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FULLY SYMMETRIC INTERPOLATORY RULES FOR MULTIPLE INTEGRALS*

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Abstract. A method is given for the direct determination of the weights for fully symmetric integration rules for the hypercube, using multivariable Lagrange interpolation polynomials. The formulas for the weights lead to new classes of efficient rules.

Key words. multiple integrals, interpolation, interpolatory rules

AMS(MOS) subject classifications. 65D02, 65D30, 65D32

1. Introduction. In this paper we consider rules for the approximate calculation of integrals in the form

$$I(f)=\int_{-1}^{1}\int_{-1}^{1}\cdots\int_{-1}^{1} f(\mathbf{x})\,dx_1\,dx_2\cdots dx_n.$$

We use $Q^{(m,n)}(f)$ to denote a rule of polynomial degree $2m+1$ for $I(f)$, so that $Q^{(m,n)}(f)\simeq I(f)$, with equality whenever $f(\mathbf{x})$ is a polynomial degree at most $2m+1$. Here, each rule $Q^{(m,n)}(f)$ is a weighted sum of *fully symmetric basic* rules $f[\lambda_{\mathbf{p}}]$, in the form

$$Q^{(m,n)}(f)=\sum_{\mathbf{p}\in P^{(m,n)}} w_{\mathbf{p}} f[\lambda_{\mathbf{p}}]. \tag{1.1}$$

The notation is similar to the notation used in [3], where $\lambda_{\mathbf{p}}=(\lambda_{p_1},\lambda_{p_2},\cdots,\lambda_{p_n})$, $P^{(m,n)}$ is the set of all distinct n-partitions of the integers $0,1,2,\cdots,m$, given by

$$P^{(m,n)}=\{(p_1,p_2,\cdots,p_n)\colon m\geqq p_1\geqq p_2\geqq\cdots\geqq p_n\geqq 0, |\mathbf{p}|\leqq m\},$$

and

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

The set $\Pi_{\mathbf{p}}$ is the set of all permutations of $\mathbf{p}$ and the inner sum is taken over all of the sign combinations that occur when $s_i=\pm1$ for those values of i with $\lambda_{q_i}\neq 0$. The *generators* $\{\lambda_i\}$ are assumed to be real, distinct and nonnegative, with $\lambda_0=0$.

We illustrate this notation for the case $m=2$ and $n=3$, where

$$\begin{aligned}Q^{(2,3)}(f)=&\,w_{(0,0,0)}f[0,0,0]+w_{(1,0,0)}f[(\lambda_1,0,0)]+w_{(2,0,0)}f[\lambda_2,0,0]\\&+w_{(1,1,0)}f[(\lambda_1,\lambda_1,0)],\end{aligned}$$

with

$$\begin{aligned}&f[(0,0,0)]=f(0,0,0),\\&f[(\lambda_i,0,0)]=f(-\lambda_i,0,0)+f(+\lambda_i,0,0)+\cdots+f(0,0,+\lambda_i),\end{aligned}$$

and

$$f[(\lambda_1,\lambda_1,0)]=f(-\lambda_1,-\lambda_1,0)+\cdots+f(+\lambda_1,+\lambda_1,0)+\cdots+f(0,+\lambda_1,+\lambda_1).$$

The last sum contains 12 terms.

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Much of the previous work on fully symmetric rules for multiple integrals has produced rules that use function evaluation points λ taken from sets with a structure that is included in the set of points used by $Q^{(m,n)}$ (see for example the rules for hypercubes listed in Chapter 8 of the book by Stroud [14]). One significant constraint on the structure used here is that for a rule of degree $2m+1$, only $m+1$ generators are allowed. A primary difference between what is developed in this paper and earlier work involves the method of rule construction. Here, we use multivariable interpolation theory to derive explicit formulas for the integration rule weights $w_{\mathbf{p}}$, and then consider what conditions on the generators $\{\lambda_i\}$ can lead to efficient rules. This is in contrast to methods that consider different classes of function evaluation point sets in order to determine which classes give efficient rules with a resulting linearly consistent system of equations for the weights. Examples of this second approach are given by Keast and Lyness [6] and Mantel and Rabinowitz [11].

The construction of one-dimensional rules using the interpolation theory is a thoroughly studied technique (see the book by Davis and Rabinowitz [1]). But, for multiple integrals, the lack of a general explicit multivariable interpolation formula of the Lagrange type has not allowed the same approach. Thacher [17] and Stenger [13] have both suggested this method but have not given any detailed analysis of specific interpolatory rules. Sylvester [15] has described interpolatory rules for simplexes using sets of function evaluation points that lie on a mesh. In the next section we show how the multivariable Lagrange interpolation formulas that were used for extrapolation in a paper by the present author [2] can be used to produce explicit formulas for the weights $w_{\mathbf{p}}$ for the rules $Q^{(m,n)}(f)$.

