Fully Symmetric Interpolatory Rules for Multiple Integrals over Infinite Regions with Gaussian Weight *

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Abstract

Fully symmetric interpolatory integration rules are constructed for multidimensional integrals over infinite integration regions with a Gaussian weight function. The points for these rules are determined by successive extensions of the one dimensional three point Gauss-Hermite rule. The new rules are shown to be efficient and only moderately unstable.

Key Words: multiple integrals, infinite regions, Gaussian weight, Kronrod-Patterson rules.

1 Introduction

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

$$I(f) = \frac{1}{(2\pi)^{n/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} ... \int_{-\infty}^{\infty} e^{-\mathbf{x}^T\mathbf{x}/2} f(\mathbf{x}) dx_1 dx_2 ... dx_n,$$

with $\mathbf{x} = (x_1, x_2, ..., x_n)^T$. This is an important problem in pure and applied science and statistics. One broad class of applications concerns the evaluation of quantum-mechanical matrix elements with Gaussian wave functions in atomic and molecular physics [14], nuclear [9] and particle physics [10]. For some applications in statistics see Evans and Swartz [6]. Integrals of this type have traditionally been estimated with product Gauss-Hermite rules or Monte-Carlo methods (see the book by Davis and Rabinowitz [1], and Evans and Swartz [6]). The purpose of this paper is to show how the general method developed by Genz [8], for the construction of fully symmetric interpolatory rules, can be used to construct efficient rules for $I(f)$. Related recent work on the development of integration rules for $I(f)$ has been done by Dellaportas and Wright [4] and Cools and Haegemans [2]. Earlier work is summarized in the books by Stroud [16] and Engels [5].

The rules $Q^{(m,n)}(f)$ that Genz [8] developed take the form

$$Q^{(m,n)}(f) = \sum_{\mathbf{p} \in P^{(m,n)}} w_{\mathbf{p}} f[\boldsymbol{\lambda}_{\mathbf{p}}].$$

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Here $\boldsymbol{\lambda}_{\mathbf{p}} = (\lambda_{p1}, \lambda_{p_2}, ..., \lambda_{p_n})$, $P^{(m,n)}$ is a set of all distinct n-partitions of the integers $0, 1, ..., m$ defined by

$$P^{(m,n)} = \{(p_1, p_2, ..., p_n) : m \geq p_1 \geq p_2 \geq ... \geq p_n \geq 0, |\mathbf{p}| \leq m\},$$

with $|\mathbf{p}| = \sum_{i=1}^{n} p_i$, and the fully symmetric sums $f[\boldsymbol{\lambda}_{\mathbf{p}}]$ defined by

$$f[\boldsymbol{\lambda}_{\mathbf{p}}] = \sum_{\mathbf{q} \in \Pi_{\mathbf{p}}} \sum_{\mathbf{s}} f(s_1 \lambda_{q_1}, s_2 \lambda_{q_2}, ... s_n \lambda_{q_n}),$$

where $\Pi_{\mathbf{p}}$ is the set of all permutations of $\mathbf{p}$ and the inner sum is taken over all of the sign combinations that occur when $s_i = \pm 1$, for those i with $\lambda_i \neq 0$. We have assumed that the generators are distinct and $\lambda_0 = 0$. If the weights $w_{\mathbf{p}}$ are given by

$$w_{\mathbf{p}} = 2^{-K} \sum_{|\mathbf{k}| \leq m - |\mathbf{p}|} \prod_{i=1}^{n} \frac{a_{k_i + p_i}}{\prod_{j=0, \neq p_i}^{k_i + p_i} (\lambda_{p_i}^2 - \lambda_j^2)},$$

where K is the number of nonzero components in $\mathbf{p}$, and

$$a_i = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} \prod_{j=0}^{i-1} (x^2 - \lambda_j^2) dx, \tag{1}$$

for $i > 0$, with $a_0 = 1$, then $Q^{(m,n)}(f)$ has polynomial degree $2m + 1$.

