbf{a}_s \end{pmatrix}. \tag{4}$$

This is termed a *generator* matrix of Λ. The elements of Λ comprise all points $\mathbf{x}$ of the form

$$\mathbf{x} = \lambda_1 \mathbf{a}_1 + \lambda_2 \mathbf{a}_2 + \ldots + \lambda_s \mathbf{a}_s = \lambda A \qquad \forall \, \lambda \in \Lambda_0; \tag{5}$$

that is, the multipliers λ_i are all integers. A generator matrix is not unique to Λ. In fact, when A is a generator matrix of Λ, so also is $A' = UA$, where U is any integer unimodular matrix. (A *unimodular matrix* satisfies $|\det U| = 1$. Premultiplication by such a matrix is equivalent to carrying out an elementary row operation on A. An *integer matrix* is one all of whose elements are integers.)

Definition. An s-dimensional *lattice rule* $Q(\Lambda)$ associated with an *integration* lattice Λ is a cubature rule over $[0, 1]^s$ that applies an equal weight $1/N$ to each of the N distinct points $\mathbf{p} \in \Lambda \cap [0, 1)^s$.

2 The Dual Lattice

Associated with any lattice Λ is its *dual* (or *reciprocal* or *polar*) lattice, conventionally denoted by $\Lambda^{\perp}$. One standard definition (the geometric definition) is

$$\mathbf{h} \in \Lambda^{\perp} \quad \text{if and only if} \quad \mathbf{h}.\mathbf{x} = \text{ integer for } \textit{all } \mathbf{x} \in \Lambda. \tag{6}$$

A corresponding definition is simply

$$\Lambda^{\perp} \text{ is the lattice generated by } B = (A^T)^{-1}, \qquad (7)$$

where A is any generator matrix of Λ. When Λ is an *integration* lattice, that is, $\Lambda \supseteq \Lambda_0$, it readily follows that $\Lambda^{\perp} \subseteq \Lambda_0$. Thus, each element of its generator matrix $B = B(\Lambda^{\perp})$ is an integer, and B is an integer matrix.

The abscissa count N of the lattice rule is a simple geometric property of the dual lattice. It is not difficult to show that the s-volume of an s-simplex generated by any $s + 1$ distinct points of Λ is an integer multiple of $|\det A|/s!$. When this integer is 1, the points in question may be defined as a *unit cell* of the lattice and may also be used as rows of a generator matrix A'.

Definition 1: The *order* of a lattice L is conventionally defined as $V_L s!$, where V_L is the s-volume of a unit cell of L.

This is the inverse of the point-density of L. A simple limiting argument, based on the density of points leads directly to the result that the number of points of $\Lambda(A)$ in $[0, 1)^s$ is simply $|\det A|^{-1}$. Since $AB^T = I$, this coincides with $|\det B|$, giving

$$N = |\det A|^{-1} = |\det B| = V^{\perp} s!, \qquad (8)$$

where $V^{\perp}$ is the s-volume of a unit cell of the dual lattice $\Lambda^{\perp}$.

Theorem 1: The abscissa count N of $Q(\Lambda)$ is the *order* of $\Lambda^{\perp}$.

With very little loss in generality, we confine our treatment to integrand functions $f(\mathbf{x})$ that are continuous on $[0, 1]^s$ and that have absolutely convergent *Fourier series* with respect to this interval. Following convention, we denote this sum by

$$\bar{f}(\mathbf{x}) = \sum_{\mathbf{h} \in \Lambda_0} \hat{f}_{\mathbf{h}} e^{2\pi i \mathbf{h}.\mathbf{x}}, \qquad (9)$$

where $\hat{f}_{\mathbf{h}}$ is a *Fourier coefficient* of $f(\mathbf{x})$ with respect to $[0, 1]^s$. We note that $\bar{f}(\mathbf{x}) = \bar{f}(\mathbf{x}+\lambda)$ for all $\lambda \in \Lambda_0$ and that, since $f(\mathbf{x})$ is continuous, $\bar{f}(\mathbf{x}) = f(\mathbf{x})$ for all $\mathbf{x} \in (0, 1)^s$.

