Symmetric Integration Rules for Hypercubes III. Construction of Integration Rules Using Null Rules

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Abstract. A new operator, which we term a "Null Rule" is defined. Its properties which are analogous to those of an integration rule are investigated. It is found to be useful in the construction of high-dimensional integration rules of moderate degree. A set of integration rules $W_{t+1}^{(n)}$ are derived which are more economical in the number of required function evaluations than the previously published $\bar{G}_{t+1}^{(n)}$.

1. Introduction. This part of this paper follows directly from Parts I and II (Lyness [1] and [2]). In Part I we introduced the n-dimensional basic rule $\mathcal{R}^{(n)}$ and the composite rule $R^{(n)}$. These rules have hypercubic symmetry, that is, they are invariant under any rotation or reflection of the hypercube into itself. In Part II we defined and discussed the projection and extension of an n-dimensional rule of degree d, to form an n'-dimensional rule ($n' \neq n$) of degree d' and determined the relation between d and d'.

In this part we exploit the formalism of Part II with a view to determining high-dimensional rules of moderate degree. As an intermediate step we define the "Null Rule" and determine some of its properties. We then use it as the basis of a recursive procedure. This procedure is used to determine a set of integration rules $W_{t+1}^{(n)}$ and several other closely related sets.

2. Null Rules. The n-dimensional rule $R^{(n)}$ is defined in terms of n-dimensional basic rules in Part I by the relation

$$R^{(n)} = \sum \xi_j \mathcal{R}_j^{(n)}, \tag{2.1}$$

where

$$\sum \xi_j = 1. \tag{2.1a}$$

It is convenient to introduce an operator which has certain of the properties of a composite rule. We term this operator an *n-dimensional null rule* $N^{(n)}$ and it is defined by the relation

$$N^{(n)} = \sum \zeta_j \mathcal{R}_j^{(n)}, \tag{2.2}$$

where

$$\sum \zeta_j = 0. \tag{2.2a}$$

All null rules have the property that they integrate any nonzero constant function (incorrectly) to give the result zero. For if $f = 1$ we find that

$$N^{(n)}f = \sum \zeta_j \mathcal{R}_j^{(n)} f = \sum \zeta_j = 0. \tag{2.3}$$

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Any null rule operator may be formed by taking the difference between two different composite rule operators. Thus the properties of null rules follow closely those of composite rules. For example, the derivation of the error expansion of the null rule (2.2) above is almost identical with the derivation of the error expansion [1, (3.2)] of the composite rule given in detail in Sections 2 and 3 of part I. We define the error coefficients

$$c_{2s_1 2s_2 \cdots 2s_n}(N^{(n)}) = \sum \zeta_j c_{2s_1 2s_2 \cdots 2s_n}(\mathcal{R}_j^{(n)}) \tag{2.4}$$

and the operator β_{2s} by

$$\beta_{2s}(N^{(n)}) = \sum \zeta_j \beta_{2s}(\mathcal{R}_j^{(n)}). \tag{2.5}$$

The expression for $\beta_{2s}(\mathcal{R}^{(n)})$ is given in equations [1, (3.4)]. In terms of these quantities we find

$$N^{(n)}f = \sum \zeta_j \mathcal{R}_j^{(n)} - \sum \zeta_j If = \sum \beta_{2s}(N^{(n)})f \tag{2.6}$$

in direct analogy to expansion [1, (3.22)]. It follows from the above definitions that

$$c_{00\cdots 0}(N^{(n)}) = 0, \tag{2.7}$$

$$\beta_0(N^{(n)})f = 0. \tag{2.8}$$

The values of these quantities if $N^{(n)}$ is replaced by a composite rule $R^{(n)}$, are 1 and $I^{(n)}f$, respectively.

We may form the convolution product of any two one-dimensional operators whether they be composite rules or null rules or both. The definition is the same as for composite rules, namely

$$T = R * S = \sum_j \xi_j \mathcal{R}_j * \sum_k \zeta_k \mathcal{R}_k = \sum_j \sum_k \xi_j \zeta_k \mathcal{R}_j * \mathcal{R}_k . \tag{2.9}$$

It should be noted that T is a null rule if either R or S or both are null rules.