There are several advantages to the use of interpolation theory for the construction of integration rules. These advantages come from the availability of explicit formulas for the rule weights. One advantage is that the question of the existence of the weights can be decided directly. A second advantage is that the question of the stability of the rules, which depends on the size of the weights, can be studied more easily. A third advantage is that the question of rule efficiency, which depends on determining conditions for some of the weights to be zero, can also be directly analyzed. These topics will be considered in the rest of the paper. An additional advantage, which we do not consider, is that error analysis can be done more directly using interpolation theory.

2. Weights for fully symmetric interpolatory rules. In this section formulas for the weights for the rules $Q^{(m,n)}(f)$ are derived. Let $X_m = \{\lambda_{\mathbf{p}}\colon |\mathbf{p}| \leqq m\}$. It was shown in [2] that a Lagrange interpolation formula for the set X_m is given by

$$L_m(\mathbf{x}) = \sum_{|\mathbf{p}| \leqq m} f(\lambda_{\mathbf{p}}) L_{m,\mathbf{p}}(\mathbf{x}) \tag{2.1}$$

where

$$L_{m,\mathbf{p}}(\mathbf{x}) = \sum_{|\mathbf{k}| \leqq m-|\mathbf{p}|} \prod_{i=1}^{n} \left(\prod_{l=0}^{p_i+k_i-1} (x_i - \lambda_l) \Big/ \prod_{l=0, \neq p_i}^{p_i+k_i} (\lambda_{p_i} - \lambda_l) \right). \tag{2.2}$$

The degree m Lagrange basis polynomials satisfy

$$L_{m,\mathbf{p}}(\lambda_{\mathbf{k}}) = \begin{cases} 1 & \text{if } \lambda_{\mathbf{k}} = \lambda_{\mathbf{p}}, \\ 0 & \text{otherwise.} \end{cases}$$

It has been shown by Thacher [16] that an interpolating polynomial of degree m for a certain class of sets of points is unique. X_m is in this class and therefore $L_m(\mathbf{x})$ is one form of the unique interpolating polynomial for $f(\mathbf{x})$ on X_m.

An example with $m=2$, $n=3$, $\lambda_0=0$, $\lambda_1=\frac{1}{2}$ and $\lambda_2=1$ is given by

$$\begin{aligned}L_2(\mathbf{x})=&f(0,0,0)L_{2,(0,0,0)}(\mathbf{x})+f(\tfrac{1}{2},0,0)L_{2,(1,0,0)}(\mathbf{x})+f(0,\tfrac{1}{2},0)L_{2,(0,1,0)}(\mathbf{x})\\&+f(0,0,\tfrac{1}{2})L_{2,(0,0,1)}(\mathbf{x})+f(1,0,0)L_{2,(2,0,0)}(\mathbf{x})+f(0,1,0)L_{2,(0,2,0)}(\mathbf{x})\\&+f(0,0,1)L_{2,(0,0,2)}(\mathbf{x})+f(\tfrac{1}{2},\tfrac{1}{2},0)L_{2,(1,1,0)}(\mathbf{x})+f(\tfrac{1}{2},0,\tfrac{1}{2})L_{2,(1,0,1)}(\mathbf{x})\\&+f(0,\tfrac{1}{2},\tfrac{1}{2})L_{2,(0,1,1)}(\mathbf{x}).\end{aligned}$$

Representative basic polynomials are

$$\begin{aligned}L_{2,(0,0,0)}(\mathbf{x})&=1-2(x_1+x_2+x_3)+2(x_1(x_1-\tfrac{1}{2})+x_2(x_2-\tfrac{1}{2})+x_3(x_3-\tfrac{1}{2}))\\&\qquad+4(x_1x_2+x_1x_3+x_2x_3),\\L_{2,(1,0,0)}(\mathbf{x})&=2x_1-4x_1(x_1-\tfrac{1}{2})-4x_1x_2-4x_1x_3,\\L_{2,(2,0,0)}(\mathbf{x})&=2x_1(x_1-\tfrac{1}{2})\end{aligned}$$

and

$$L_{2,(1,1,0)}(\mathbf{x})=4x_1x_2.$$

Interpolatory rules for $f(\mathbf{x})$ are obtained by integrating (2.1), but we are interested in fully symmetric rules so we define

$$F_m(\mathbf{x})=\sum_{|\mathbf{p}|\leqq m} f[\lambda_{\mathbf{p}}]M_{m,\mathbf{p}}(\mathbf{x}), \tag{2.3}$$

where $M_{m,\mathbf{p}}$ is obtained from $L_{m,\mathbf{p}}$ by replacing each x by x^2 and each λ by λ^2. Let $[\mathbf{p}]$ denote the number of nonzero components $\mathbf{p}$.

THEOREM 2.1. *If* $w_{\mathbf{p}}=2^{-[\mathbf{p}]}I(M_{m,\mathbf{p}})$, *then* $Q^{(m,n)}(f)$ *is a rule of polynomial degree* $2m+1$.