If the only restrictions on the *generator* set $\{\lambda_i\}$ are that the generators be distinct with $\lambda_0 = 0$, then the number of values of the integrand f needed for the rule $Q^{(m,n)}$ is $V^{(m,n)} = \sum_{\mathbf{p} \in P^{(m,n)}} N_{\mathbf{p}}^{(n)}$, where $N_{\mathbf{p}}^{(n)} = 2^{|\mathbf{i}|} n! / ((n - |\mathbf{i}|)! i_1! i_2! ... i_K!)$, when $\mathbf{p} \in P^{(m,n)}$ has K distinct nonzero components $j_1, j_2, ..., j_K$, with respective multiplicities $i_1, i_2, ..., i_K$. The numbers $V^{(m,n)}$ increase rapidly with m and n, but $V^{(m,n)}$ can be significantly reduced if the set $\{\lambda_i\}$ is carefully chosen so that some of the weights $w_{\mathbf{p}}$ are zero, eliminating associated terms in the sum for $V^{(m,n)}$. When the integration region is the unweighted hypercube $[-1, 1]^n$, then a simple method for selecting $\{\lambda_i\}$ that leads to efficient rules is to use the points determined by Patterson [15] for unweighted one dimensional integrals over [-1,1]. These points are determined by successive optimal Kronrod [12] extensions of the one-point Gauss-Legendre rule, whereby a $(2n + 1)$-point rule is obtained from an n-point rule by adding $n + 1$ points, chosen to maximize the degree of the $(2n + 1)$-point rule. The two aims of this paper are to show a) how a generalization of Patterson's method can be used to produce successive extensions of the one point Gauss-Hermite rule, and b) that the points for these extended rules can be used for generators of good rules for $I(f)$. In the next section we consider the problem of generalizing Patterson's method for integrals over $(-\infty, \infty)$ with Gaussian weight, and in the final section we show that the points for the new extended rules provide stable and efficient rules for $I(f)$.

2 Extended Rules for $(-\infty, \infty)$

In this section we focus on the one dimensional integral $G(f) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} f(x) dx$. We let $Q^{(m)} \equiv Q^{(m,1)}$ denote a rule for $G(f)$ of polynomial degree $2m + 1$. In order to notate the extension process we are about to describe, we use $Q^{(m)}[i_1 + i_2 ... + i_k]$ to denote a degree $2m + 1$ rule for $G(f)$ which uses $\sum_{j=1}^{k} i_j$ points, and was constructed by successively extending lower degree rules with $\sum_{j=1}^{l} i_j$ points for $l = 1, 2, ..., k$.

We begin with the one point Gauss-Hermite rule for $G(f)$, $Q^{(0)}[1](f) = f(0)$, which has degree 1. Following Patterson's method, we can try to extend this rule by adding two symmetrically placed points $\pm\lambda_1$ to produce the rule

$$Q^{(2)}[1+2](f) = w_0^{(1)} f(0) + w_1^{(1)} f[\lambda_1].$$

The weights $w_0^{(1)}$ and $w_1^{(1)}$, and λ_1 are determined to maximize the degree of $Q^{(3)}$. The well-known solution is $\lambda_1 = \sqrt{3}$, $w_0^{(0)} = 2/3$ and $w_1^{(1)} = 1/6$. $Q^{(2)}[1+2]$ is just the three-point degree five Gauss-Hermite rule for $G(f)$.

The next step in Patterson's extension process is to try adding two new generators to determine a rule in the form

$$Q^{(5)}[1+2+4](f) = w_0 f(0) + w_1 f[\lambda_1] + w_2 f[\lambda_2] + w_3 f[\lambda_3],$$

with maximal degree. The solution is a degree eleven rule, but unfortunately the new generators are not both real. This is a well known problem. The Kronrod extensions to the m-point Gauss-Hermite rules with real generators only exist when $m = 1, 2, 4$ (see Kahaner and Monegato [11] and Gautschi [7]). But we will show that $Q^{(2)}[1+2]$ does have higher degree extensions with real generators, and that these rules can be extended further to yield an embedded family of rules for $G(f)$. We first provide some additional theoretical background and notation.

Suppose a $(2\mu+1)$-point rule for $G(f)$ is given in the form $R(f) = \sum_{i=0}^{\mu} w_i f[\lambda_i]$, and we want to extend it by adding 2ν points $\pm\lambda_{\mu+1}, \pm\lambda_{\mu+2}, ..., \pm\lambda_{\mu+\nu}$, choosing the new generators to maximize the degree of the extended rule. Then the additional generators are determined by the conditions

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} \prod_{j=0}^{\mu} (x^2 - \lambda_j^2) \prod_{j=\mu+1}^{\mu+\nu} (x^2 - \lambda_j^2) x^{2k} dx = 0,$$

$k = 0, 1, .., \nu - 1$. If we let $S(x) = x^{2\nu} + s_{\nu-1} x^{2\nu-2} + ... + s_0$ be the polynomial with roots $\pm\lambda_{\mu+1}, \pm\lambda_{\mu+2}, ..., \pm\lambda_{\mu+\nu}$, then the ν conditions given determine a linear system for the coefficients of S. If this linear system has a solution S, a rootfinding procedure can then be applied to S to determine the new generators.