Equation [1, (3.25)] expresses the error coefficients of an n-dimensional convolution product $R_1 * R_2 * \cdots * R_n$ of one-dimensional composite rules R_i in terms of the error coefficient of each one-dimensional composite rule. This result and its proof is unaltered if any or all the composite rules R_i are replaced by null rules. In particular, [1, (3.26)], which is a special case of [1, (3.25)], may be applied to a null rule, giving the result

$$c_{2s_1 2s_2 \cdots 2s_n}((N^{(1)})^n) = c_{2s_1}(N^{(1)}) c_{2s_2}(N^{(1)}) \cdots c_{2s_n}(N^{(1)}). \tag{2.10}$$

3. The Projection and Extension of Null Rules. It is convenient to introduce a particular n-dimensional null operator $\mathcal{O}^{(n)}$. This operator has the defining property

$$\mathcal{O}^{(n)} f(x_1, x_2, \cdots, x_n) = 0 \tag{3.1}$$

together with the consequent properties

$$\mathcal{O}^{(i)} * \mathcal{R}(\alpha_1, \alpha_2, \cdots, \alpha_j) = \mathcal{O}^{(i+j)}, \tag{3.2}$$

$$\mathcal{O}^{(i)} + \mathcal{R}(\alpha_1, \alpha_2, \cdots, \alpha_i) = \mathcal{R}(\alpha_1, \alpha_2, \cdots, \alpha_i). \tag{3.3}$$

The projection of basic rules and composite rules was defined in Section 2 of Part I in terms of a projection operator. We define the projection of a null rule in the same way as the projection of a composite rule, in terms of the projections of its constituent basic rules. Thus

$$\mathcal{P}\left(\sum \zeta_i \mathcal{R}_i^{(n)}\right) = \sum \zeta_i \left(\mathcal{P}\mathcal{R}_i^{(n)}\right) \tag{3.4}$$

the final term being defined in [2, (2.2)]. This indicates that a null rule projects onto a null rule. We note that an important property of projection is retained, namely,

$$N^{(r)} f(x_1, x_2, \cdots, x_{r-1}) = (\mathcal{P}(N^{(r)})) f(x_1, x_2, \cdots, x_{r-1}). \tag{3.5}$$

In keeping with this definition we see that

$$\mathcal{P}\mathcal{O}^{(n)} = \mathcal{O}^{(n-1)} \tag{3.6}$$

and that we may define a zero-dimensional null operator $\mathcal{O}^{(0)}$ in analogy to $\mathcal{I}$ of [2, (2.6)] with the properties (3.2) and (3.3) above. In addition, all null rules project onto $\mathcal{O}^{(0)}$. Thus

$$\mathcal{P}(N^{(1)}) = \mathcal{O}^{(0)}. \tag{3.7}$$

We may derive an expression for the projection of the convolution product $S_1^{(s)} * S_2^{(t)}$ of two null rules or a null rule and a composite rule $S_1^{(s)}$ and $S_2^{(t)}$. This expression is precisely the same as if $S_1^{(s)}$ and $S_2^{(t)}$ were composite rules (given in [2, (2.9)]), and is

$$\mathcal{P}(S_1^{(s)} * S_2^{(t)}) = \frac{1}{s+t} \{ s\mathcal{P}(S_1^{(s)}) * S_2^{(t)} + tS_1^{(s)} * \mathcal{P}(S_2^{(t)}) \} \tag{3.8}$$

whether $S_1^{(s)}$, $S_2^{(t)}$ be null rules or composite rules. Applying this to the n-dimensional product null rule $(N^{(1)})^n$ we find

$$\mathcal{P}((N^{(1)})^n) = \mathcal{O}^{(n-1)}. \tag{3.9}$$

This result contrasts with the corresponding result for a composite rule [2, (2.10)], namely,

$$\mathcal{P}((R^{(1)})^n) = (R^{(1)})^{n-1}. \tag{3.10}$$

The extension of a null rule to a higher dimension is another null rule defined n terms of the extension of basic rules as follows:

$$E_s^{s+1}(\nu) N^{(s)} = E_s^{s+1}(\nu) \sum \zeta_i \mathcal{R}_i^{(s)} = \sum \zeta_i E_s^{s+1}(\nu) \mathcal{R}_i^{(s)}, \tag{3.11}$$

where $E_s^{s+1}(\nu)\mathcal{R}_i^{(s)}$ is as defined in [2, (3.5)]. The formula for the extension of the s-dimensional null product rule $(N^{(1)})^s$ is simpler than [2, (3.13)] the corresponding formula for the composite rule $(R^{(1)})^s$. It appears that

$$E_s^n(\nu)(N^{(1)})^s = \frac{n!}{s!(n-s)!} \mathcal{R}(\nu)^{n-s} * (N^{(1)})^s. \tag{3.12}$$