Proof. We need to show that $Q^{(m,n)}(f)=I(f)$ for all $f(\mathbf{x})=\mathbf{x}^{\mathbf{k}}$ with $|\mathbf{k}|\leqq 2m+1$. If $\mathbf{k}$ has any component k_i that is odd then $I(\mathbf{x}^{\mathbf{k}})=0$, and $Q^{(m,n)}(\mathbf{x}^{\mathbf{k}})=0$ because every term of the form $\lambda_{\mathbf{q}}^{\mathbf{k}}$ in the sums (1.2) for $Q^{(m,n)}$ has a corresponding term $-\lambda_{\mathbf{q}}^{\mathbf{k}}$, and those terms cancel each other. Therefore we need to consider only $f(\mathbf{x})=\mathbf{x}^{2\mathbf{k}}$ with $|\mathbf{k}|\leqq m$. Now, because an interpolating polynomial for X_m is unique, $L_m(\mathbf{x})$ reproduces any polynomial of degree m or less, and so $F_m(\mathbf{x})$ reproduces any even polynomial of degree $2m$ or less. Therefore $F_m(\mathbf{x})=\mathbf{x}^{2\mathbf{k}}$ whenever $|\mathbf{k}|\leqq m$. Notice also that the inner sum in equation (1.2) for $f[\lambda_{\mathbf{p}}]$ reduces to $2^{[\mathbf{p}]}\lambda_{\mathbf{p}}^{2\mathbf{k}}$ when $f(\mathbf{x})=\mathbf{x}^{2\mathbf{k}}$ because the sign changes do not affect the value of $f(\mathbf{x})$ and so there are $2^{[\mathbf{p}]}$ identical terms in the sum. Finally, notice that $I(M_{m,\mathbf{p}})=I(M_{m,\mathbf{q}})$ for all $\mathbf{q}\in\Pi_{\mathbf{p}}$ because the integral value for any polynomial is unchanged by a permutation of the coordinate indices. These results combined give the following sequence of equalities:

$$\begin{aligned}I(\mathbf{x}^{2\mathbf{k}})&=I(F_m(\mathbf{x}))\\&=\sum_{|\mathbf{p}|\leqq m} I(M_{m,\mathbf{p}}(\mathbf{x}))\lambda_{\mathbf{p}}^{2\mathbf{k}}\\&=\sum_{|\mathbf{p}|\leqq m} w_{\mathbf{p}}2^{[\mathbf{p}]}\lambda_{\mathbf{p}}^{2\mathbf{k}}\\&=\sum_{\mathbf{p}\in P^{(m,n)}} w_{\mathbf{p}}f[\lambda_{\mathbf{p}}]\\&=Q^{(m,n)}(\mathbf{x}^{2\mathbf{k}}),\end{aligned}$$

whenever $|\mathbf{k}|\leqq m$. This completes the proof.

If we let

$$a_i = \int_{-1}^{1} \prod_{j=0}^{i-1} (x^2 - \lambda_j^2)\, dx$$

then

$$w_{\mathbf{p}} = 2^{-[\mathbf{p}]} \sum_{|\mathbf{k}| \le m - |\mathbf{p}|} \prod_{i=1}^{n} \left(a_{k_i+p_i} \Big/ \prod_{j=0, \ne p_i}^{k_i+p_i} (\lambda_{p_i}^2 - \lambda_j^2) \right). \tag{2.4}$$

For the rest of this paper we use "FSI rule" to indicate a fully symmetric interpolatory rule $Q^{(m,n)}$ with weights determined by formula (2.4).

Notice that when the generator sequence is fixed for a number of values of m the interpolatory rule sequence $\{Q^{(m,n)}\}$, with n fixed, is a sequence of imbedded rules, in the sense that each rule uses all of the integrand values used by the previous rules. Successive elements in such a sequence are often used in practical calculations for error estimation. For $n > 1$ the ordering of the generator sequence is important, because a different ordering produces a different set of rules. If no specific ordering of the generators is required then there are $(m+1)!$ different rules of the same degree for the selected generators. The ordering of the generators determines the distribution of the integrand evaluation points, which can affect the size and sign of the weights, and so could have an effect on the stability of the generated rules. An example of the effect of generator ordering on rule stability will be given in the next section.

We also mention that although we have only considered integrals over the hypercube the theory developed so far applies directly to any other class of fully symmetric integrals defined over a product region.

3. Efficient fully symmetric interpolatory rules. Much of the study of multidimensional rules has been concerned with finding rules that are as efficient as possible, in the sense that as few integrand values as possible are used for each value of n and m. In order to illustrate the use of the formulas from the previous section we show how relatively simple conditions on the generators can lead to significant reductions in the total integrand evaluation numbers for FSI rules.

