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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.

Keywords: Multiple integrals; Infinite regions; Gaussian weight; Kronrod–Patterson rules

AMS classification: 65 D30, 65 D32

1. Introduction

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

$$I(f) = \frac{1}{(2\pi)^{n/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \mathrm{e}^{-x^{\mathrm{T}}x/2} f(\boldsymbol{x}) \mathrm{d}x_1 \, \mathrm{d}x_2 \cdots \mathrm{d}x_n,$$

with $\boldsymbol{x} = (x_1, x_2, \ldots, x_n)^{\mathrm{T}}$. 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 [6]. Integrals of this type have traditionally been estimated with product Gauss–Hermite rules or Monte–Carlo methods (see [1,6]). 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

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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

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

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

$$P^{(m,n)} = \{(p_1, p_2, \ldots, p_n) : m \geqslant p_1 \geqslant p_2 \geqslant \cdots \geqslant p_n \geqslant 0,\ |\boldsymbol{p}| \leqslant m\},$$

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

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

where $\Pi_{\boldsymbol{p}}$ is the set of all permutations of $\boldsymbol{p}$ 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 $w_{\boldsymbol{p}}$ are given by

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

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

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

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 $V^{(m,n)} = \sum_{\boldsymbol{p}\in P^{(m,n)}} N_{\boldsymbol{p}}^{(n)}$, where $N_{\boldsymbol{p}}^{(n)} = 2^{|\boldsymbol{i}|} n!/((n - |\boldsymbol{i}|)! i_1! i_2! \ldots i_K!)$, when $\boldsymbol{p} \in P^{(m,n)}$ has K distinct nonzero components $j_1, j_2, \ldots, j_K$, with respective multiplicities $i_1, i_2, \ldots, i_K$. 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 $w_{\boldsymbol{p}}$ 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 $G(f) = (1/\sqrt{2\pi})\int_{-\infty}^{\infty} e^{-x^2/2} f(x)dx$. 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 $Q^{(m)}[i_1 + i_2 + \cdots + i_k]$ 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 $l = 1,2,\ldots,k$.

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 $\lambda_1 = \sqrt{3}$, $w_0^{(0)} = \frac{2}{3}$ and $w_1^{(1)} = \frac{1}{6}$. $Q^{(2)}[1+2]$ 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 [7,11]). 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 $\pm\lambda_{\mu+1}, \pm\lambda_{\mu+2}, \ldots, \pm\lambda_{\mu+\nu}$, choosing the new generators to maximize the degree of the extended rule. Then the additional generators are determined by the conditions

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

$k = 0,1,\ldots,\nu-1$. If we let $S(x) = x^{2\nu} + s_{\nu-1}x^{2\nu-2} + \cdots + s_0$ be the polynomial with roots $\pm\lambda_{\mu+1}$, $\pm\lambda_{\mu+2}, \ldots, \pm\lambda_{\mu+\nu}$, then the ν conditions given determine a linear system for the coefficients of S. If this linear system has a solution S, a root finding 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 $k = 0,1,\ldots,\mu-1$, 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 $v=2$. We need to satisfy the condition

$$\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} e^{-x^2/2}x^2(x^2-3)(x^4+s_1x^2+s_0)x^{2k}\,dx=0,$$

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 $v=3$. After a little algebra we found $S(x)=x^6-(105/4)x^4+(315/2)x^2-(315/4)$, which has six real roots: $\lambda_2\approx\pm4.184956$, $\lambda_3\approx\pm0.7410953$ and $\lambda_4\approx\pm2.8612800$ (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 $v=4$. In this case $S(x)=x^8-(104/3)x^6+658x^4-2940x^2+1785$, which has eight real roots $\hat{\lambda}_2\approx\pm4.497915$, $\hat{\lambda}_3\approx\pm0.8462881$, $\hat{\lambda}_4\approx\pm3.735572$ and $\hat{\lambda}_5\approx\pm2.684040$. 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 v 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 $S(x)=x^{10}-(8\,845\,705/102\,946)x^8+(125\,244\,020/51\,473)x^6-(1\,373\,974\,085/51\,473)x^4+(5\,691\,209\,975/51\,473)x^2-(11\,757\,510\,985/102\,946)$. We also found a further extension with 16 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 20 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 10 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 Figs. 1 and 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

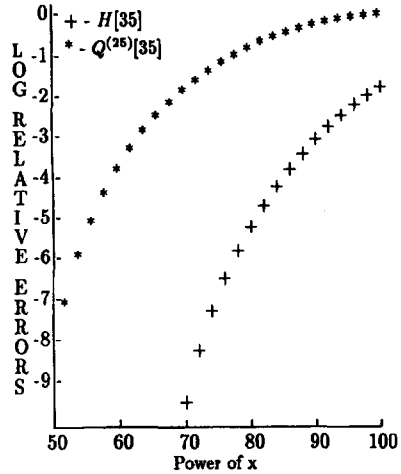

Fig. 1. $Q^{(25)}[35](x^k)$ and $H[35](x^k)$ errors.