In Sections 5 and 6 we shall make use of null rules of the type

$$S = (E_s^n(\alpha) - E_s^n(0))\mathcal{R}(\alpha)^s. \tag{3.13}$$

We note that

$$S \Rightarrow (E_s^{s+1}(\alpha) - E_s^{s+1}(0))\mathcal{R}(\alpha)^s \Rightarrow \mathcal{O}^{(s)}. \tag{3.14}$$

Moreover, it follows from (3.12) and [2, (3.13)] that

$$(3.15) \qquad (E_s^{s+1}(\alpha) - E_s^{s+1}(0))\mathcal{R}(\alpha)^s = (\mathcal{R}(\alpha) - \mathcal{R}(0))^{s+1}.$$

4. The Degree of a Null Rule. The degree $d = 2t + 1$ of a composite rule $R^{(n)}$ has been defined both in Part I in terms of its error coefficients, and in Part II in terms of the functions which it integrates exactly. One of these definitions states that the degree of a rule is $2t + 1$ or greater if

$$(4.1) \qquad c_{00\cdots0}(R^{(n)}) = 1,$$

$$(4.2) \qquad c_{2s_12s_2\cdots2s_n}(R^n) = 0, \qquad 1 < \sum_{i=1}^{n} 2s_i < 2t + 1,$$

and the other states that the rule is of degree $2t + 1$ or greater if

$$(4.3) \qquad R^{(n)}f = I^{(n)}f \quad \text{when} \quad f \in \Phi_{t+1}^{(n)},$$

the set $\Phi_{t+1}^{(n)}$ being defined in [2, (4.4)].

In constructing rules of degree $2t + 1$ it is useful to be able to use the property that if R_1 and R_2 are of a particular degree, so is $\lambda R_1 + (1 - \lambda)R_2$. This trivial property follows directly from either of the above definitions.

The definition of the degree of a null rule is chosen so that it retains this property. The definition is as follows:

Definition. A null rule $N^{(n)}$ is of degree $2t + 1$ or greater if

$$(4.4) \qquad c_{2s_12s_2\cdots2s_n}(N^{(n)}) = 0, \qquad \sum_{i=1}^{n} 2s_i < 2t + 1.$$

From this follows trivially the alternative definition corresponding to (4.3) above, namely, that a null rule $N^{(n)}$ is of degree $2t + 1$ or greater if

$$(4.5) \qquad R^{(n)}f = 0 \quad \text{when} \quad f \in \Phi_{t+1}^{(n)}.$$

We may construct a rule $R^{(n)}$ by combining null rules $N_i^{(n)}$ and composite (or basic) rules $R_i^{(n)}$ as follows:

$$R^{(n)} = \sum \xi_i R_i^{(n)} + \sum \lambda_i N_i^{(n)},$$

where

$$\sum \xi_i = 1.$$

It follows from the definitions (4.1) to (4.5) that if all the $N_i^{(n)}$ and $R_i^{(n)}$ are of degree d, the rule $R^{(n)}$ is also of this degree.

It is useful to express the degree of the product null rule $(N^{(1)})^n$ in terms of the degree of the one-dimensional rule $N^{(1)}$. To do this we make use of the definition (4.4) and the expansion (2.10). If $N^{(1)}$ is of degree $2t + 1$, it follows that

$$c_{2s}(N^{(1)}) = 0, \qquad 2s \leqq 2t.$$

Thus the product

$$c_{2s_1}(N^{(1)})c_{2s_2}(N^{(1)}) \cdots c_{2s_n}(N^{(1)}) = 0 \quad \text{if any} \quad 2s_i < 2t + 2.$$

This product is therefore zero if the sum of the n positive numbers $2s_1, 2s_2, \cdots,$