If $\mathbf{p} \in P^{(m,n)}$ has k distinct nonzero components then it has the form

$$\mathbf{p} = (j_1, \cdots, j_1, j_2, \cdots, j_2, \cdots, j_k, \cdots, j_k, 0, \cdots, 0).$$

If there are i_1 of the j_2's, i_2 of the j_2's, $\cdots$, i_k of the j_k's then $[\mathbf{p}] = |\mathbf{i}|$, and the number of integrand values needed for $f[\lambda_{\mathbf{p}}]$ is given by

$$N_{\mathbf{p}}^{(m,n)} = 2^{|\mathbf{i}|} n!/((n - |\mathbf{i}|)!\, i_1!\, i_2! \cdots i_k!).$$

The total number of integrand values needed for an FSI rule of degree $2m+1$ with no zero weights is

$$E^{(m,n)} = \sum_{\mathbf{p} \in P^{(m,n)}} N_{\mathbf{p}}^{(m,n)}. \tag{3.1}$$

This number can be reduced if the generator sequence is chosen to make some of the weights zero, thereby eliminating some of the terms in the sum. Some ways of doing this will be considered in the rest of this section.

One way to make $w_{\mathbf{p}} = 0$ is to choose the generators so that $a_{k_i+p_i} = 0$ for at least one component k_i in all $\mathbf{k}$ with $|\mathbf{k}| \le m - |\mathbf{p}|$. Let G denote an *ordered* set of generators, $G = \{\lambda_0, \lambda_1, \cdots, \lambda_m\}$ and let $\mathbf{z}(\mathbf{p}) = (z_1, \cdots, z_n)$ with z_i defined by

$$z_i = \begin{Bmatrix} 0 \\ l \end{Bmatrix} \quad \text{if} \int_{-1}^{1} \prod_{j=0}^{p_i+k-1} (x^2 - \lambda_j^2)\, dx \quad \begin{cases} \ne 0 & \text{for } k = 0, \\ = 0 & \text{for } k = 0, 1, \cdots, l-1. \end{cases}$$

THEOREM 3.1. *An* FSI *rule using a generator set G has a weight $w_{\mathbf{p}}=0$ if $|\mathbf{p}|+|\mathbf{z}(\mathbf{p})|>m$.*

Proof. The definition of $\mathbf{z}(\mathbf{p})$ implies that if $z_i \neq 0$ then $a_{k_i+p_i}=0$ for $k_i=0, 1, \cdots, z_i-1$. All of these terms in the sum (2.4) have $|\mathbf{k}|+|\mathbf{p}|\leqq m$. Combining this with the assumption $|\mathbf{p}|+|\mathbf{z}(\mathbf{p})|>m$ implies $|\mathbf{k}|<|\mathbf{z}(\mathbf{p})|$, so for each term in the sum (2.4) there must be at least one i for which $k_i<z_i$, and so for such an i, $a_{k_i+p_i}=0$. Therefore all terms in the sum for $w_{\mathbf{p}}$ are zero.

In order to consider a simple but very useful application of Theorem 3.1 let $t(\mathbf{p})$ denote the number of occurrences of $p_i=2$ in $\mathbf{p}$.

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

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

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

Proof. For each $p_i=2$ in $\mathbf{p}$ we have $z_i\geqq 1$ in $\mathbf{z}(\mathbf{p})$, so $|\mathbf{z}(\mathbf{p})|\geqq t(\mathbf{p})$. Using the assumption $|\mathbf{p}|-m+t(\mathbf{p})>0$, this implies $|\mathbf{p}|+|\mathbf{z}(\mathbf{p})|>m$.

Notice that the points $-\lambda_*, 0, \lambda_*$ are simply the three-point Gauss–Legendre rule points. As an example of the use of Corollary 3.2 consider $m=6$. In Table 3.1 the partitions of the integers 0–6 for $n>5$ (trailing zeros and commas omitted) that would be used for weight indices for an FSI rule of degree 13 are given.

TABLE 3.1
Weight indices for an FSI *rule with $m=6$.*

0										
1										
2	11									
3	21			111						
4	31	22		211			1111			
5	41	32		311	221		2111		11111	
6	51	42	33	411	321	222	3111	2211	21111	111111

Corollary 3.2 says that any index $\mathbf{p}$ in the last row of Table 3.1 that has one component equal to 2 and any index $\mathbf{p}$ in the previous row with two components equal to 2 will have $w_{\mathbf{p}}=0$. When $n=6$ an FSI rule with no restriction on G requires $E^{(6,6)}=8989$ integrand values, but an FSI rule using G_*, has zero weights for the indices (42), (221), (321), (222), (2211), and (21111) and uses only 4869 integrand values. Lyness [7], [8] has also shown how a systematic use of λ_*, can lead to efficient rules, although most of these rules do not use the same function values as the FSI rules discussed here.