When $R(f)$ is a Gauss-Hermite rule, we have

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} \prod_{j=0}^{\mu} (x^2 - \lambda_j^2) x^{2k} dx = 0,$$

for $k = 0, 1, .., \mu - 1$, so we require $\nu > \mu$ if we want to be able to determine $S(x)$. The case $\mu = \nu + 1$ produces the standard Kronrod [12] extensions to the Gauss rules.

In order to illustrate this process for $G(f)$ we consider the case where $\mu = 1$ and $\nu = 2$. We need to satisfy the condition

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} x^2 (x^2 - 3)(x^4 + s_1 x^2 + s_0) x^{2k} dx = 0,$$

for $k = 0$ and $k = 1$. Using $G(x^{2k}) = \prod_{i=1}^{k} (2i - 1)$, with $G(1) = 1$, we find $S(x) = x^4 - 10x^2 - 5$. The two new generators are determined by $\lambda_2^2 = 5 + \sqrt{30}$ and $\lambda_3^2 = 5 - \sqrt{30}$, but λ_3 is not real. This analysis shows that the standard Kronrod extension to the three-point Gauss-Hermite rule does not exist, so Patterson's extension method cannot be used

to construct an imbedded sequence of rules for $G(f)$ in the same manner that Patterson used to construct rules for $\int_{-1}^{1} f(x)dx$.

For application to rules for $I(f)$, we really wanted to have some extension to $Q^{(2)}[1+2](f)$, so we considered the case $\nu = 3$. After a little algebra we found $S(x) = x^6 - \frac{105}{4}x^4 + \frac{315}{2}x^2 - \frac{315}{4}$, which has six real roots: $\lambda_2 \approx \pm 4.184956$, $\lambda_3 \approx \pm 0.7410953$ and $\lambda_4 \approx \pm 2.8612800$ (these numbers will be given to 16 decimal digits in the next section). The resulting Kronrod "rich" rule, which we call $Q^{(7)}[1+2+6]$, has degree 15. We also found another Kronrod rich formula extending $Q^{(2)}[1+2]$, with $\nu = 4$. In this case $S(x) = x^8 - \frac{104}{3}x^6 + 658x^4 - 2940x^2 + 1785$, which has eight real roots $\hat{\lambda}_2 \approx \pm 4.497915$, $\hat{\lambda}_3 \approx \pm 0.8462881$, $\hat{\lambda}_4 \approx \pm 3.735572$ and $\hat{\lambda}_5 \approx \pm 2.684040$. The resulting rule, $Q^{(9)}[1+2+8]$, has degree 19. We continued this process of trying to extend the rules that we had already found, at each stage selecting the smallest ν that would yield a resulting $S(x)$ with real roots. Building on $Q^{(7)}[1+2+6]$ we found that we could add ten more generators to produce a 19-point degree 29 rule $Q^{(14)}[1+2+6+10]$, with $S(x) = x^{10} - \frac{8845705}{102946}x^8 + \frac{125244020}{51473}x^6 - \frac{1373974085}{51473}x^4 + \frac{5691209975}{51473}x^2 - \frac{11757510985}{102946}$. We also found a further extension with sixteen more generators to produce a 35-point, degree 51 rule $Q^{(25)}[1+2+6+10+16]$. Building on $Q^{(9)}[1+2+8]$ we found a different degree 51 rule, by adding twenty more generators to produce the 31-point $Q^{(25)}[1+2+8+20]$.

The largest-degree rules that we found are $Q^{(31)}[1+2+6+10+22]$ and $Q^{(33)}[1+2+6+10+24]$. Other rules with real roots were found which did not have sequences of increasing numbers of roots, such as $Q^{(31)}[1+2+8+4+18+10+10]$. Also, we found that we could build sequences which start with higher-degree Gauss-Hermite points, such as $Q^{(12)}[5+10]$ and $Q^{(15)}[7+12]$ (note that starting with a 3-point rule is the same as the $[1+2]$ sequence). These latter rules are not as efficient for constructing multidimensional rules, as discussed below.

In general, we found that we could not obtain sequences with more than 5-7 steps, and in any event were limited by degree 67 in obtaining solutions with real roots. Also, in obtaining the rules of higher degree, the matrix equations whose solutions yield the roots were increasingly ill conditioned. In some cases, well over ten digits of precision were lost, so that even double precision arithmetic (64 bits) was not reliable. These latter rules were obtained using quadruple and/or multiple precision arithmetic, combined with the use of Hermite polynomial expansions for $S(x)$.