For a general cubature rule Q, an expression for the error functional $Qf - If$ in terms of the Fourier coefficients of the integrand function f is readily derived by using the classical Poisson summation formula. In the case of a lattice rule, this derivation is almost trivial. We

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apply the operator $Q(\Lambda)$ to each term of the Fourier series (9) separately. The calculation of $Q(\Lambda)g_{\mathbf{h}}$, where $g_{\mathbf{h}}(\mathbf{x}) = \mathrm{e}^{2\pi i \mathbf{h}.\mathbf{x}}$, turns out to be elementary. When $\mathbf{h}$ is an element of the dual lattice $\Lambda^{\perp}$, then, in view of (6) above, $\mathbf{h}.\mathbf{x} = \text{integer}$ for all $\mathbf{x} \in \Lambda$; since $Q(\Lambda)$ samples only these points, it follows that $Q(\Lambda)g_{\mathbf{h}} = 1$. When $\mathbf{h}$ is not an element of $\Lambda^{\perp}$, a marginally more sophisticated argument reduces $Q(\Lambda)g_{\mathbf{h}}$ to zero. Thus, applying the operator $Q(\Lambda)$ to the Fourier series (9), we find many terms are annihilated. Specifically,

$$Q(\Lambda)f - If = \sum_{\mathbf{h} \in \Lambda_0}{}' \hat{f}_{\mathbf{h}} Q(\Lambda)g_{\mathbf{h}} = \sum_{\mathbf{h} \in \Lambda^{\perp}}{}' \hat{f}_{\mathbf{h}}. \tag{10}$$

This constitutes a useful expression for the discretization error associated with a lattice rule in terms of the Fourier coefficients of the integrand function.

The dual lattice $\Lambda^{\perp}$ then provides directly two basic properties of the lattice rule $Q(\Lambda)$. According to (8) above, the abscissa count $N(Q)$ is a simple multiple of the volume of the basic cell of $\Lambda^{\perp}$; and each element of this dual lattice represents a nonvanishing term in expression (10) for the discretization error. That is; the dual lattice comprises a chart or diagram of the discretization error made by a lattice rule.

3 Lattice Rules of Specified Trigonometric Degree

In this paper, we use the following conventional definition. A *trigonometric polynomial* of degree d is a function of the form

$$f(\mathbf{x}) = \sum_{||\mathbf{h}|| \le d} a_{\mathbf{h}} \mathrm{e}^{2\pi i \mathbf{h}.\mathbf{x}}. \tag{11}$$

Clearly, the coefficients $a_{\mathbf{h}}$ are simply the Fourier coefficients $\hat{f}_{\mathbf{h}}$ and $a_0 = \hat{f}_0 = If$. A trivial change of emphasis in this definition produces the following equivalent definition.

A trigonometric polynomial is a function having only a finite number of nonzero Fourier coefficients. It is of degree d, or equivalently of *enhanced degree* $\delta = d + 1$ if

$$\hat{f}_{\mathbf{h}} = 0 \qquad \text{when} \qquad ||\mathbf{h}|| \ge \delta. \tag{12}$$

It is of *strict* enhanced degree δ when it is not also of enhanced degree $\delta - 1$.

A cubature rule of enhanced degree δ is one that integrates all trigonometric polynomials of enhanced degree δ exactly. (We term this to be of *strict* enhanced degree δ if it is not also of enhanced degree $\delta + 1$.)