One generator sequence that has been considered for multiple integration rules in varying degrees of generality in several published papers is the Gauss point sequence (see Lyness and Keast [9] for the most detail and also Stroud [14] for a number of examples). Let $q=[(m+1)/2]$ (integer part) and let $G_G=\{0, \lambda_{1G}, \cdots, \lambda_{qG}, \lambda_{q+1}, \cdots, \lambda_m\}$, where the Gauss points $\lambda_{1G}, \cdots, \lambda_{qG}$ are the positive zeros of the degree $m+1$ Legendre polynomial, and $\lambda_{q+1}, \cdots, \lambda_m$ are any distinct positive numbers also distinct from the Gauss points.

COROLLARY 3.3. *An* FSI *rule with generators G_G has $w_{\mathbf{p}}=0$ if $p_i>q$ for any i.*

Proof. This corollary follows easily from Theorem 3.1; an equivalent result has also been proved by Lyness and Keast [9, Thm. 4.9].

If Corollary 3.3 is applied to the case $m=6(q=3)$ and $n=6$ then it follows that when Gauss points are used for generators, the weights with indices (4), (5), (6), (41), (51), (42) and (411) are zero with the resulting rule requiring 8113 integrand values. This is less efficient than an FSI rule using G_*. However, when $n=2(E^{(6,2)}=85)$, the G_* rule requires 77 values compared to 49 for a G_G rule.

One generator sequence somewhat less familiar than the Gauss sequence is the infinite sequence that begins with 0 and λ_*, and has the remaining λ_i's determined by the condition $a_i=0$ when $i=4, 5, 8, 9, 10, 11, \cdots, 2^k, 2^{k+1}, \cdots, 2^k+2^{k-1}-1, \cdots$. Let $G_P=\{0, \lambda_*, \lambda_{2P}, \cdots, \lambda_{mP}\}$ denote the first $m+1$ elements from this sequence that has been studied by Patterson [12] and leads to an embedded family of efficient rules for one-dimensional integrals. It is difficult to compactly characterize the $\mathbf{p}$ values that give zero weights when using G_P but Theorem 3.1 can be applied for each $\mathbf{p}$ individually. If the previous example (Table 3.1) is used with $n=6$, the weights with indices (41), (51), (42), (411), (221), (321), (222), (2211) and (21111) are zero, and the resulting FSI rule uses 4149 integrand values, but if $n=2$, the resulting rule uses 61 values. As can be seen from this example the G_P sequence gives zero weights for many indices occurring in the last line of the right side of the table and some in the lower left part of the table, in contrast to the G_G sequence which gives zero weights for indices in the lower left part of the table only. As n increases the basic rules for the indices on the right part of the table tend to require more integrand values, so that G_P rules should be more efficient than the G_G rules. This hypothesis is confirmed by the results in Table 3.2, where the total integrand values for four families of FS rules for a range of n and m values are given. The G_{GM} and G_{KL} families will be referred to in § 4.

Most of the extra gain in efficiency for the Patterson point FSI rules is achieved because of the use of the generator $\lambda_1=\lambda_*$, and it is likely that, for $n>3$, even more efficient FSI rules could be found for each (m, n) pair by a more careful choice of the generators $\lambda_2, \lambda_3, \cdots, \lambda_m$. But one useful feature of G_P is that it is obtained from an infinite sequence that is independent of m. In practice this means that for many applications (m not too large) a computer program for computing the sequence $Q^{(m,n)}$ using G_P need only store the same few generators for all n.

An important practical question with FSI rules concerns their stability. It is well known that when $n=1$ the Gauss point rules have all weights positive, and all the Patterson point rules that have so far been computed have positive weights for $w(x)=1$ on $[-1, 1]$. When $n>1$ many of the published rules for multiple integrals (see Stroud [14]) have weights that change sign and have large variations in size. In the rest of this section we report some experimental results concerning the stability of FSI rules using the generators G_P and G_G. In order to investigate the stability of FSI rules for this case define the scaled absolute weight sum $|W|$ by

$$|W|=2^{-n}\sum_{\mathbf{p}\in P^{(m,n)}}|w_{\mathbf{p}}|N_{\mathbf{p}}^{(m,n)}.$$

Notice that $|W|\geqq 1$, with $|W|=1$ if all weights are positive. $|W|$ is a worst case roundoff error magnification factor, and if for some rule $|W|=1$ the rule is stable, or, using the terminology of Mantel and Rabinowitz [11], the rule is a *good* rule. In Table 3.3 computed values $|W|$ (with only one digit given after the decimal point) for the Patterson (above) and Gauss (below) point FSI rules are displayed for a range of values of m and n.