$2s_n$ is less than $n(2t+2)$ for in that case at least one number $2s_i$ is less than $(2t+2)$ and the corresponding term $c_{2s_i}(N^{(1)})$ is zero. Using (2.10) this shows that

$$c_{2s_1 2s_2 \cdots 2s_n}((N^{(1)})^n) = 0, \qquad \sum 2s_i < n(2t+2) - 1,$$

and the definition of degree (4.4) shows that the degree of $(N^{(1)})^n$ is $n(2t+2)-1$. We state this result as a theorem;

THEOREM 4.1. *If the null rule $N^{(1)}$ is of degree d, the product null rule $(N^{(1)})^n$ is of degree $d' = n(d+1) - 1$.*

The null rule $\mathcal{O}^{(s)}$ is of any degree since $\mathcal{O}^{(s)}f$ is zero for any function. This gives the following result:

THEOREM 4.2. *If*

$$N^{(n)} \Rightarrow \mathcal{O}^{(s)},$$

then $N^{(n)}$ is of degree at least $2s+1$.

5. A Set of Null Rules $S_{t+1}^{(m)}$. In Part II it was shown that starting with a t-dimensional rule $R_{t+1}^{(t)}$ of degree $2t+1$ we could construct a greater dimensional rule of the same degree by using the formula for rule extension. Thus the rules $E_t^{t+1}(0)R_{t+1}^{(t)}$, $E_{t+1}^{t+2}(0)E_t^{t+1}(0)R_{t+1}^{(t)}$ could be considered as the results of a recursive procedure

$$R_{t+1}^{(n)} = E_{n-1}^{n}(0)R_{t+1}^{(n-1)}, \qquad n > t, \tag{5.1}$$

which commenced with the rule $R_{t+1}^{(t)}$. However, this first rule might be difficult to construct and it would be useful if we could derive a recursive procedure of this type which started with a one-dimensional rule $R_{t+1}^{(t)}$ of degree $2t+1$. In this section we investigate this possibility. We base this attempt on the following theorem:

THEOREM 5.1. *If $R_{t+1}^{(m-1)}$ is an $(m-1)$-dimensional rule of degree $2t+1$ and if $S_{t+1}^{(m)}$ is an m-dimensional null rule having the properties*

$$\mathcal{P}(S_{t+1}^{(m)}) = \mathcal{O}^{(m-1)}, \tag{5.2}$$

$$S_{t+1}^{(m)}f = I^{(m)}f \quad \textit{when} \quad f \in \phi_{t+1}^{m}, \tag{5.3}$$

it follows that

$$R^{(m)} = E_{m-1}^{m}(0)R_{t+1}^{(m-1)} + S_{t+1}^{(m)} \tag{5.4}$$

is an m-dimensional rule of degree $2t+1$.

Proof. If $R^{(m)}$ is given by (5.4) above it follows, using (5.2), that

$$\mathcal{P}(R^{(m)}) = R_{t+1}^{(m-1)} + \mathcal{O}^{(m-1)} = R_{t+1}^{(m-1)}. \tag{5.5}$$

Since $R_{t+1}^{(m-1)}$ is of degree $2t+1$, we have

$$R_{t+1}^{(m-1)}f = I^{(m-1)}f \quad \text{when} \quad f \in \Phi_{t+1}^{(m-1)}. \tag{5.6}$$

The elements of $\Phi_{t+1}^{(m-1)}$ are functions of $m-1$ variables. So using equation [2, (2.3)] and [2, (4.2)] we have

$$R^{(m)}f = \mathcal{P}(R^{(m)})f = R_{t+1}^{(m-1)}f = I^{(m-1)}f = I^{(m)}f \quad \text{when} \quad f \in \Phi_{t+1}^{(m-1)}. \tag{5.7}$$

We now consider $f \in \phi_{t+1}^{m}$. These are functions of m variables having $x_1^2x_2^2 \cdots x_m^2$ as a factor. The rule $E_{m-1}^{m}(0)R^{(m-1)}$ evaluates these functions at points at which they are zero. Thus

$$E^m_{m-1}(0)R^{(m-1)}_{t+1}f = 0 \quad \text{when} \quad f \in \phi^m_{t+1}. \tag{5.8}$$

(This is a special case of Theorem 3.1A of Lyness [3].) Equation (5.8) together with (5.3) above gives

$$R^{(m)}f = E^m_{m-1}(0)R^{(m-1)}_{t+1}f + S^{(m)}_{t+1}f = I^{(m)}f \quad \text{when} \quad f \in \phi^m_{t+1}. \tag{5.9}$$

Since

$$\Phi^{(m)}_{t+1} = \Phi^{(m-1)}_{t+1} \cup \phi^m_{t+1}, \tag{5.10}$$

(5.9) and (5.7) together combine to give

$$R^{(m)}f = I^{(m)}f \quad \text{when} \quad f \in \Phi^{(m)}_{t+1} \tag{5.11}$$

and this is the condition that $R^{(m)}$ is of degree $2t + 1$. This establishes Theorem 5.1.