For any positive integer δ, the right hand side of equation (10) may be re-expressed, giving

$$Q(\Lambda)f - If = \sum_{\substack{\mathbf{h} \in \Lambda^{\perp} \\ 1 \leq ||\mathbf{h}|| < \delta}} \hat{f}_{\mathbf{h}} + \sum_{\substack{\mathbf{h} \in \Lambda^{\perp} \\ ||\mathbf{h}|| \geq \delta}} \hat{f}_{\mathbf{h}}. \tag{13}$$

When $f(\mathbf{x})$ is a polynomial of enhanced degree δ, (12) asserts that each Fourier coefficients appearing in the second summation is zero. Thus, when in addition $\Lambda^{\perp}$ contains no elements for which $1 \leq ||\mathbf{h}|| < \delta$, the entire right hand side vanishes; it follows that the lattice rule $Q(\Lambda)$ integrates $f(\mathbf{x})$ exactly and is *ipso facto* of enhanced degree δ. Thus, the enhanced degree of the lattice rule $Q(\Lambda)$ depends only on the location of the elements of the dual lattice $\Lambda^{\perp}$. Specifically, we have the following theorem.

Theorem. The *strict* enhanced degree δ of $Q(\Lambda)$ is

$$\delta = \min_{\substack{\mathbf{h} \in \Lambda^{\perp} \\ \mathbf{h} \neq 0}} ||\mathbf{h}||. \tag{14}$$

For brevity, and for subsequent generalization, it is convenient to define an s-dimensional crosspolytope

$$O_{\delta} : \mathbf{x} \in R^{(s)} \cap ||\mathbf{x}|| < \delta. \tag{15}$$

This is the strict convex hull of the 2^s points $(\pm\delta, \pm\delta, ..., \pm\delta)$; when $s = 3$, this is a regular octahedron. Two subsets that include only points in the unit lattice are denoted by

$$\Omega_{\delta} : \mathbf{h} \in \Lambda_0 \cap ||\mathbf{h}|| < \delta \tag{16}$$

$$\Omega_{\delta}' : \mathbf{h} \in \Omega_{\delta} \cap ||\mathbf{h}|| \neq \mathbf{0}. \tag{17}$$

Note that the summation range in (11) above is simply $\mathbf{h} \in \Omega_{\delta}$ and that the strict enhanced degree (14) above is

$$\delta = \max_{\Lambda^\perp \cap \Omega'_{\delta'} = \bigcirc} \delta'. \tag{18}$$

Using terminology taken from lattice theory (see, for example, [GrLe87]), we may reexpress these results as follows.

Definition 2: A lattice Λ is *admissible* with respect to a (radially) symmetric region Ω if the only element of Λ in the interior of Ω is the origin. This is abbreviated to Ω-*admissible*.

Theorem 2: The lattice rule $Q(\Lambda)$ is of enhanced degree δ if and only if $\Lambda^\perp$ is Ω_δ-*admissible*.

As in other branches of cubature, one can define an *optimal* (lattice) rule of specified trigonometric degree as a (lattice) rule of that degree whose abscissa count N is as small as is possible. Note that we have defined, for every positive integer δ, both optimal rules and optimal *lattice* rules. Since the first population includes the second as a subset, the abscissa count for an optimal rule cannot exceed the abscissa count for a corresponding optimal lattice rule.

Optimal rules are known and listed in the Appendix for the following (s, δ) pairs: for all s with $\delta = 1, 2, 3, 4$; for all δ with $s = 1, 2$; and for $(s, \delta) = (3, 6)$. While some of the known optimal rules are not lattice rules, there exists for each pair (s, δ) mentioned above an optimal rule that is also a lattice rule. In addition, optimal *lattice* rules are known for $s = 3$ when δ is any multiple of 6. For *other* assignments of (s, δ), to the author's knowledge, no rules have been established to be optimal.

In addition, many lattice rules (particularly in three and four dimensions) have appeared in the literature. These have resulted from computer searches over only part of the relevant population, so they remain only candidates for optimality. The construction (See [CoLy01]) of the most recent, and currently the most thorough, list of rules follows an approach suggested by the definition of an optimal rule given above. A large population of Ω_δ-admissible rules $\Lambda^\perp$ was examined, and those having lowest order $N(\Lambda^\perp)$ were retained. This was, in effect, an attempt to carry out a lattice-packing problem on a computer. These rules have been termed *K-optimal* rules.

