Fully Symmetric Interpolatory Rules for Multiple Integrals over Hyper-Spherical Surfaces

Alan Genz
Department of Mathematics
Washington State University
Pullman, WA 99164-3113 USA
alangenz@wsu.edu

Abstract

Fully symmetric interpolatory integration rules are constructed for multidimensional integrals over U_n, the surface of an n-dimensional hyper-sphere. Explicit formulas for the weights are given for odd degrees 3–13. The new rules are efficient and only moderately unstable. Two randomization methods are described.

Key Words: multiple integrals, sphere, surface integral.

1 Introduction

This paper deals with the construction of numerical methods for the estimation of integrals in the form

$$I(f) = \int_{U_n} f(\mathbf{z}) d\sigma,$$

where $\mathbf{z} = (z_1, z_2, \ldots, z_n)$, $U_n = \{\mathbf{z}|\mathbf{z} \in \mathcal{R}^n, z_1^2 + z_2^2 \cdots + z_n^2 = 1\}$, and where σ is an element of surface on U_n. This is an important problem in pure and applied science, which has been studied by various authors. The books by Stroud [7] and Mysovskikh [5] both contain a number of formulas, and the paper by Keast and Diaz [4] provides a general method for constructing fully symmetric rules. Recent work by Xu [9] provides some fully symmetric rules with explicit formulas for the rule weights.

The purpose of this paper is to show how to modify a method for construction of the numerical integration rules described by Sylvester [8], for integration over an $n-1$–dimensional simplex T_{n-1}. The modified T_{n-1} rules can then be transformed to provide a family of rules for integration over U_n. Sylvester's integration rules for T_{n-1} are interpolatory rules, with explicit formulas for the rule weights, so the transformed rules for U_n also have explicit formulas for the weights. The resulting integration rules are new for the cases where the polynomial degree of precision is greater than 7. The rule construction method also allows the construction of two types of randomized rules, using methods previously described by the present author (Genz [2]) for randomized rules over $\mathcal{R}^n$ with Gaussian weight.

2 Interpolatory Rules for U_n

Let T_{n-1} be the $n-1$-simplex defined by $T_{n-1} = \{\mathbf{x} \mid \mathbf{x} \in \mathcal{R}^{n-1}, 0 \le x_1 + x_2 \cdots + x_{n-1} \le 1\}$, and, for any $\mathbf{x} \in T_{n-1}$, define $x_n = 1 - x_1 - x_2 \cdots - x_{n-1}$. Also, let $\mathbf{t_p} = (t_{p_1}, t_{p_2}, \ldots, t_{p_n})$, and let $\mathbf{p} = (p_1, p_2, \ldots, p_n)$. If real numbers $t_0, t_1, \ldots, t_m$ are given, satisfying the condition

$$|\mathbf{t_p}| = t_{p_1} + t_{p_2} + \cdots + t_{p_n} = 1, \quad \text{whenever} \quad |\mathbf{p}| = p_1 + p_2 + \cdots + p_n = m,$$

for non-negative integers $p_1, \ldots, p_n$, then the Lagrange interpolation formula (Sylvester [8]) for a function $g(\mathbf{x})$ on T_{n-1} is given by

$$L^{(m,n-1)}(g, \mathbf{x}) = \sum_{|\mathbf{p}|=m} \prod_{i=1}^{n} \prod_{j=0}^{p_i-1} \frac{x_i - t_j}{t_{p_i} - t_j} \;\; g(\mathbf{t_p}).$$

$L^{(m,n-1)}(g, \mathbf{x})$ is the unique polynomial of degree m which interpolates $g(\mathbf{x})$ at all of the $\binom{m+n-1}{m}$ points in the set $\{\mathbf{x} \mid \mathbf{x} = (t_{p_1}, \ldots, t_{p_{n-1}}), |\mathbf{p}| = m\}$. Sylvester provided families of points, satisfying the condition $|\mathbf{t_p}| = 1$ when $|\mathbf{p}| = m$, in the form $t_i = \frac{i+\mu}{m+\mu n}$, for $i = 0, 1, \ldots, m$, and μ real. If $0 \le \mu \le 1$, all interpolation points for $L^{(m,n-1)}(g, \mathbf{x})$ are in T_{n-1}. Sylvester derived families of interpolatory rules for integration over T_{n-1} by integrating $L^{(m,n-1)}(g, \mathbf{x})$.