A converse of Theorem 5.1 is true. This is

THEOREM 5.2. *If $R^{(m)}_{t+1}$ and $R^{(m-1)}_{t+1}$ are any two m- and $(m - 1)$-dimensional integration rules of degree $2t + 1$, then the null rule*

$$S^{(m)} = R^{(m)}_{t+1} - E^m_{m-1}(0)R^{(m-1)}_{t+1} \tag{5.12}$$

has the properties

$$S^{(m)}f = I^{(m)}f \quad \textit{when} \quad f \in \phi^m_{t+1}, \qquad \mathcal{P}(S^{(m)}) = \mathcal{O}^{(m-1)}. \tag{5.13}$$

The proof uses the argument of the proof of Theorem 5.1 in the reverse order and is not given explicitly here.

The value of these theorems as the basis of a method of constructing integration rules depends on the difficulty involved in calculating a particular null rule $S^{(m)}_{t+1}$ which satisfies (5.2) and (5.3). It appears that to satisfy (5.3) is the principal difficulty. For once we have found either a rule or a null rule $T^{(m)}$ which satisfies the nonlinear equations (5.3), that is

$$T^{(m)}f = I^{(m)}f \quad \text{when} \quad f \in \phi^m_{t+1} \tag{5.14}$$

We need only set

$$S^{(m)}_{t+1} = T^{(m)} - E^m_{m-1}(0)(\mathcal{P}(T^{(m)})) \tag{5.15}$$

and it is apparent that $S^{(m)}_{t+1}$ satisfies (5.3) and also that

$$\mathcal{P}(S^{(m)}_{t+1}) = \mathcal{P}(T^{(m)}) - \mathcal{P}(T^{(m)}) = \mathcal{O}^{(m-1)} \tag{5.16}$$

so that $S^{(m)}_{t+1}$ satisfies (5.2) also.

In the next section we indicate a systematic approach and calculate a set of integration rules using this procedure. Before doing this, we examine the construction of the sets of integration rules determined in Part II. We determine possible $S^{(m)}_{t+1}$ which, used recursively in the relation

$$R^{(m)}_{t+1} = E^m_{m-1}(0)R^{(m-1)}_{t+1} + S^{(m)}_{t+1}, \tag{5.17}$$

lead to these sets of integration rules.

The rules $(G_{t+1})^n$ are generated by setting

$$R_{t+1}^{(1)} = G_{t+1} = \sum \zeta_i \mathfrak{R}(\beta_i), \tag{5.18}$$

$$S_{t+1}^{(m)} = (G_{t+1})^m - E_{m-1}^m(0)(G_{t+1})^{m-1}. \tag{5.19}$$

The rules $E_t^n(0)G_{t+1}^t$ may be generated using (5.18) and

$$\begin{aligned} S_{t+1}^{(m)} &= (G_{t+1})^m - E_{m-1}^m(0)(G_{t+1})^{m-1}, \qquad & m \leqq t, \\ S_{t+1}^{(m)} &= \mathcal{O}^{(m)}, & m > t. \end{aligned} \tag{5.20}$$

The rules $\bar{G}_{t+1}^{(n)}$ may be generated using (5.18) and

$$\begin{aligned} S_{t+1}^{(m)} &= (G_{t+1})^m - E_{m-1}^m(0)(G_{t+1})^{m-1}, \qquad m \leqq t-1, \\ S_{t+1}^{(t)} &= \frac{1}{(3\beta_1^2)^t}[(E_{t-1}^t(\beta_1) - E_{t-1}^t(0))\{\mathfrak{R}(\beta_1)\}^{t-1}], \\ S_{t+1}^{(m)} &= \mathcal{O}^{(m)}, \qquad m > t. \end{aligned} \tag{5.21}$$

These sets of rules were not in fact determined by this procedure. This is the reason for the somewhat obvious form of (5.19).