We also considered the proficiency of these rules for evaluating integrals of the form $\int_{-\infty}^{\infty} e^{-x^2/2}x^k dx$ for "missing powers," *i.e.,* those whose degree k exceeds that of the exact quadrature. The results are shown in Fig. 2.1 and Fig. 2.2 for $Q^{(25)}[1+2+6+10+16]$ and $\hat{Q}^{(25)}[1+2+8+20]$, respectively. In both cases, the relative error is quite small, though not as small as the result obtained from Gauss-Hermite quadrature using the same number of integrand evaluations. For the figures we use $H[k]$ to denote a k-point (degree 2k-1) Gauss-Hermite rule. The relative errors shown here are also not as small as those obtained by Patterson [15] using the Kronrod extensions of the one-point Gauss-Legendre rule. In the latter case, for large enough k, the Kronrod extensions gave even lower relative errors than the Gauss-Legendre rule with the same number of integrand evaluations.

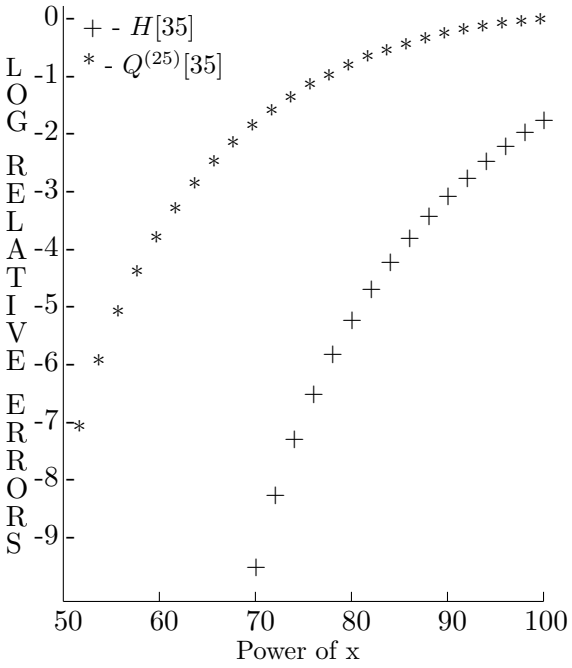

Fig. 2.1: $Q^{(25)}[35](x^k)$ and $H[35](x^k)$ Errors.

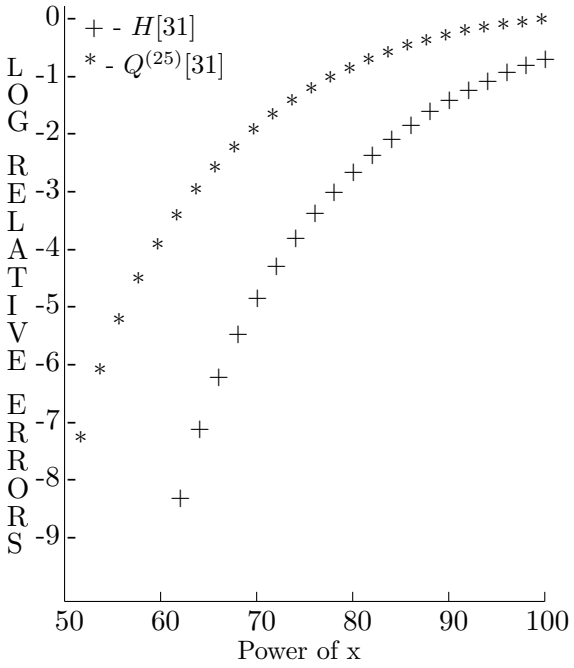

Fig. 2.2: $Q^{(25)}[31](x^k)$ and $H[31](x^k)$ Errors.

3 Efficient Multidimensional Rules

We now consider the use of the generators determined in the previous section for rules for $I(f)$. For reference, we restate Genz's [8] Theorem 3.1 and Corollary 3.2.

Theorem 3.1 *A fully symmetric interpolatory rule using a generator set* $G = \{\lambda_0, \lambda_1, ..., \lambda_m\}$ *has weight* $w_{\mathbf{p}} = 0$ *whnever* $|\mathbf{p}| + |\mathbf{z}(\mathbf{p})| > m$.

Corollary 3.2 *If* $G_* = \{0, \lambda_*, \lambda_2, ..., \lambda_m\}$, *where*

$$\int_{-1}^{1} x^2(x^2 - \lambda_*^2)dx = 0$$

and $\lambda_2, ..., \lambda_m$ *are any positive numbers distinct from* λ_*, *then* $w_{\mathbf{p}} = 0$ *whenever* $|\mathbf{p}|+|t(\mathbf{p})| > m$.