Fully symmetric interpolatory integration rules for U_n can be obtained by a simple change of variables. Make the substitutions $x_i = z_i^2$, and $t_i = u_i^2$ in $L^{(m,n-1)}(g, \mathbf{x})$, and define

$$M^{(m,n)}(f, \mathbf{z}) = \sum_{|\mathbf{p}|=m} \prod_{i=1}^{n} \prod_{j=0}^{p_i-1} \frac{z_i^2 - u_j^2}{u_{p_i}^2 - u_j^2} \;\; f\{\mathbf{u_p}\}.$$

where $f\{\mathbf{u}\}$ is a *symmetric sum* defined by

$$f\{\mathbf{u}\} = 2^{-c(\mathbf{u})} \sum_{\mathbf{s}} f(s_1 u_1, s_2 u_2, \ldots, s_n u_n),$$

with $c(\mathbf{u})$ the number of nonzero entries in $(u_1, u_2, \ldots, u_n)$, and the sum $\sum_{\mathbf{s}}$ taken over all of the sign combinations that occur when $s_i = \pm 1$, for those i with $u_i \ne 0$.

Theorem 2.1 *If*

$$w_{\mathbf{p}} = I(\prod_{i=1}^{n} \prod_{j=0}^{p_i-1} \frac{z_i^2 - u_j^2}{u_{p_i}^2 - u_j^2}),$$

then

$$Q^{(m,n)}(f) = \sum_{|\mathbf{p}|=m} w_{\mathbf{p}} f\{\mathbf{u_p}\}.$$

is an integration rule of polynomial degree $2m+1$ *for* U_n.

Proof. Let $\mathbf{z^k} = z_1^{k_1} z_2^{k_2} \cdots z_n^{k_n}$. I and R are both linear functionals, so it is sufficient to show that $Q^{(m,n)}(\mathbf{z^k}) = I(\mathbf{z^k})$ whenever $|\mathbf{k}| \leq 2m+1$. If $\mathbf{k}$ has any component k_i that is odd, then $I(\mathbf{z^k}) = 0$, and $Q^{(m,n)}(\mathbf{z^k}) = 0$ because every term $\mathbf{u_q^k}$ in each of the symmetric sums $f\{\mathbf{u_p}\}$ has a canceling term $-\mathbf{u_q^k}$. Therefore, the only monomials that need to be considered are of the form $\mathbf{z^{2k}}$, with $|\mathbf{k}| \leq m$. The uniqueness of $L^{(m,n-1)}(g, \mathbf{x})$ implies $L^{(m,n-1)}(\mathbf{x^k}, \mathbf{x}) = \mathbf{x^k}$ whenever $|\mathbf{k}| \leq m$, so $M^{(m,n)}(\mathbf{z^{2k}}, \mathbf{z}) = \mathbf{z^{2k}}$, whenever $|\mathbf{k}| \leq m$. Combining these results:

$$\begin{aligned} I(f) &= I(M^{(m,n)}(f, \mathbf{z})) \\ &= \sum_{|\mathbf{p}|=m} I\Big(\prod_{i=1}^{n} \prod_{j=0}^{p_i-1} \frac{z_i^2 - u_j^2}{u_{p_i}^2 - u_j^2}\Big) f\{\mathbf{u_p}\} \\ &= \sum_{|\mathbf{p}|=m} w_{\mathbf{p}} f\{\mathbf{u_p}\} \\ &= Q^{(m,n}(f), \end{aligned}$$

whenever $f(\mathbf{z}) = \mathbf{z^k}$, with $|\mathbf{k}| \leq 2m+1$, so $Q^{(m,n)}(f)$ has polynomial degree $2m+1$.