As was mentioned in the previous section the size and sign of the weights can be affected by the ordering of the generators. There are $q!$ different orderings for a degree $2m+1$ FSI rule using G_G, and a significant variation in the number $|W|$ was found

TABLE 3.2
The number of integrand values for four families of FS *rules.*

Degree	Family	Dimension 2	3	4	5	6	7	8	9	10
7	G_P	17	39	81	151	257	407	609	871	1201
	G_G	21	57	121	221	365	561	817	1141	1541
	G_{KL}	17	45	97	181	305	477	705	997	1361
	G_{GM}	17	33	57	93	149	241	401	693	1245
9	G_P	33	87	193	391	727	1303	2177	3463	5281
	G_G	25	93	257	581	1145	2045	3393	5317	7961
	G_{KL}	25	77	193	421	825	1485	2497	3973	6041
	G_{GM}	29	71	145	263	441	703	1089	1671	2585
11	G_P	33	135	385	903	1889	3655	6657	11527	19105
	G_G	45	195	617	1583	3509	6987	12817	22039	35965
	G_{KL}	41	151	417	983	2089	4103	7553	13159	21865
	G_{GM}	45	137	337	713	1353	2369	3905	6153	9385
13	G_P	61	201	633	1733	4149	8961	17905	33661	60205
	G_G	49	263	1025	3143	8113	18439	38017	72583	130225
	G_{KL}	49	223	737	1975	4625	9871	19649	36967	66289
	G_{GM}	65	239	697	1715	3717	7311	13329	22875	37389
15	G_P	89	375	1169	3263	8361	19687	42913	87535	168825
	G_G	77	461	1977	6673	18949	47253	106481	221209	429995
	G_{KL}	73	369	1329	3897	9913	22753	48353	96475	184233
17	G_P	97	471	1889	5983	16449	41191	95809	209071	431265
	G_G	81	569	2881	11273	36433	101881	254465	580589	1229265
	G_{KL}	81	465	1953	6489	18353	46177	106305	228265	463377
19	G_P	145	703	2721	9583	29489	80671	201537	468687	1027025
	G_G	117	895	4873	20563	71869	217479	587153	1444635	3290245
	G_{KL}	113	731	3201	11211	33649	90139	221057	504843	1086961
21	G_P	161	1039	4545	15983	50849	148207	396929	985935	2295969
	G_G	121	1051	6561	31355	122425	409195	1209345	3233835	7957433
23	G_P	161	1135	6081	25423	87521	267823	753537	1974927	4859169
	G_G	185	1567	10209	51735	215545	770815	2438785	6976215	18334713

for different orderings. For example, if the generators are used in increasing order $(\lambda_{1G} < \cdots < \lambda_{qG})$ for $(2m+1, n) = (19, 6)$, then $|W| \simeq 10^{12}$, but with another ordering $|W| \simeq 10^3$. In Table 3.3 the Gauss generator values for $|W|$ are preceded in each row by a permutation of $12 \cdots q$. This permutation (of the increasing value generator order) gives minimal or near minimal values of $|W|$, for $2 \leqq n \leqq 10$. The G_P FSI rules are much less sensitive to generator permutations. With these rules $\lambda_{1P} = \lambda_*$, followed by λ_{2P} and λ_{3P} (which may be interchanged), then λ_{4P}, λ_{5P}, λ_{6P} and λ_{7P} (which may be permuted in any one of 4! possible ways). Interchanges of λ_{2P} and λ_{3P} have no significant effect on $|W|$ for the n and m values used in Table 3.3. Permuting generators 4–7 gives a range of $|W|$ for $m > 3$ with a factor of about 2 or 3 separating the largest and smallest values. If the increasing order sequence $(\lambda_{4P} < \lambda_{5P} < \lambda_{6P} < \lambda_{7P})$ is associated with the permutation 1234, then near minimal or minimal values for $|W|$ occur for any permutation of the form $XYZ3$. The numbers given in Table 3.3 were produced using the permutation 1243. Both types of rules become only moderately unstable as m and n increase. The results indicate that for the larger values of n and m two or

TABLE 3.3
$|W|$ *for* FSI *rules using Patterson/Gauss points.*

Degree	Perm.	2	3	4	5	6	7	8	9	10
		Dimension								
7		1.6	3.2	4.4	8.1	17.2	31.9	53.6	83.7	123.5
	12	1.8	3.2	8.4	16.7	27.5	40.9	56.9	75.4	96.5
9		1.0	3.0	7.8	14.0	24.0	41.9	80.3	143.4	240.3
	12	1.0	1.8	5.4	12.5	23.3	38.9	64.2	99.4	151.4
11		1.0	2.0	4.1	14.5	34.3	65.9	110.0	206.3	381.1
	123	1.5	3.5	11.4	25.8	49.4	88.3	149.0	243.2	382.9
13		1.3	3.0	7.2	12.5	29.2	76.4	166.5	316.0	552.3
	132	1.0	1.9	4.8	13.2	41.8	102.9	218.4	484.0	995.1
15		1.9	3.8	8.5	21.8	43.2	84.9	167.6	387.8	804.4
	1423	1.3	3.6	10.1	20.4	41.0	102.6	247.5	526.6	992.3
17		1.5	3.8	8.3	16.9	48.1	111.3	231.2	436.8	932.2
	1324	1.0	2.4	8.8	28.0	72.7	166.0	341.7	651.6	1182.2
19		1.4	2.0	8.6	22.9	74.1	110.4	284.1	645.4	1283.2
	13524	1.2	2.8	10.5	30.0	82.8	207.0	481.1	1010.9	1942.0
21		1.0	3.5	9.4	23.2	62.8	141.8	311.0	669.6	1581.9
	13524	1.0	2.6	7.1	17.1	45.5	119.7	282.8	608.2	1291.3
23		1.0	2.6	8.2	24.1	55.2	148.8	366.8	835.7	1739.2
	142536	1.2	4.0	16.8	58.2	172.0	452.9	1070.9	2339.2	4679.4