Here the vector $\mathbf{z}(\mathbf{p}) = (z(p_1), z(p_2), ..., z(p_n))$ is defined by $z(i) = l$ if $a_{i+k} = 0$ for $k = 0, 1, ..., l-1$, with $z(0) = 0$. The moments a_i are defined by equation (1) in Section 1, instead of using the unweighted [-1,1] integrals in [8]. The appropriate generalization of Corollary 3.2 uses the three-point Gauss-Hermite $\lambda_1 = \sqrt{3} = \lambda_*$ which satisfies the equivalent condition

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-x^2/2} x^2(x^2 - \lambda_*^2)dx = 0.$$

The same definition of $t(\mathbf{p})$ as the number of occurrences of $p_i = 2$ in $\mathbf{p}$ is used.

The use of $\lambda_1 = \lambda_*$ in a rule $Q^{(m,n)}$ leads to a significant reduction in $V^{(m,n)}$. This reduction is more pronounced when m and n are large. For example, when $m = 6$ and $n = 6$, $w_{\mathbf{p}} = 0$ for $\mathbf{p}$ = (4,2,0,0,0,0), (2,2,1,0,0,0), (3,2,1,0,0,0), (2,2,2,0,0,0), (2,2,1,1,0,0) and (2,1,1,1,1,0), and $V^{(6,6)}$ is reduced from 8989 to 4869. But when $m = 4$ and $n = 2$, $w_{\mathbf{p}} = 0$ only for $\mathbf{p} = (2, 2)$, so $V^{(4,2)}$ is reduced only from 41 to 37.

The use of the generators for one of the extended rule sequences $Q^{(m)}$ (assuming $\lambda_1 = \lambda_*$) further reduces the integrand value count. The manner in which this occurs is determined (using Theorem 3.1) by position of the zeros in the sequence of a_i's. For $Q^{(25)}[1+2+6+10+16]$, we have $a_i = 0$ for $i = 2$, 5-7, 10-14 and 18-25. For $Q^{(25)}[1+2+8+20]$, we have $a_i = 0$ for $i = 2$, 6-9 and 16-25. This information can be used to check for zero weights when a rule is applied and so avoid computation of the fully symmetric sums $f[\boldsymbol{\lambda}_\mathbf{p}]$ for those weights. For rules such as $Q^{(12)}[5+10]$ and $Q^{(15)}[7+12]$, the condition for vanishing weights is satisfied far less often, rendering these much less useful for multidimensional quadrature.

We let $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$, for $0 \le m \le 25$, be the rules determined by the generators for $Q^{(25)}[1+2+6+10+16]$ and for $Q^{(25)}[1+2+8+20]$, respectively. For $Q_P^{(m,n)}$ the z sequence is $\{z(i)\} = \{0,0,1,0,0,3,2,1,0,0,5,4,3,2,1,0,0,0,8,7,6,5,4,3,2,1\}$, and for $\hat{Q}_P^{(m,n)}$ the relevant sequence is $\{\hat{z}(i)\} = \{0,0,1,0,0,0,4,3,2,1,0,0,0,0,0,0,10,9,8,7,6,5,4,3,2,1\}$.

In Table 3.1 we give the required number of integrand values $V^{(m,n)}$ for rules $Q^{(m,n)}$ (no restriction on the generators except $\lambda_0 = 0$), for selected m and n values.

Table 3.1: The Number of Integrand Values Needed for $Q^{(m,n)}$ Rules

m	n: 3	4	5	6	7	8	9	10
3	63	129	231	377	575	833	1159	1561
4	129	321	681	1289	2241	3649	5641	8361
5	231	681	1683	3653	7183	13073	22363	36365
6	377	1289	3653	8989	19825	40081	75517	134245
7	575	2241	7183	19825	48639	108545	224143	433905
8	833	3649	13073	40081	108545	265729	598417	1256465
9	1159	5641	22363	75517	224143	598417	1462563	3317445
10	1561	8361	36365	134245	433905	1256465	3317445	8097453
11	2047	11969	56695	227305	795455	2485825	7059735	18474633
12	2625	16641	85305	369305	1392065	4673345	14218905	39753273
13	3303	22569	124515	579125	2340495	8405905	27298155	81270333
14	4089	29961	177045	880685	3800305	14546705	50250765	158819253
15	4991	39041	246047	1303777	5984767	24331777	89129247	298199265
16	6017	50049	335137	1884961	9173505	39490049	152951073	540279585
17	7175	63241	448427	2668525	13726991	62390545	254831667	948062325
18	8473	78889	590557	3707509	20103025	96220561	413442773	1616336765
19	9919	97281	766727	5064793	28875327	145198913	654862247	2684641785
20	11521	118721	982729	6814249	40754369	214828609	1014889769	4354393801

The following Tables 3.2 and 3.3 give the required number of integrand values for the rules $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$, respectively. We can see from these Tables that the use of the generalized Patterson extended generator sequences can provide a significant reduction in the computation needed for fully symmetric rule approximations to $I(f)$. The rules $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$ require similar numbers of f values, with $\hat{Q}_P^{(m,n)}$ requiring approximately 30% more f values for large m. These numbers are significantly smaller than the numbers $V^{(m,n)}$ in Table 3.1, particularly when m and n are large. For $m > 8$ (approximately), the rules $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$ are also more efficient than the rules described by Cools and Haegemans [2], where a degree $2m+1$ rule requires $V^{(m-1,n)} + 2^n$ f values.