3 Explicit Formulas for Interpolatory Rules for U_n

If a particular choice of the u_i $(= \sqrt{\frac{i+\mu}{m+\mu n}})$ sequence is specified, then explicit formulas for the weights can be determined by repeated use of the formula (Stroud [7], p. 221)

$$\int_{U_n} x_1^{k_1} x_2^{k_2} \cdots x_n^{k_n} d\sigma = 2 \frac{\Gamma(\frac{k_1+1}{2})\Gamma(\frac{k_2+1}{2}) \cdots \Gamma(\frac{k_n+1}{2})}{\Gamma(\frac{|\mathbf{k}|+n}{2})}.$$

The most efficient interpolatory rules for U_n, in terms of fewest integrand values, come from the closed ($\mu = 0$) interpolation formulas. The closed rules have many points with several zero-valued components and therefore have fewer terms in the symmetric sums. The rest of this section will focus on the closed case, and will provide explicit weight formulas for this case.

Denote the surface content for U_n by $V_n = \int_{U_n} d\sigma = 2\Gamma(\frac{1}{2})^n / \Gamma(\frac{n}{2})$, and notice that $w_{\mathbf{p}} = w_{\mathbf{q}}$ if $\mathbf{q}$ is a permutation of $\mathbf{p}$, so it is sufficient to determine only those weights $w_{\mathbf{p}}$ for $Q^{(m,n)}(f)$ for which $\mathbf{p}$ is a distinct $n-$partition of m.

First consider the degree three ($m = 1$) case. In this case, $u_0 = 0$ and $u_1 = 1$, and the interpolatory rule uses $2n$ integration rule points. The only distinct weight is

$$w_{(1,0,\ldots,0)} = \int_{U_n} z_1^2 d\sigma = 2\frac{\Gamma(\frac{3}{2})\Gamma(\frac{1}{2})^{n-1}}{\Gamma(\frac{n+2}{2})} = \frac{1}{n}V_n.$$

This rule appears in the book by Stroud ([7], p. 294).

The degree five ($m = 2$) case uses $u_0 = 0$, $u_1 = \frac{1}{\sqrt{2}}$ and $u_2 = 1$, and the interpolatory rule uses $2n + 2n(n-1) = 2n^2$ integration rule points. The two distinct weights are

$$\begin{aligned}
w_{(2,0,\ldots,0)} &= \int_{U_n} \frac{z_1^2(z_1^2 - \frac{1}{2})}{\frac{1}{2}} d\sigma = 4\frac{\Gamma(\frac{5}{2})\Gamma(\frac{1}{2})^{n-1}}{\Gamma(\frac{n+4}{2})} - 2\frac{\Gamma(\frac{3}{2})\Gamma(\frac{1}{2})^{n-1}}{\Gamma(\frac{n+2}{2})} \\
&= 2\frac{\frac{3}{2}\frac{1}{2}}{\frac{n+2}{2}\frac{n}{2}}V_n - \frac{\frac{1}{2}}{\frac{n}{2}}V_n = \frac{4-n}{n(n+2)}V_n, \\
w_{(1,1,0,\ldots,0)} &= \int_{U_n} \frac{z_1^2 z_2^2}{\frac{1}{2}\frac{1}{2}} d\sigma = 2\frac{\Gamma(\frac{3}{2})^2\Gamma(\frac{1}{2})^{n-2}}{\frac{1}{2}\frac{1}{2}\Gamma(\frac{n+4}{2})} = 4\frac{\frac{1}{2}\frac{1}{2}}{\frac{n+2}{2}\frac{n}{2}}V_n = \frac{4}{n(n+2)}V_n.
\end{aligned}$$

This rule also appears in Stroud's book ([7], p. 294, and in Mysovskih's book [5]).