4 Connection with the Lattice-Packing Problem

Parts of classical lattice theory are concerned with packing symmetric regions into lattices. One version of the lattice packing-problem treats a fixed region, Ω, and searches for the densest lattice that has only one point within the region. We recall from (8) above that the order of a lattice is an inverse measure of its density. The lattice-packing problem is concerned with Ω-*admissible* lattices L having the smallest *order $N(L)$*.

Much of the theory is classical. In particular, Minkowski's elegant theorem of 1904 assures us that, when Ω is a convex symmetric region, a necessary (but usually not sufficient) condition for L to be Ω-admissible is

$$vol(\Omega) \leq 2^s N(L). \tag{19}$$

The quantity

$$\rho(L, \Omega) = vol(\Omega)/2^s N(L) \tag{20}$$

is termed the *packing factor* of L with respect to Ω. In view of Minkowski's theorem, $\rho(L, \Omega) \leq 1$ when Ω is a symmetrical convex region.

The classical theory establishes the existence of critical lattices. L_C (having order N_C) is a *critical* lattice with respect to Ω if no other Ω-admissible lattice L having order $N < N_C$ exists. The corresponding packing factor

$$k(\Omega) = \rho(L_C, \Omega) = vol(\Omega)/2^s N_C \tag{21}$$

is then termed the *lattice constant* for the region Ω. For the s-dimensional octahedron O_δ, the only lattice constants known are 1,1,18/19 for $s = 1,2,3$, respectively.

5 The Cubature Rule Rho-Index

Theorems 1 and 2, with their associated definitions, indicate that a near-optimal or an optimal lattice rule $Q(\Lambda)$ is characterized by an Ω_δ-admissible lattice $\Lambda^\perp$ that has a low order or an optimally low order $N(\Lambda^\perp)$. Thus, we may present our theory from the viewpoint of the classical lattice-packing problem. In our application, we treat the region Ω_δ, and the population of lattices L has to be restricted to *integer* lattices $\Lambda^\perp$. It is natural to define

a *rho-index*, $\rho(Q)$, for the lattice rule $Q(\Lambda)$ as the packing factor (20) above of $\Lambda^{\perp}$ with respect to Ω_{δ}. Since $vol(\Omega_{\delta}) = 2^s \delta^s / s!$, we have the following definition.

Definition:

$$\rho(Q) = \frac{(\delta(Q))^s}{s! N(Q)}, \tag{22}$$

where $\delta(Q)$ is the *strict* enhanced degree of Q and $N(Q)$ its abscissa count.

While the justification for this index has been presented above in terms of lattice rules and lattice theory, this same definition clearly applies to any cubature rule, since it depends only on the abscissa count and the enhanced degree. The bounds $\rho(Q) < 1$ and $\rho(Q) < k(\Omega_{\delta})$ apply directly only to lattice rules. A completely independent bound, however, applies to the rho-index of any cubature formula. This is based on the well-known Moller-Cools bound $N_{ME}(s, \delta)$. This is a lower bound on the abscissa count of an s-dimensional cubature rule of enhanced degree δ, based on the properties of the set of moment equations (ME) such a rule must satisfy. Explicit expressions for these bounds and recurrence relations for their evaluation are given in [CoSl96]. It is trivial to show that $N_{ME}(s, \delta) \geq \delta^s / s!$; equality may occur only when $s \leq 2$. Applying this somewhat crude bound on N_{ME} to Definition (22), we find $\rho(Q) \leq 1$ for all quadrature rules. In fact, of course, for specific s and δ, the known values of $N_{ME}(s, \delta)$ may be employed, leading to significantly smaller upper bounds on the rho-index.

It is straightforward to show that the rho-index of the m-copy version $Q^{(m)}$ of any cubature rule Q coincides with the rho-index of Q. This follows generally because $\delta(Q^{(m)}) = m\delta(Q)$ and $N(Q^{(m)}) = m^s N(Q)$.

We summarize the properties of $\rho(Q)$ discussed above.

Theorem: In the notation of this section, we have the following:

For all cubature rules Q, $\rho(Q^{(m)}) = \rho(Q)$ for all positive integer m.