Table 3.2: The Number of Integrand Values Needed for $Q_P^{(m,n)}$ Rules

m	n: 3	4	5	6	7	8	9	10
3	39	81	151	257	407	609	871	1201
4	93	201	401	749	1317	2193	3481	5301
5	165	441	993	2021	3837	6897	11833	19485
6	237	761	2033	4725	9941	19441	35929	63405
7	381	1305	3793	9765	22725	48689	97561	185085
8	513	2129	6913	19281	48401	111841	241201	490625
9	703	3065	11323	35357	96967	241329	556707	1206645
10	919	4489	17643	59957	179791	485329	1202691	2779549
11	1183	6185	27003	98837	317607	919697	2440227	6012829
12	1719	8745	39403	156037	540207	1671441	4718595	12337869
13	2031	12057	57563	238333	878615	2905457	8731875	24194869
14	2463	15321	80123	356797	1390567	4865009	15494691	45435829
15	2979	20681	110647	516933	2139931	7918801	26602383	82198957
16	3513	25985	152817	746193	3219401	12526977	44321601	144016017
17	4191	32025	198587	1044885	4763447	19395505	71876307	244900077
18	4731	39233	259747	1425481	6850203	29355329	113924451	405821737
19	6315	48321	333187	1941769	9731627	43506753	176518947	656830057
20	7539	62321	427219	2575825	13603523	63565729	268514499	1040480737

Table 3.3: The Number of Integrand Values Needed for $\hat{Q}_P^{(m,n)}$ Rules

m	n: 3	4	5	6	7	8	9	10
3	39	81	151	257	407	609	871	1201
4	93	201	401	749	1317	2193	3481	5301
5	171	449	1003	2033	3851	6913	11851	19505
6	267	817	2123	4857	10123	19681	36235	63785
7	435	1457	4123	10377	23747	50273	99883	188345
8	591	2409	7683	21045	51943	118289	252091	507965
9	799	3577	12963	39629	106711	261425	594939	1274725
10	985	5209	20733	69413	203969	540337	1317477	3003069
11	1279	7089	31783	116585	370191	1053793	2747703	6663449
12	1533	9545	46113	185677	640965	1960593	5452329	14033109
13	1899	12129	64923	283009	1056107	3475521	10323867	28201569
14	2625	16169	88613	417421	1676041	5904593	18697773	54198069
15	3215	21153	121407	599377	2571439	9677889	32592735	100055537
16	4223	27201	161007	843769	3833903	15336129	54839295	178115417
17	5111	36449	216607	1163833	5578135	23613313	89337951	306464057
18	6191	46241	290447	1608793	7981823	35486465	141527103	511442777
19	6983	59041	381407	2186665	11287335	52330625	218821983	830570857
20	7883	71545	501639	2958829	15723795	75854129	331313199	1316337797

Another issue that arises 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, which is a worst-case roundoff error magnification factor. We use $C^{(m,n)}$ to denote this

stability factor for a fully symmetric interpolatory rule $Q^{(m,n)}$, with

$$C^{(m,n)} = \sum_{\mathbf{p} \in P^{(m,n)}} N_{\mathbf{p}}^{(n)} |w_{\mathbf{p}}|.$$

A completely stable rule has $C = 1$, but there is no known general method for constructing efficient rules for $I(f)$ with $C = 1$. The product Gauss-Hermite rules do have $C = 1$, but the number $(m+1)^n$ of the f values needed for a degree $2m+1$ product Gauss-Hermite rule grows so rapidly with n that using these rules becomes infeasible for practical calculations when $n > 3$. or 4.