The degree 7 ($m = 3$) rule uses $u_0 = 0$, $u_1 = \frac{1}{\sqrt{3}}$, $u_2 = \frac{\sqrt{2}}{\sqrt{3}}$ and $u_3 = 1$, and the interpolatory rule uses $2n + 4n(n-1) + 4n(n-1)(n-2)/3$ points. Similar algebraic work shows that the three distinct weights are

$$\begin{aligned}
w_{(3,0,\ldots,0)} &= \int_{U_n} \frac{z_1^2(z_1^2 - \frac{1}{3})(z_1^2 - \frac{2}{3})}{\frac{2}{3}\frac{1}{3}} d\sigma = \frac{2n^2 - 15n + 43}{2n(n+2)(n+4)}V_n, \\
w_{(2,1,0,\ldots,0)} &= \int_{U_n} \frac{z_1^2(z_1^2 - \frac{1}{3})z_2^2}{\frac{2}{3}\frac{1}{3}^2} d\sigma = \frac{9(5-n)}{2n(n+2)(n+4)}V_n, \\
w_{(1,1,1,0,\ldots,0)} &= \int_{U_n} \frac{z_1^2 z_2^2 z_3^2}{\frac{1}{3}^3} d\sigma = \frac{27}{n(n+2)(n+4)}V_n.
\end{aligned}$$

This rule is apparently new.

Table 3.1 provides a summary of these formulas, and also includes formulas for the degree 9, 11, and 13 weights. The *generator* for a weight $w_{\mathbf{p}}$ is a point $\mathbf{z_p}$ with $z_{p_1} \geq z_{p_2} \geq \ldots \geq z_{p_n} \geq 0$. The (*fully symmetric*) set of integration rule points for $w_{\mathbf{p}}$ is the set of all permutations of $\mathbf{z_p}$ with all possible $\pm$ sign combinations. The rules for $2m + 1 > 5$ are new. All formulas have been checked using a computer algebra system. To save space in the Table 3.1, all of the zero entries for each generator have been truncated, and the weight(s) given for each m have been scaled by dividing by the common factor $\frac{V_n}{n(n+2)\cdots(n+2m-2)}$.

Table 3.1: Points and Weights for Fully Symmetric Interpolatory Rules for U_n

m	Truncated Generator	Scaled Weight
1	(1)	1
2	(1)	$4-n$
	$(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})$	4
3	(1)	$(2n^2-15n+43)/2$
	$(\frac{\sqrt{2}}{\sqrt{3}},\frac{1}{\sqrt{3}})$	$9(5-n)/2$
	$(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})$	27
4	(1)	$(4-n)(n^2-6n+40)$
	$(\frac{\sqrt{3}}{2},\frac{1}{2})$	$16(n^2-8n+36)/3$
	$(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})$	$4(n-2)(n-12)$
	$(\frac{\sqrt{2}}{2},\frac{1}{2},\frac{1}{2})$	$32(6-n)$
	$(\frac{1}{2},\frac{1}{2},\frac{1}{2},\frac{1}{2})$	256
5	(1)	$(8n^4-90n^3+995n^2-5300n+11947)/8$
	$(\frac{2}{\sqrt{5}},\frac{1}{\sqrt{5}})$	$-25(2n^3-19n^2+188n-631)/8$
	$(\frac{\sqrt{3}}{\sqrt{5}},\frac{\sqrt{2}}{\sqrt{5}})$	$-25(2n^3-39n^2+208n-441)/12$
	$(\frac{\sqrt{3}}{\sqrt{5}},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}})$	$125(2n^2-17n+111)/6$
	$(\frac{\sqrt{2}}{\sqrt{5}},\frac{\sqrt{2}}{\sqrt{5}},\frac{1}{\sqrt{5}})$	$125(n^2-16n+33)/4$
	$(\frac{\sqrt{2}}{\sqrt{5}},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}})$	$625(7-n)/2$
	$(\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}},\frac{1}{\sqrt{5}})$	3125
6	(1)	$(4-n)(10n^4-71n^3+1733n^2-9442n+42420)/10$
	$(\frac{\sqrt{5}}{\sqrt{6}},\frac{1}{\sqrt{6}})$	$18(2n^4-19n^3+343n^2-2186n+6900)/5$
	$(\frac{\sqrt{2}}{\sqrt{3}},\frac{1}{\sqrt{3}})$	$9(n^4-23n^3+194n^2-1444n+1200)/2$
	$(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{2}})$	$4(n^4-26n^3+257n^2-658n+4620)$
	$(\frac{\sqrt{2}}{\sqrt{3}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}})$	$-54(n^3-9n^2+134n-540)$
	$(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{6}})$	$-36(n^3-21n^2+134n-420)$
	$(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}})$	$-27(n^3-30n^2+188n+48)$
	$(\frac{1}{\sqrt{2}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}})$	$432(n^2-9n+80)$
	$(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{3}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}})$	$324(n^2-18n+44)$
	$(\frac{1}{\sqrt{3}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}})$	$3888(8-n)$
	$(\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}},\frac{1}{\sqrt{6}})$	46656