For all cubature rules Q, $\rho(Q) < \delta^s / s! N_{ME} < 1$.

For all lattice rules Q, $\rho(Q) < k(\Omega_{\delta}) = \delta^s / s! N_C < 1$.

6 The Rho-Index as a Function of Degree

In the figures, ρ is plotted against δ for several existing and hypothetical three-dimensional and four-dimensional rules. An individual cubature rule is represented by a point.

This type of plot was introduced by Cools and Lyness [CoLy01], and these examples are taken from that article. The horizontal line in Figure 1 at $\rho = 18/19$ represents an upper bound on the rho-index for any *lattice* rule; the square symbols represent an upper bound on the rho-index for any cubature rule. These are based on the inequalities in the previous theorem; they do *not* represent known quadrature rules in general. The circular symbols represent the K-optimal rules listed in [CoLy01]; the crosses represent rules published before 1990, which remained the best published until 2001.
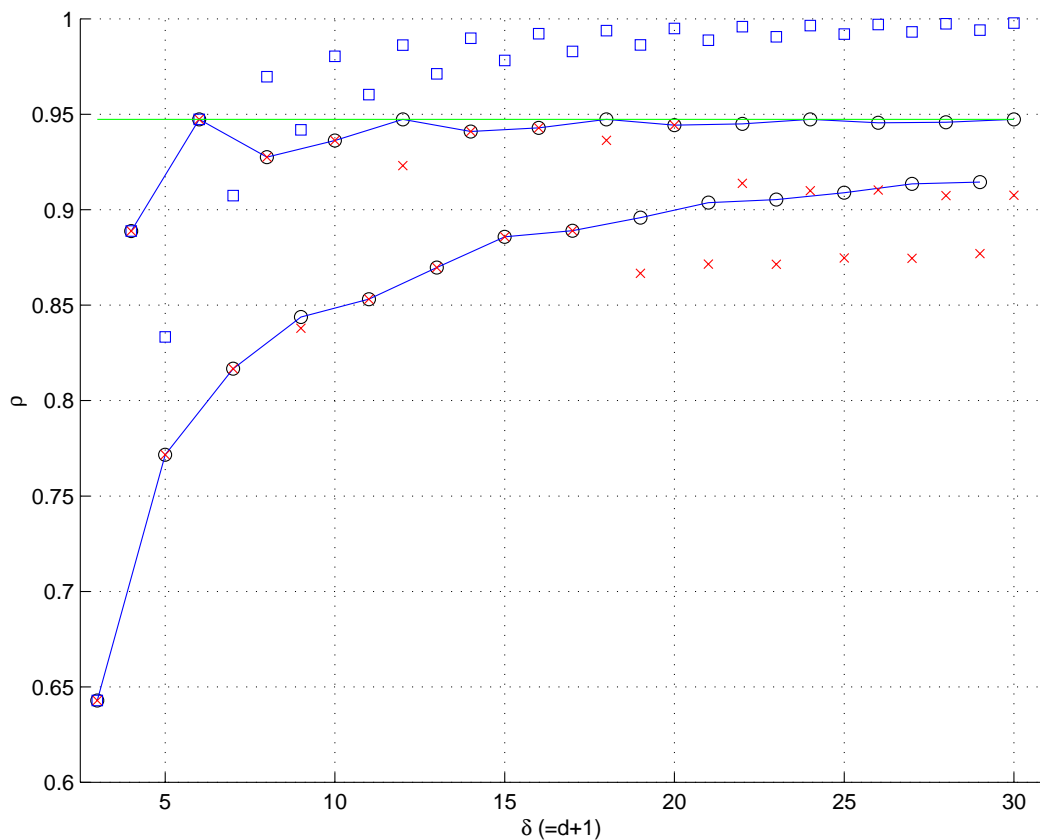

Figure 1: The rho-index of some optimal three-dimensional rules.

One may note a fundamental dichotomy between results for even and for odd degree.