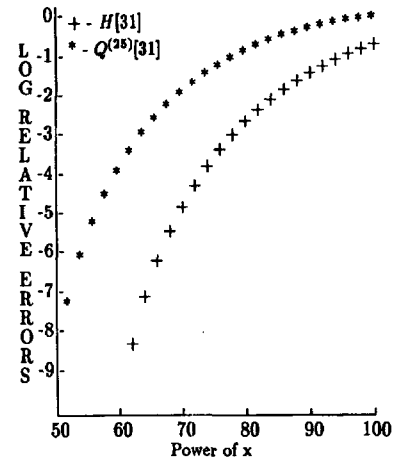

Fig. 2. $Q^{(25)}[31](x^k)$ and $H[31](x^k)$ errors.

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.

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 Theorem 3.1 and Corollary 3.2. of Genz's [8].

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

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

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

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

Here the vector $z(\boldsymbol{p}) = (z(p_1), z(p_2), \ldots, z(p_n))$ is defined by $z(i) = l$ if $a_{i+k} = 0$ for $k = 0, 1, \ldots, l-1$, with $z(0) = 0$. The moments a_i are defined by Eq. (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

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

The same definition of $t(\boldsymbol{p})$ as the number of occurrences of $p_i = 2$ in $\boldsymbol{p}$ 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 $n = 6$, $w_p = 0$ for

$\boldsymbol{p} = (4,2,0,0,0,0)$, $(2,2,1,0,0,0)$, $(3,2,1,0,0,0)$, $(2,2,2,0,0,0)$, $(2,2,1,1,0,0)$ and $(2,1,1,1,1,0)$, and $V^{(6,6)}$ is reduced from 8989 to 4869. But when $m=4$ and $n=2$, $w_p = 0$ only for $\boldsymbol{p} = (2,2)$, 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 $f[\ _p]$ 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 $0 \leqslant m \leqslant 25$, 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 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 1
The number of integrand values needed for $Q^{(m,n)}$ rules

	n							
m	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	13 073	22 363	36 365
6	377	1289	3653	8989	19 825	40 081	75 517	134 245
7	575	2241	7183	19 825	48 639	108 545	224 143	433 905
8	833	3649	13 073	40 081	108 545	265 729	598 417	1 256 465
9	1159	5641	22 363	75 517	224 143	598 417	1 462 563	3 317 445
10	1561	8361	36 365	134 245	433 905	1 256 465	3 317 445	8 097 453
11	2047	11 969	56 695	227 305	795 455	2 485 825	7 059 735	18 474 633
12	2625	16 641	85 305	369 305	1 392 065	4 673 345	14 218 905	39 753 273
13	3303	22 569	124 515	579 125	2 340 495	8 405 905	27 298 155	81 270 333
14	4089	29 961	177 045	880 685	3 800 305	14 546 705	50 250 765	158 819 253
15	4991	39 041	246 047	1 303 777	5 984 767	24 331 777	89 129 247	298 199 265
16	6017	50 049	335 137	1 884 961	9 173 505	39 490 049	152 951 073	540 279 585
17	7175	63 241	448 427	2 668 525	13 726 991	62 390 545	254 831 667	948 062 325
18	8473	78 889	590 557	3 707 509	20 103 025	96 220 561	413 442 773	1 616 336 765
19	9919	97 281	766 727	5 064 793	28 875 327	145 198 913	654 862 247	2 684 641 785
20	11 521	118 721	982 729	6 814 249	40 754 369	214 828 609	1 014 889 769	4 354 393 801

Tables 2 and 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 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 2
The number of integrand values needed for $Q_P^{(m,n)}$ rules

	n							
m	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	11 833	19 485
6	237	761	2033	4725	9941	19 441	35 929	63 405
7	381	1305	3793	9765	22 725	48 689	97 561	185 085
8	513	2129	6913	19 281	48 401	111 841	241 201	490 625
9	703	3065	11 323	35 357	96 967	241 329	556 707	1 206 645
10	919	4489	17 643	59 957	179 791	485 329	1 202 691	2 779 549
11	1183	6185	27 003	98 837	317 607	919 697	2 440 227	6 012 829
12	1719	8745	39 403	156 037	540 207	1 671 441	4 718 595	12 337 869
13	2031	12 057	57 563	238 333	878 615	2 905 457	8 731 875	24 194 869
14	2463	15 321	80 123	356 797	1 390 567	4 865 009	15 494 691	45 435 829
15	2979	20 681	110 647	516 933	2 139 931	7 918 801	26 602 383	82 198 957
16	3513	25 985	152 817	746 193	3 219 401	12 526 977	44 321 601	144 016 017
17	4191	32 025	198 587	1 044 885	4 763 447	19 395 505	71 876 307	244 900 077
18	4731	39 233	259 747	1 425 481	6 850 203	29 355 329	113 924 451	405 821 737
19	6315	48 321	333 187	1 941 769	9 731 627	43 506 753	176 518 947	656 830 057
20	7539	62 321	427 219	2 575 825	13 603 523	63 565 729	268 514 499	1 040 480 737