Table 3.2 shows the required number of integrand values for the rules $Q^{(m,n)}$ for selected values of m and n. For comparison, integrand value numbers are also provided for some other rule families. In the "Xu" rows, the numbers are given for the rules described by Xu

[9]. These rules, given for odd m only, require $2^n\binom{n+\lfloor m/2\rfloor}{\lfloor m/2\rfloor}$ integrand values for a degree $2m+1$ rule. In spite of the rapidly increasing 2^n factor, these rules often require fewer integrand values than the $Q^{(m,n)}$ rules. For large n, the $Q^{(m,n)}$ rules require $O(\frac{(2n)^m}{m!})$ integrand values compared to $O(\frac{2^n n^{\lfloor m/2\rfloor}}{\lfloor m/2\rfloor!})$ integrand values for the Xu rules. For a fixed m and sufficiently large n, the $Q^{(m,n)}$ rules will require fewer points.

Table 3.2: Numbers of Integrand Values Needed for Spherical Surface Rules

Degree	Rule	n: 3	4	5	6	7	8	9	10
3	$Q^{(1,n)}$	6	8	10	12	14	16	18	20
	Xu	8	16	32	64	128	256	512	1024
5	$Q^{(2,n)}$	18	24	50	72	98	128	162	200
	Mys.	20	30	42	56	72	90	110	132
7	$Q^{(3,n)}$	38	88	90	292	462	688	978	1340
	Mys.	52	90	142	210	296	402	530	682
	Mys.	26	64	130	232	378	576	834	1160
	Stroud	26	48	82	136	226	384	674	1224
	Xu	32	80	192	448	1024	2304	5120	11264
9	$Q^{(4,n)}$	66	184	450	432	1666	2816	4482	6800
	Mys.	38	104	250	532	1022	1808	2994	4700
11	$Q^{(5,n)}$	102	360	1002	2364	2702	9424	16722	28004
	Keast	70	168	362	740	1486	2992	6098	12604
	Xu	80	240	672	1792	4608	11520	28160	67584
13	$Q^{(6,n)}$	146	600	1970	5336	12642	18048	53154	97880
15	$Q^{(7,n)}$	198	952	3530	10836	28814	68464	116370	299660
	Xu	160	560	1792	5376	15360	42240	112640	292864
17	$Q^{(8,n)}$	258	1208	5890	17376	59906	157184	374274	715040
19	$Q^{(9,n)}$	326	1992	9290	35436	115598	332688	864146	2060980
	Xu	280	1120	4032	13440	42240	126720	366080	1025024
21	$Q^{(10,n)}$	402	2712	14002	58728	209762	658048	1854882	4780008

The rows labelled with "Mys." give the number of integrand values needed for some rules listed in the book by Mysovskih [5]. For degree 7, there are numbers for two general rules listed: the first rule uses $n(n+1)+(n+1)(n+2)(n+3)/3$ integrand values and the second uses $2n(2n^2-3n+4)/3$ integrand values. For degree 7, the row labelled "Stroud" gives numbers (2^n+2n^2) for rules listed in the book by Stroud [7], p. 295. For degree 11, the row labelled "Keast" gives numbers $(2n+2^n(n+1)+4n(n-1)(n+1)/3)$ for a rule derived by Keast [4], p. 418. The Mysovskih and Stroud books also list a number of other rules for specific values of the rule degree and n (mostly for low rule degree and small n) that are not included in Table 3.2.