This might not be noticed if these results had been presented in terms of N rather than ρ because N is generally a monotonic rapidly increasing function of δ. This dichotomy occurs in the bound (the square symbols), and this is clearly evident in the figures. This effect occurs also in the K-optimal sequence, but in the figures we have deliberately deemphasised it by connecting the symbols for odd δ and the symbols for even δ separately.

The figures may be used to illustrate a historical perspective. In three dimensions, any product trapezoidal rule has $\rho = 1/6$ for all δ, and the classical centre and vertex rule has $\rho = 2/3$ for even δ. These rules have been widely used by scientists since the advent of computing machines. Only the second sequence, if plotted in Figure 1, would appear within the frame of the figure. These would lie on a horizontal line $\rho = 2/3$ close to the lower margin of the figure. Continuing the historical perspective, a sequence of rules due to Noskov and his collaborators in the late 1980s appear as crosses. (See, for example, [Mys88] and [Nos88].) Later, the K-optimal rules appeared in 2001. It remains to establish to what extent the bounds indicated by the square symbols are attainable. But it is clear from the figure that, for $\delta \geq 10$, they are unattainable by lattice rules.

A similar picture emerges in the four dimensional-case. Here the two classical rules have rho-values $1/24$ and $1/6$, respectively, and representers of these two elementary rules would not appear within the frame of Figure 2.

The reader will have noticed that the most of the results of interest appear to lie within a horizontal strip. The upper edge is clearly $\rho = 1$. The somewhat irregular lower bound of this strip is in keeping with the preceding theorem. It follows from that theorem that, for all $k \geq 2$ and $n \geq 1$ the optimal rho-values for $\delta = n, kn, k^2 n, k^3 n, \ldots$ form a non- decreasing sequence. Thus the overall sequence of optimal rho-values contains many non-decreasing subsequences. This overall sequence appears to increase in general, but in a spasmodic way.
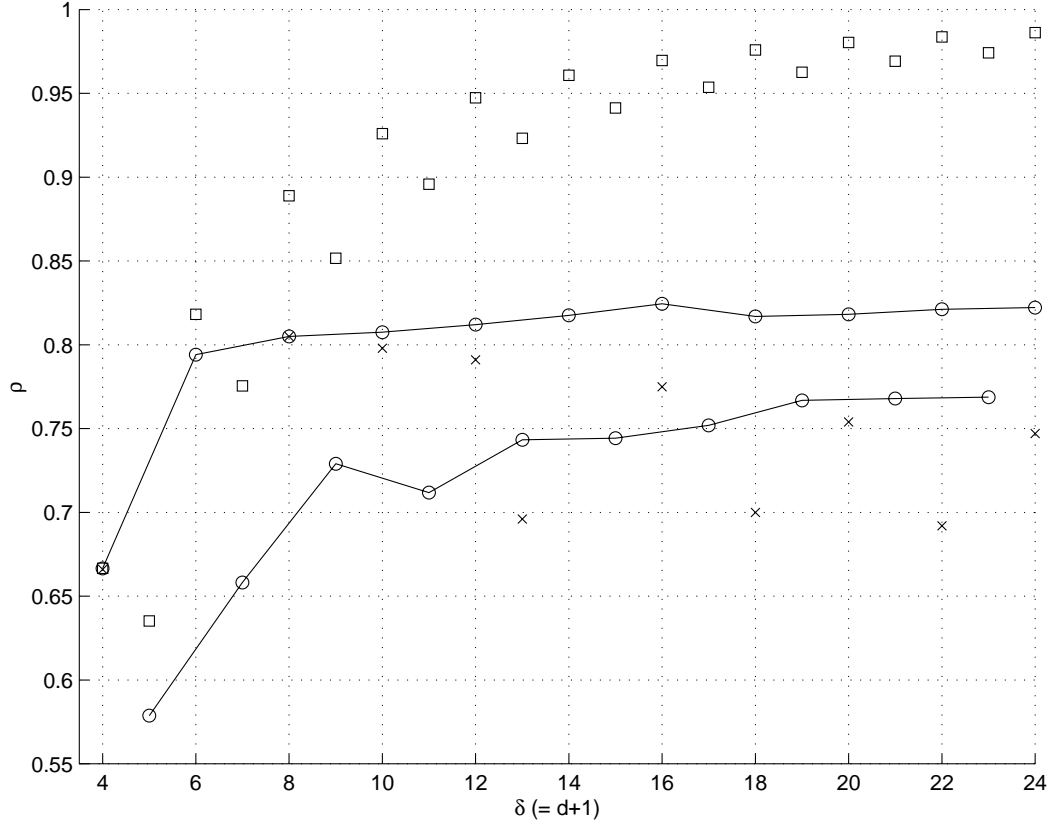
Figure 2: The rho-index of some optimal four-dimensional rules.