6. The Rules $W_{t+1}^{(n)}$. We construct in this section a set of integration rules $W_{t+1}^{(n)}$ using the procedure of the previous section. To do this we construct certain of the $S_{t+1}^{(m)}$. There is of course a very wide choice about how to do this. In this example, we have to make several arbitrary choices. These are made with a view to being as economical as is convenient in the number of points used by the constructed rule; the criterion of convenience here is based on the amount of analytic work involved. Thus the rules constructed will not be minimal rules. Nor will they be unduly extravagant rules in terms of the number of points required.

We set

$$S_{t+1}^{(m)} = \mathcal{O}^{(m)}, \qquad m \geqq t+1, \tag{6.1}$$

and we expand the relation (5.17) to give

$$W_{t+1}^{(n)} = E_t^{(n)}(0)S_{t+1}^{(t)} + E_{t-1}^{(n)}(0)S_{t+1}^{(t-1)} + E_{t-2}^{(n)}(0)S_{t+1}^{(t-2)} + E_{t-3}^{(n)}(0)W_{t+1}^{(t-3)}. \tag{6.2}$$

For the sake of definiteness, we set $W_{t+1}^{(t-3)}$ to be $(G_{t+1})^{t-3}$ though there are better choices. Thus

$$S_{t+1}^{(m)} = (G_{t+1})^m - E_{m-1}^m(0)(G_{t+1})^{m-1}, \qquad m \leqq t-4. \tag{6.3}$$

We now determine null rules $S_{t+1}^{(m)}$ $(m = t-2,\ t-1,\ t)$. The choice of $W_{t+1}^{(t-3)}$ does not directly affect the form of $S_{t+1}^{(m)}$ $(m > t-4)$. At a later stage we may if we like make a different choice for $W_{t+1}^{(t-3)}$ without having to recalculate $S_{t+1}^{(m)}$ $(m > t-4)$.

We deal with these out of order, taking $S_{t+1}^{(t-1)}$ first. We consider a null rule of the form

$$S_{t+1}^{(t-1)} = \lambda_{t-1}(E_{t-2}^{t-1}(\alpha_{t-1}) - E_{t-2}^{t-1}(0))(\mathfrak{R}(\alpha_{t-1})). \tag{6.4}$$

This satisfies condition (5.2), namely,

$$\mathcal{P}(S_{t+1}^{(t-1)}) = \mathcal{O}^{(t-2)}. \tag{6.5}$$

The two elements of ϕ_{t+1}^{t-1} are $x_1^2x_2^2 \cdots x_{t-1}^2$ and $x_1^4x_2^2 \cdots x_{t-1}^2$. Thus condition (5.3) gives two equations which we use to determine λ_{t-1} and α_{t-1}. These equations are

$$S_{t+1}^{(t-1)}x_1^2x_2^2 \cdots x_{t-1}^2 = I^{(t-1)}x_1^2x_2^2 \cdots x_{t-1}^2,$$
$$S_{t+1}^{(t-1)}x_1^4x_2^2 \cdots x_{t-1}^2 = I^{(t-1)}x_1^4x_2^2 \cdots x_{t-1}^2. \quad (6.6)$$

Substituting (6.4) and the values of $I^{(t-1)}f$ we find

$$\lambda_{t-1}\alpha_{t-1}^{2t-2} = 1/3^{t-1},$$
$$\lambda_{t-1}\alpha_{t-1}^{2t} = 1/5\cdot 3^{t-1}, \quad (6.7)$$

which have the solution

$$\lambda_{t-1} = (5/9)^{t-1}, \quad (6.8)$$

$$\alpha_{t-1} = \sqrt{(3/5)}. \quad (6.9)$$

Thus we set

$$S_{t+1}^{(t-1)} = (5/9)^{t-1}(E_{t-2}^{t-1}(\sqrt{(3/5)}) - E_{t-2}^{t-1}(0))(\mathcal{R}(\sqrt{(3/5)}))^{t-2} \quad (6.10)$$