three significant digits could be lost when computing $Q^{(m,n)}(f)$ in finite precision using either generator sequence, as long as the appropriate permutation is used. For $n=2$, some conjectures are that G_G is good with m even and, G_P is good when $2m+1 = 3(2^i)-1$ for any $i>0$. It also seems possible that for fixed n increasing m with G_P, $|W|$ is bounded from above. If this is true then $Q^{(m,n)}(f)$ converges to $I(f)$, if $f(\mathbf{x})$ continuous [4, Cor. 4.3.7]. Generally, the results in this section show that there are families of FSI rules that are relatively stable and reasonably efficient. Any of the FSI rules discussed in this section can be easily computed using the same straightforward computer program, that requires only m, n and $\{\lambda_i\}$ for inputs.

4. Weights for modified rules. In this section formulas for the weights for rules that have not been derived as interpolatory rules, but have a structure that is close to that for the interpolatory rules already described, are considered. It might be possible that an interpolatory theory can be developed for these rules if it can be shown how to construct explicit formulas for Lagrange interpolation polynomials for the integrand evaluation point sets used by these rules. There are numerous published examples of rules of this type (see Stroud [14]), and families of this type have been developed by Lyness [7], [8], McNamee and Stenger [10], Lyness and Keast [9], and Genz and Malik [3]. As an example, consider a rule of degree 13 with $n=6$, with the FS basic rule indices for an FSI rule given in Table 3.1. The six-dimensional degree 13 rule described by Lyness and Keast [9] has almost the same structure, but the FS basic rules with indices (321), (3111), (2211) and (21111) in the FSI rule are replaced by those with indices (333), (2222), (3333) and (22222). This FS rule is considerably more efficient (4625 integrand values) than the G_G generator FSI rule, but the weights for the modified rule cannot be determined using the direct methods described in the previous section and a (block triangular) linear system of 22 equations in the 22 unknown weights must be solved. In this section it is shown how the weights for such modified rules can be obtained more directly from the weights for FSI rules.

The question of what replacement modifications to an FSI rule are allowed so that the resulting rule can still be of the same degree is a complicated one that will not be considered in detail here. Keast and Lyness [6] consider this question from the point of view of asking what is the minimal structure necessary for a FS rule of specified degree; the rules that they develop satisfy certain minimal structure conditions and are as efficient as is possible using the Gauss point generator sequence. Mantel and Rabinowitz [11] also consider this question for rules that are not necessarily fully symmetric but only for $s=2$ and $s=3$.

Consider a modified FS rule in the form

$$Q'(f)=\sum_{\mathbf{p}\in P^{(m,n)}} w'_{\mathbf{p}} f[\boldsymbol{\lambda}_{\mathbf{p}}]+\sum_{i=1}^{a} W_i f[\boldsymbol{\lambda}_{\mathbf{p}_i}].$$

THEOREM 4.1. *A modified* FS *rule has degree* $2m+1$ *if the weights are given by*

$$w'_{\mathbf{p}}=w_{\mathbf{p}}-\sum_{i=1}^{a} W_i \sum_{\mathbf{j}\in\Pi\mathbf{p}_i} M_{m,\mathbf{p}}(\boldsymbol{\lambda}_{\mathbf{j}}),$$

where $w_{\mathbf{p}}=2^{-[\mathbf{p}]}I(M_{m,\mathbf{p}}(\mathbf{x}))$.

Proof. Apply $Q'(f)$ to $f(\mathbf{p})=\mathbf{x}^{2\mathbf{k}}$ to obtain

$$\begin{aligned}
Q'(\mathbf{x}^{2\mathbf{k}})&=\sum_{|\mathbf{p}|\leq m} w'_{\mathbf{p}}2^{[\mathbf{p}]}\boldsymbol{\lambda}_{\mathbf{p}}^{2\mathbf{k}}+\sum_{i=1}^{a} W_i\sum_{\mathbf{j}\in\Pi\mathbf{p}_i} 2^{[\mathbf{p}]}\boldsymbol{\lambda}_{\mathbf{j}}^{2\mathbf{k}}\\
&=\sum_{|\mathbf{p}|\leq m} w'_{\mathbf{p}}2^{[\mathbf{p}]}\boldsymbol{\lambda}_{\mathbf{p}}^{2\mathbf{k}}+\sum_{i=1}^{a} W_i\sum_{\mathbf{j}\in\Pi\mathbf{p}_i} 2^{[\mathbf{p}]}\sum_{|\mathbf{p}|\leq m} M_{m,\mathbf{p}}(\boldsymbol{\lambda}_{\mathbf{j}})\boldsymbol{\lambda}_{\mathbf{p}}^{2\mathbf{k}}\\
&=\sum_{|\mathbf{p}|\leq m} 2^{[\mathbf{p}]}\boldsymbol{\lambda}_{\mathbf{p}}^{2\mathbf{k}}\left(w'_{\mathbf{p}}+\sum_{i=1}^{a} W_i\sum_{\mathbf{j}\in\Pi\mathbf{p}_i} M_{m,\mathbf{p}}(\boldsymbol{\lambda}_{\mathbf{j}})\right).
\end{aligned}$$