A practical issue when using an integration rule is stability. A standard measure of the stability of an integration rule is the sum of the absolute values of the rule weights. This is a worst-case roundoff error magnification factor. Denote this stability factor for a fully symmetric interpolatory rule $Q^{(m,n)}$ by

$$C^{(m,n)} = \sum_{|\mathbf{p}|=m} N_{\mathbf{p}}^{(m,n)} |w_{\mathbf{p}}| / V_n,$$

where $N_{\mathbf{p}}^{(m,n)}$ is the number of points needed for the sum $f\{\mathbf{z_p}\}$. A completely stable rule has $C = 1$, but there is no general method known for constructing efficient rules for $I(f)$ with $C = 1$. In Table 3.3 the approximate stability factors for the rules $Q^{(m,n)}$ are shown. Although these stability factors increase slowly with m and n, it can be seen that there will not be a significant loss of precision through roundoff error magnification when these rules are used.

Table 3.3: Approximate $Q^{(m,n)}$ Rule Stability Factors

m	n: 2	3	4	5	6	7	8	9	10
1	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0	1.0
2	1.0	1.0	1.0	1.3	1.5	1.7	1.8	1.9	2.0
3	1.0	1.0	1.0	1.0	1.6	2.1	2.6	3.0	3.4
4	1.0	1.2	1.4	1.6	1.7	2.4	3.3	4.1	5.0
5	1.0	1.1	1.5	2.1	2.8	3.3	4.4	5.7	7.1
6	1.4	1.9	2.3	3.0	4.3	5.5	6.7	8.4	10.4
7	1.1	1.8	3.0	4.5	6.5	8.8	11.1	13.4	16.2
8	2.7	3.7	4.8	7.1	10.2	13.9	18.0	22.3	26.7
9	1.5	4.1	7.6	11.9	17.2	23.1	29.9	37.3	45.3
10	6.3	8.6	12.9	20.4	29.5	39.7	51.0	63.6	77.6

4 Stochastic Interpolatory Rules for U_n

It is useful to have methods for computing error estimates for integration rules that are used in practical computations. One traditional method for error estimation relies on the use of differences between successive values in the sequence $Q^{(1,n)}(f), Q^{(2,n)}(f), \ldots$. This method could be used with the family of rules described in the previous section, but it is sometimes unreliable, and sometimes infeasible for large values of m and n. A second class of methods for error estimation uses randomization. There are two common methods for randomization of integration rules. The first method uses random copies of the complete rule, and the second method uses comparisons between the integrand at random points from the integration region and the polynomial model for the rule. The use of these two error estimation methods for the $Q^{(m,n)}$ rules is discussed in the following subsections.

4.1 Complete $Q^{(m,n)}$ Rule Randomizations

Define

$$Q^{(m,n)}(f,Z) = \sum_{|\mathbf{p}|=m} w_{\mathbf{p}} f\{\mathbf{u}_{\mathbf{p}}, Z\},$$

where Z is an $n \times n$ orthogonal matrix, and $f\{\mathbf{u}_{\mathbf{p}}, Z\}$ denotes the application of the transformation Z to each of the points used in the original symmetric sum $f\{\mathbf{u}_{\mathbf{p}}\}$. All rule points for $Q^{(m,n)}(f,Z)$ are on the $n-$sphere surface and are linear transformations of the original points, so $Q^{(m,n)}(f,Z)$ also has polynomial degree $2m+1$. Denote the average of N random copies of $Q^{(m,n)}(f,Z)$ by

$$\bar{Q}_N^{(m,n)}(f) = \frac{1}{N}\sum_{i=1}^{N} Q^{(m,n)}(f, Z_i).$$

If random orthogonal matrices Z_i are generated with Haar distribution from the set of all matrices in the orthogonal group (see Stewart [6], 1980), then the "stochastic" rule $\bar{Q}_N^{(m,n)}(f)$ is an unbiased degree $2m+1$ estimate for $I(f)$. A robust unbiased degree $2m+1$ error estimate $\bar{Q}_N^{(m,n)}(f)$ is provided by the Monte Carlo standard error

$$E_N(f) = \Big(\frac{1}{N(N-1)}\sum_{i=1}^{N}(Q^{(m,n)}(f,Z_i) - \bar{Q}_N^{(m,n)}(f))^2\Big)^{\frac{1}{2}}.$$