The stability factor for a fully symmetric interpolatory rule $Q^{(m,n)}$ depends on the choice and ordering of the generators. The generators for the rules $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$ are fixed but we have some choice in how they are ordered. The generators for these rules were produced in subsets, and permuting the generators within each subset does not effect the cost or degree of the resulting rule. For example, with $Q_P^{(m,n)}$, generators within each of the subsets $\{\lambda_2, \lambda_3, \lambda_4\}$, $\{\lambda_5, \lambda_6, \lambda_7, \lambda_8, \lambda_9\}$ and $\{\lambda_{10}, \lambda_{11}, \lambda_{12}, \lambda_{13}, \lambda_{14}, \lambda_{15}, \lambda_{16}, \lambda_{17}\}$ can be permuted without changing the cost or degree of the resulting rules, so there are 3!5!8! possible generator orderings. We found that permuting the generators can produce significant changes in the stability factors. We did not carry out a complete search over all possible generator permutations to determine the optimal permutation for each m and n, but we found a heuristic that produces what appears to be nearly minimal (within a factor of 2 or 3) stability factors. Within each subset we alternate large and small generators, beginning each subset with the largest generator. In Table 3.4 we list the generators to sixteen decimal digits, ordered according to this heuristic, for the rules $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$. These generators were computed in quadruple precision (128 bits). We then checked the computed sequence $\{a_i\}$ to see if those a_i that were supposed to be zero (theoretically) were small relative to the corresponding moments $G(x^{2i})$. We believe the generators given Table 3.4 are accurate to all sixteen decimal digits. For practical reasons, we have only included information for $m \leq 20$ in Tables 3.1-3 and 3.5-6, even though these generators can be used to produce rules with $m \leq 25$ (maximum degree 51). The original definition of a fully symmetric interpolatory rule given in Section 1 suggests that we need $m+1$ generators for a rule of degree $2m+1$. However, the higher order generators, which theoretically could be any distinct positive numbers (also distinct from the generators given in Table 3.4), do not need to be specified. Theorem 3.1 guarantees that the weight is zero for any fully symmetric sum that uses one of the extra generators.

In Tables 3.5 and 3.6 we list approximate stability factors for the rules $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$, obtained using the generators in the order given in Table 3.4. Although these stability factors increase slowly with m and n, we can see that there will not be a significant loss of precision through roundoff error magnification when these rules are used. The $\hat{Q}_P^{(m,n)}$ stability factors tend to be a little smaller for the the larger m values. There has been no systematic study of stability factors for other rules for $I(f)$. Cools and Haegemans [2] did not compute stability factors for the rules that they developed. The rules described by Dellaportas and Wright [4] are designed to have stability factor one, but were constructed only for degree ≤ 9. These rules form an imbedded sequence that ends in a product Gauss-Hermite rule. Although higher degree rules can be constructed, they may be infeasible to use for large m values. Capstick and Keister [1] considered generalizing the approach of McNamee and Stenger [13] to develop rules for $I(f)$ and found many of the new rules to be poorly conditioned.

Table 3.4: Generators for $Q_P^{(m,n)}$ and $\hat{Q}_P^{(m,n)}$ Rules

i	Generators λ_i for $Q_P^{(m,n)}$	Generators $\hat{\lambda}_i$ for $\hat{Q}_P^{(m,n)}$
0	0	0
1	0.17320508075688773D+01	0.17320508075688773D+01
2	0.41849560176727319D+01	0.49791465117195582D+01
3	0.74109534999454084D+00	0.84628809835102170D+00
4	0.28612795760570581D+01	0.37355715460409573D+01
5	0.63633944943363700D+01	0.26840395601585692D+01
6	0.12304236340273060D+01	0.90508037980317400D+01
7	0.51870160399136561D+01	0.47371420996884380D+00
8	0.25960831150492022D+01	0.80130130598043254D+01
9	0.32053337944991945D+01	0.12435457006528093D+01
10	0.90169397898903025D+01	0.71482776511870860D+01
11	0.24899229757996061D+00	0.22210157242456798D+01
12	0.79807717985905609D+01	0.63725842092196923D+01
13	0.22336260616769417D+01	0.31782891110545301D+01
14	0.71221067008046167D+01	0.56545621267720157D+01
15	0.36353185190372782D+01	0.43394221426603945D+01
16	0.56981777684881096D+01	
17	0.47364330859522971D+01	