Comparison with

$$I(\mathbf{x}^{2\mathbf{k}})=\sum_{|\mathbf{p}|\leq m} w_{\mathbf{p}}2^{[\mathbf{p}]}\boldsymbol{\lambda}_{\mathbf{p}}^{2\mathbf{k}}$$

gives the desired result.

So far no restriction has been placed on the weights W_i and points $\boldsymbol{\lambda}_{\mathbf{p}_i}$. If the modifications are supposed to increase the efficiency of the modified rule these points should be chosen so that some of the $w'_{\mathbf{p}}$ values are zero for $|\mathbf{p}|\leq m$. The following system must therefore be satisfied:

$$\sum_{i=1}^{a} W_i D_i = w_{\mathbf{p}}, \quad \text{for all } \mathbf{p}\in T, \tag{4.1}$$

where

$$D_i=\sum_{\mathbf{j}\in\Pi\mathbf{p}_i} M_{m,\mathbf{p}}(\boldsymbol{\lambda}_{\mathbf{j}}),$$

and T is some set of $\mathbf{p}$'s with $|\mathbf{p}|\leq m$. In the simplest case, where $a=1$, one solution is $W_1=w_{\mathbf{p}}/D_1$, given $\mathbf{p}$ and any $\mathbf{p}_1$ with $|\mathbf{p}|\leq m<|\mathbf{p}_1|$. This is possible as long as $D_1\neq 0$.

When $a>1$ the nonlinear system (4.1) is similar in form to the systems that are often used to derive integration rules. However, for many rules that have been developed the appropriate a is considerably less than the number of equations in the original system for the modified weights, so the approach suggested here could give a reduction in the work necessary for the construction of such rules. For example, with the six-dimensional degree 13 Keast-Lyness modified Gauss generator rule discussed at the beginning of this section, $a=4$ compared to the original 22.

One example of the $a=1$ case involves the rules described by Genz and Malik [3], where $\mathbf{p}_1=(m, m, \cdots, m)$ and it is shown how to determine $\lambda_1, \cdots, \lambda_m$ and W_1 to make $w'_{\mathbf{p}}=0$ for all $\mathbf{p}$ with $|\mathbf{p}|=m$. Since $\Pi_{\mathbf{p}_1}=\{\mathbf{p}_1\}$, the modified weights are given directly by

$$w'_{\mathbf{p}}=w_{\mathbf{p}}-W_1 M_{m,\mathbf{p}}(\lambda_{\mathbf{p}_1}),$$

for all $\mathbf{p}$ with $|\mathbf{p}|<m$. These rules are more efficient than an FSI rule with the same generators for a number of values of m and n because a single 2^n point FS basic rule replaces all of the FS basic rules with $|\mathbf{p}|=m$.

However, the unmodified rules discussed in § 3 are already quite efficient when compared to other published rules. If the total integrand value numbers from Table 3.2 for the G_P FSI rules are compared with the numbers for the modified G_G rules given by Keast [5, Table 4] and denoted in Table 3.2 by G_{KL}, it can be easily seen that only for the $(2m+1, n)$ pairs $(9,2)$, $(13,2)$, $(15,2)$, $(17,2)$, $(19,2)$, $(9,3)$, $(15,3)$ and $(17,3)$ are the G_{KL} rules more efficient. On the other hand the modified rules described by Genz and Malik [3] (G_{GM} in Table 3.2) are more efficient for $5<2m+1<15$ and $1<n<11$ than the G_P FSI rules except when $(2m+1, n)=(11,2)$, $(11,3)$, $(13,3)$ and $(13,4)$. There is at present no information about the stability of the G_{KL} rules or the G_{GM} rules. For $n>3$ and $2m+1>13$ the G_P FSI rules are at present the most efficient rules known for the hypercube. They are also "fairly" good rules, because $|W|$ does not appear to grow too rapidly with m.

5. Concluding remarks. The main result of this paper is to show how the weights for large classes of rules for the approximate calculation of fully symmetric multiple integrals can be obtained as integrals of multivariable polynomials. The formulas developed lead easily to the description of a new imbedded family of FS rules based on the Patterson generators that are simple, efficient and only moderately unstable. Error formulas for the interpolatory rules have not been considered, but it is possible that the formulas already provided will also help in their development.

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