7 Concluding Remark

Much of the underlying theory presented here is not new. It has been assembled in a way that emphasizes the connection with classical lattice theory and leads naturally to the rho-index and its plot as a function of δ. The author has found these plots be interesting and aesthetically satisfying; they illustrate much of the present state of the art in a compact and unambiguous way.

8 Appendix

This appendix contains parameters that define one optimal rule for every (s, δ) pair for which an optimal rule is known to the author. Other optimal rules of the same enhanced degree

may be constructed by displacement of the coordinate system, coordinate interchange, and coordinate sign reversal. These last two, applied to a lattice rule, produce another, generally distinct lattice rule.

An s-dimensional rank-1 lattice rule may be expressed in the form

$$Qf = Q[1, N, \mathbf{z}, s]f := \frac{1}{N} \sum_{j=1}^{N} f\left(\left\{\frac{j\mathbf{z}}{N}\right\}\right), \tag{23}$$

where N is an integer that exceeds 1 and $\mathbf{z}$ is a nonzero element of the unit lattice Λ_0.

For all dimensions $s \geq 1$, the following assignments of N and $\mathbf{z}$ give *optimal* rules of the stated enhanced degree δ.

$$\begin{aligned}
\delta &= 1; & N &= 1; & \mathbf{z} &= (0, 0, \ldots, 0) \\
\delta &= 2; & N &= 2; & \mathbf{z} &= (1, 1, \ldots, 1) \\
\delta &= 3; & N &= 2s + 1; & \mathbf{z} &= (1, 2, \ldots, s) \\
\delta &= 4; & N &= 4s; & \mathbf{z} &= (1, 3, \ldots, 2s - 1).
\end{aligned}$$

In addition, for $s = 3$, an optimal rule is defined by the assignment

$$\delta = 6; \ N = 38; \ \mathbf{z} = (1, 7, 27),$$

and for $s = 3$ and $\delta = 6m$, the m-copy of this rule (which, when $m > 1$, cannot be expressed in form (23)) is an optimal *lattice* rule.

For $s = 2$, the following assignments give optimal rules for all positive enhanced degree δ.

$$\begin{aligned}
\delta \ odd; & \quad N = (\delta^2 + 1)/2; & \mathbf{z} &= (1, \delta) \\
\delta \ even; & \quad N = \delta^2/2; & \mathbf{z} &= (1, \delta + 1)
\end{aligned}$$

Finally, simple expressions for the abscissa count bound $N_{ME}(s, \delta)$ include

$$
\begin{aligned}
N_{ME}[1, \delta] &= \delta && (24) \\
N_{ME}[2, \delta] &= \delta^2/2 && \delta \text{ even} \\
&= (\delta^2 + 1)/2 && \delta \text{ odd} \\
N_{ME}[3, \delta] &= \delta(\delta^2 + 2)/6 && \delta \text{ even} \\
&= \delta(\delta^2 + 5)/6 && \delta \text{ odd} \\
N_{ME}[4, \delta] &= \delta^2(\delta^2 + 8)/24 && \delta \text{ even} \\
&= (\delta^4 + 14\delta^2 + 9)/24 && \delta \text{ odd}.
\end{aligned}
$$

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