Table 3
The number of integrand values needed for $\hat{Q}_P^{(m,n)}$ rules

	n							
m	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	11 851	19 505
6	267	817	2123	4857	10 123	19 681	36 235	63 785
7	435	1457	4123	10 377	23 747	50 273	99 883	188 345
8	591	2409	7683	21 045	51 943	118 289	252 091	507 965
9	799	3577	12 963	39 629	106 711	261 425	594 939	1 274 725
10	985	5209	20 733	69 413	203 969	540 337	1 317 477	3 003 069
11	1279	7089	31 783	116 585	370 191	1 053 793	2 747 703	6 663 449
12	1533	9545	46 113	185 677	640 965	1 960 593	5 452 329	14 033 109
13	1899	12 129	64 923	283 009	1 056 107	3 475 521	10 323 867	28 201 569
14	2625	16 169	88 613	417 421	1 676 041	5 904 593	18 697 773	54 198 069
15	3215	21 153	121 407	599 377	2 571 439	9 677 889	32 592 735	100 055 537
16	4223	27 201	161 007	843 769	3 833 903	15 336 129	54 839 295	178 115 417
17	5111	36 449	216 607	1 163 833	5 578 135	23 613 313	89 337 951	306 464 057
18	6191	46 241	290 447	1 608 793	7 981 823	35 486 465	141 527 103	511 442 777
19	6983	59 041	381 407	2 186 665	11 287 335	52 330 625	218 821 983	830 570 857
20	7883	71 545	501 639	2 958 829	15 723 795	75 854 129	331 313 199	1 316 337 797

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

$$C^{(m,n)} = \sum_{p \in P^{(m,n)}} N_p^{(n)} |w_p|.$$

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 4 we list the generators to 16 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 4 are accurate to all 16 decimal digits. For practical reasons, we have only included information for $m \leqslant 20$ in Tables 1–3, 5 and 6, even though these generators can be used to produce rules with $m \leqslant 25$ (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 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 5 and 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 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 $\leqslant 9$. 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 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 5
Approximate $Q_P^{(m,n)}$ rule stability factors

	n							
m	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 6
Approximate $\hat{Q}_P^{(m,n)}$ rule stability factors

	n							
m	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 $f(\boldsymbol{x}) = \sqrt{1 + \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}$. 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 7.

Table 7
Absolute errors for the $Q_P^{(m,n)}$ rules for $\sqrt{1 + \boldsymbol{x}^{\mathrm{T}}\boldsymbol{x}/2}$

	n							
m	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 only moderately unstable as the degree of polynomial precision increases.

References

[1] S. Capstick and B.D. Keister, Multidimensional quadrature algorithms at higher degree and/or dimension, *J. Comput. Phys.*, to appear.
[2] R. Cools and A. Haegemans, An imbedded family of cubature formulas for n-dimensional product regions, *J. Comput. Appl. Math.* **51** (1994) 251–262.
[3] P.J. Davis and P. Rabinowitz, *Methods of Numerical Integration* (Academic Press, New York, 1984).
[4] P. Dellaportas and D. Wright, Positive imbedded integration in Bayesian analysis, *Statist. Comput.* **1** (1991) 1–12.
[5] H. Engels, *Numerical Quadrature and Cubature* (Academic Press, New York, 1980).
[6] M. Evans and T. Swartz, Some integration strategies for problems in statistical inference, *Comput. Sci. Statist.* **24** (1992) 310–317.
[7] W. Gautschi, Gauss–Kronrod quadrature — a survey, in: G.V. Milovanović, Ed., *Numerical Methods and Approximation Theory III* (Faculty of Electronic Engineering, University of Niš, Niš, 1988) 39–66.
[8] A. Genz, Fully symmetric interpolatory rules for multiple integrals, *SIAM J. Numer. Anal.* **23** (1986) 1273–1283.
[9] K.L.G. Heyde, *The Nuclear Shell Model* (Springer, Berlin, 1990).
[10] N. Isgur and G. Karl, P-wave baryons in the quark model, *Phys. Rev. D* **18** (1978) 4187–4205.
[11] D.K. Kahaner and G. Monegato, Nonexistence of extended Gauss–Laguerre and Gauss–Hermite quadrature rules with positive weights, *J. Appl. Math. Phys.(ZAMP)* **29** (1978) 983–986.
[12] A.S. Kronrod, *Nodes and Weights of Quadrature Formulas* (Consultants Bureau, New York, 1965).
[13] J. McNamee and F. Stenger, Construction of fully symmetric numerical integration formulas, *Numer. Math.* **10** (1967) 327–344.
[14] P.O'D. Offenhartz, *Atomic and Molecular Orbital Theory* (McGraw-Hill, New York, 1970).
[15] T.N.L. Patterson, The optimum addition of points to quadrature formulae, *Math. Comp.* **22** (1968) 847–856.
[16] A.H. Stroud, *The Approximate Calculation of Multiple Integrals* (Prentice Hall, Englewood Cliffs, NJ, 1971).