The contribution of this null rule to the rule $W_{t+1}^{(n)}$ of (6.2) is $E_{t-1}^{n}(0)S_{t+1}^{(t-1)}$ and so uses all points used by the basic rules

$$\mathcal{R}(0)^{n-s} * \mathcal{R}(\sqrt{(3/5)})^s, \qquad s = 0, 1, \cdots, t-1.$$

The null rule $S_{t+1}^{(t)}$ may be constructed in the same way. We choose

$$S_{t+1}^{(t)} = \lambda_t(E_{t-1}^{t}(\alpha_t) - E_{t-1}^{t}(0))(\mathcal{R}(\alpha_t))^{t-1} \quad (6.11)$$

which satisfies condition (5.2). The set ϕ_{t+1}^{t} contains only one function $x_1^2x_2^2 \cdots x_t^2$. Applying condition (5.3) we find

$$S_{t+1}^{(t)}x_1^2x_2^2 \cdots x_t^2 = I^{(t)}x_1^2x_2^2 \cdots x_t^2 \quad (6.12)$$

which gives

$$\lambda_t\alpha_t^{2t} = 1/3^t. \quad (6.13)$$

The null rule $S_{t+1}^{(t)}$ appears in $W_{t+1}^{(n)}$ in the combination $E_t^{n}(0)S_{t+1}^{(t)}$ and uses all the points used by the basic rules

$$\mathcal{R}(0)^{n-s} * \mathcal{R}(\alpha_t)^s, \qquad s = 0, 1, \cdots, t.$$

We choose α_t so that these points coincide as far as possible with those used by $E_{t-1}^{n}(0)S_{t+1}^{(t-1)}$ and so we set

$$\alpha_t = \sqrt{(3/5)}, \quad (6.14)$$

$$\lambda_t = (5/9)^t, \quad (6.15)$$

giving

$$S_{t+1}^{(t)} = (5/9)^t(E_{t-1}^{t}(\sqrt{(3/5)}) - E_{t-1}^{t}(0))(\mathcal{R}(\sqrt{(3/5)}))^{t-1}. \quad (6.16)$$

In the special case $t = 2$, the construction of $S_{t+1}^{(m)}$ is now complete. The resulting rule is given previously in Part II and is $E_2^{n}(0)(G_3)^2$.

The construction of $S_{t+1}^{(t-2)}$ is more complicated. We deal in detail with the case $t \geqq 4$. We write down a null rule of rather a complicated form

$$
\begin{aligned}
S_{t+1}^{(t-2)} = {} & \sum_i \eta_i (E_{t-3}^{t-2}(\gamma_i) - E_{t-3}^{t-2}(0))(\mathfrak{R}(\gamma_i))^{t-3} \\
& + \eta_0 (E_{t-3}^{t-2}(\sqrt{(3/5)}) - E_{t-3}^{t-2}(0)) * (\mathfrak{R}(\sqrt{(3/5)})^{t-3} \qquad (6.17) \\
& + \frac{\zeta}{t-2} (E_{t-3}^{t-2}(\alpha) - E_{t-3}^{t-2}(0))((t-3)\mathfrak{R}(\beta) + \mathfrak{R}(\alpha)) * (\mathfrak{R}(\alpha))^{t-4}).
\end{aligned}
$$

Here α, β, γ_i, ζ, η_0 and η_i are parameters. This expression satisfies the requirement (5.2), namely,

$$\mathcal{P}(S_{t+1}^{(t-2)}) = \mathcal{O}^{(t-3)}.$$

It is also necessary to satisfy requirement (5.3) which gives the four nonlinear equations

$$
\begin{aligned}
& S_{t+1}^{(t-2)} x_1^2 x_2^2 \cdots x_{t-2}^2 = I^{(t-2)} x_1^2 x_2^2 \cdots x_{t-2}^2, \\
(6.18) \qquad & S_{t+1}^{(t-2)} x_1^4 x_2^2 \cdots x_{t-2}^2 = I^{(t-2)} x_1^4 x_2^2 \cdots x_{t-2}^2, \\
& S_{t+1}^{(t-2)} x_1^6 x_2^2 \cdots x_{t-2}^2 = I^{(t-2)} x_1^6 x_2^2 \cdots x_{t-2}^2, \\
(6.19) \qquad & S_{t+1}^{(t-2)} x_1^4 x_2^4 x_3^2 \cdots x_{t-2}^2 = I^{(t-2)} x_1^4 x_2^4 x_3^2 \cdots x_{t-2}^2.
\end{aligned}
$$