Table 3.5: Approximate $Q_P^{(m,n)}$ Rule Stability Factors

m	n: 3	4	5	6	7	8	9	10
3	1.7	2.3	2.9	4.8	7.6	11.8	17.6	25.4
4	2.6	3.8	5.0	6.1	8.5	14.5	23.8	37.3
5	2.4	3.5	5.0	7.5	9.7	13.4	23.3	40.4
6	1.9	2.6	4.0	7.2	11.8	16.6	24.2	39.0
7	1.5	3.4	7.0	11.1	18.3	27.1	38.0	51.8
8	1.8	4.5	8.8	14.4	21.7	36.0	55.4	80.0
9	2.3	4.8	8.3	13.4	21.3	33.6	60.5	97.8
10	2.0	3.5	7.2	13.6	25.4	43.1	72.0	119.7
11	1.4	2.7	7.2	16.7	33.3	59.4	95.5	150.3
12	1.3	3.7	9.1	19.4	36.4	63.8	107.4	174.6
13	1.6	4.6	9.8	18.4	33.9	61.3	110.8	196.4
14	1.4	3.7	7.1	15.5	32.4	66.2	123.8	233.5
15	1.4	2.7	6.5	15.5	37.2	79.6	146.2	267.5
16	2.2	4.1	9.5	22.0	45.7	89.3	161.5	284.6
17	3.4	5.9	12.4	24.6	45.2	87.0	165.1	305.9
18	3.3	5.8	11.8	22.1	43.2	85.3	175.5	347.9
19	3.1	5.0	10.2	22.8	49.2	102.5	205.5	402.8
20	3.4	7.2	14.8	31.2	63.5	125.2	232.6	432.0

Table 3.6: Approximate $\hat{Q}_P^{(m,n)}$ Rule Stability Factors

m	n: 3	4	5	6	7	8	9	10
3	1.1	1.5	2.0	3.6	6.3	10.3	15.9	23.5
4	1.4	2.2	2.9	3.7	5.6	10.0	17.6	29.1
5	2.1	3.2	4.2	5.3	6.3	8.0	14.4	27.6
6	1.9	2.8	4.2	6.3	8.6	10.9	13.7	22.2
7	1.5	2.1	3.0	5.8	9.2	14.1	20.1	27.8
8	1.1	2.1	4.2	7.1	11.7	17.9	25.8	35.2
9	1.0	2.5	5.2	8.6	13.3	20.3	31.7	46.2
10	1.1	2.7	5.2	8.4	13.0	18.8	30.7	49.5
11	2.7	4.1	6.4	10.1	15.9	24.8	35.9	58.0
12	3.5	4.6	6.7	11.8	20.4	34.7	53.8	82.2
13	3.4	4.2	6.5	11.6	21.2	38.1	62.8	101.7
14	4.1	6.5	10.4	17.0	27.5	44.2	70.8	112.3
15	5.8	10.0	15.3	22.7	35.5	57.1	91.0	138.1
16	6.6	11.5	18.0	27.0	41.3	63.8	100.4	166.0
17	5.5	9.2	15.3	25.8	45.0	76.7	120.7	186.2
18	3.7	8.2	14.9	28.5	51.2	90.4	149.9	234.1
19	3.4	10.3	22.0	40.0	68.6	113.2	185.5	291.6
20	4.0	12.2	26.0	46.3	76.1	123.3	208.4	339.2

We conclude this section with a simple illustrative example. Consider the test integrand $f(\mathbf{x}) = \sqrt{1 + \mathbf{x}^T\mathbf{x}/2}$. We applied both of the new rule sequences to this problem. Similar results were obtained, and we show the errors for the $Q_P^{(m,n)}$ rules in Table 3.7.

Table 3.7: Absolute Errors for the $Q_P^{(m,n)}$ Rules for $\sqrt{1 + \mathbf{x}^T\mathbf{x}/2}$

m	n: 3	4	5	6	7	8	9	10
3	0.001321	0.004151	0.007935	0.013249	0.020764	0.031178	0.045178	0.063429
4	0.002317	0.002534	0.001791	0.000122	0.003524	0.008873	0.016780	0.028003
5	0.000194	0.000387	0.001146	0.001766	0.001879	0.001044	0.001278	0.005766
6	0.000316	0.000336	0.000468	0.000791	0.001282	0.001803	0.002079	0.001682
7	0.000002	0.000239	0.000552	0.000943	0.001448	0.002099	0.002891	0.003741
8	0.000086	0.000186	0.000194	0.000052	0.000287	0.000868	0.001738	0.002934
9	0.000099	0.000121	0.000085	0.000019	0.000018	0.000056	0.000343	0.000963
10	0.000030	0.000012	0.000033	0.000088	0.000138	0.000188	0.000275	0.000475
11	0.000022	0.000008	0.000020	0.000051	0.000071	0.000073	0.000048	0.000027
12	0.000001	0.000025	0.000055	0.000076	0.000076	0.000052	0.000003	0.000060

4 Concluding Remarks

We have developed two new families of fully symmetric interpolatory integration rules that can be used to numerically estimate multidimensional integrals over infinite regions with a Gaussian weight function. The higher degree rules are the most efficient rules known for this problem. The new rules are are only moderately unstable as the degree of polynomial precision increases.

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