4.2 Polynomial Model Randomizations for $Q^{(m,n)}$ Rules

The method described in this section was initially developed by Haber ([3], 1969) for interpolatory rules and generalized by Genz ([2], 1998) for fully symmetric interpolatory rules. Define

$$e_m(f,\mathbf{z}) = f\{\mathbf{z}\} - M^{(m,n)}(f,\mathbf{z}),$$

for a point $\mathbf{z} \in U_n$. If $f(\mathbf{z}) = \mathbf{z}^{\mathbf{k}}$ and $|\mathbf{k}| \le 2m+1$, then $e_m(f,\mathbf{z}) = 0$. The expected value for $e_m(f,\mathbf{z})$ is

$$I(e_m(f,\mathbf{z})) = I(f\{\mathbf{z}\}) - I(M^{(m,n)}(f,\mathbf{z})) = I(f) - Q^{(m,n)}(f).$$

Therefore, if N random points $\{\mathbf{z}_i\}$ are chosen uniformly from U_n, then the sum

$$\bar{E}_N(f) = \frac{V_n}{N}\sum_{i=1}^{N} e_m(f,\mathbf{z}_i)$$

is an unbiased degree $2m+1$ stochastic error estimate rule for $Q^{(m,n)}(f)$. An unbiased error estimate for $\hat{E}_N(f)$ is provided by the Monte Carlo standard error

$$S_N(f) = \Big(\frac{1}{N(N-1)}\sum_{k=1}^{N}(V_n e_m(f,\mathbf{z}_i) - \bar{E}_N(f))^2\Big)^{\frac{1}{2}}.$$

This randomization method provides an error estimate, along with an error estimate for the error estimate. This type of method is more commonly used with estimates for $I(f)$ in the form

$$r_m(f, \mathbf{z}) = V_n(f\{\mathbf{z}\} - M^{(m,n)}(f, \mathbf{z})) + Q^{(m,n)}(f).$$

If random points $\{\mathbf{z}\}$ are chosen uniformly from U_n, then $r_m(f, \mathbf{z})$ is an unbiased degree $2m+1$ stochastic rule for $I(f)$. This method for randomizing a polynomial rule is a type of "control variates" method (see Davis and Rabinowitz [1], p. 389) for reducing variance. In many cases the sum $\bar{E}_N(f) + Q^{(m,n)}(f)$ will be a better estimate for $I(f)$ than $Q^{(m,n)}(f)$. A simple heuristic for these cases is to compare of $S_N(f)$ with $\bar{E}_N(f)$. In those cases where $S_N(f)$ is smaller than $\bar{E}_N(f)$, $\bar{E}_N(f) + Q^{(m,n)}(f)$ should be a better estimate for $I(f)$ than $Q^{(m,n)}(f)$, and then $S_N(f)$ provides an error estimate for $\bar{E}_N(f) + Q^{(m,n)}(f)$. The primary extra computational cost for $\bar{E}_N(f)$, compared to the cost of computing $Q^{(m,n)}(f)$ alone, is the extra $2^n N$ f values needed for the N values of $f\{\mathbf{z}\}$, each of which require 2^n f values. The use of these stochastic rules for large values of n (e.g. $n > 15$) might be infeasible.

5 Concluding Remarks

A new family of fully symmetric interpolatory integration rules have been derived. The rules can be used to numerically estimate multidimensional integrals over the surface of a hypersphere. The higher degree rules are new, and explicit formulas are given for the weights. The rules are only moderately unstable as the degree of polynomial precision increases. If the rule cost is measured in terms of the number of integrand values, the new rules are efficient, because of their use of fully symmetric sum generators with many components equal to zero. Two randomized error estimation methods have also derived for the rules.

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