These equations give

$$
\begin{aligned}
& \zeta \beta^2 \alpha^{2t-6} + \sum \eta_i \gamma_i^{2t-4} + \eta_0 (3/5)^{t-2} = 1/3^{t-2}, \\
(6.20) \quad & \frac{\zeta}{t-2} [\beta^4 \alpha^{2t-6} + (t-3)\beta^2 \alpha^{2t-4}] + \sum \eta_i \gamma_i^{2t-2} + \eta_0 (3/5)^{t-1} = 1/5 \cdot 3^{t-3}, \\
& \frac{\zeta}{t-2} [\beta^6 \alpha^{2t-6} + (t-3)\beta^4 \alpha^{2t-4}] + \sum \eta_i \gamma_i^{2t} + \eta_0 (3/5)^{t} = 1/7 \cdot 3^{t-3}, \\
(6.21) \quad & \frac{\zeta}{t-2} [2\beta^2 \alpha^{2t-4} + (t-4)\beta^2 \alpha^{2t-2}] + \sum \eta_i \gamma_i^{2t} + \eta_0 (3/5)^{t} = 1/5^2 \cdot 3^{t-4},
\end{aligned}
$$

respectively.

Taking the difference of the final two equations we find

$$\frac{\zeta}{t-2} \beta^2 \alpha^{2t-6} (\beta^2 - \alpha^2) = \left(\frac{1}{7 \cdot 3} - \frac{1}{5 \cdot 5} \right) \frac{1}{3^{t-4}}. \qquad (6.22)$$

We are now in a position to justify the choice (6.17). Since there are four equations of the type (5.3) we need four adjustable parameters. Thus we might have hoped at that stage that the first term with two values of i would suffice. Since we are using all the points required by the second term we include it as it brings in another adjustable parameter η_0 at no cost in the number of points. However, (6.22) indicates that we need another type of rule. For if we were to set ζ in (6.17) to be zero, equation (6.22) would be a contradiction. (This is a direct verification of Theorem 3.4 of Lyness [3].) The precise form of this additional term is obtained if we include in $S_{t+1}^{(t-2)}$ a basic rule $\mathfrak{R}(\beta) * (\mathfrak{R}(\alpha))^{t-3}$ but not $\mathfrak{R}(\alpha)^{t-2}$. There are now enough parameters to include only one term in the summation in the first term of (6.17) and to omit the suffix i.

The solutions to equations (6.20) and (6.21) are two two-parameter systems; we use parameters η_0 and λ; we set

$$A = \frac{3\cdot 4}{7\cdot 25(t-2)}\{1 - \eta_0(\tfrac{9}{5})^{t-2}\}^{-1} \tag{6.23}$$

and

$$S_A = +1 \quad \text{if} \quad A > 0, \qquad S_A = -1 \quad \text{if} \quad A < 0. \tag{6.24}$$

Then the parameters in (6.17) are:

$$\begin{aligned} \alpha^2 &= 3/5 + (-\lambda \pm \sqrt{(S_A + \lambda^2)})\sqrt{|A|}, \\ \beta^2 &= 3/5 + (-\lambda \mp (t-3)\sqrt{(S_A + \lambda^2)})\sqrt{|A|}, \\ \gamma^2 &= 3/5 + A/(\lambda\sqrt{|A|}), \end{aligned} \tag{6.25}$$

$$\begin{aligned} \zeta &= \{1 - \eta_0(9/5)^{t-2}\}/(1 + S_A\lambda^2)3^{t-2}\beta^2\alpha^{2t-6}, \\ \eta &= S_A\lambda^2\{1 - \eta_0(9/5)^{t-2}\}/(1 + S_A\lambda^2)3^{t-2}\gamma^{2t-4}. \end{aligned} \tag{6.26}$$

In the case of rules of degree 7 ($t = 3$) the null rule $S_{t+1}^{(t-2)}$ is not of this form. The set ϕ_4^1 contains only three functions. Thus in place of (6.17) we set

$$S_4^{(1)} = \sum_{i=1}^{j} \eta_i(E_0^1(\gamma_i) - E_0^1(0))\mathcal{G} + \eta_0(E_0^1(\sqrt{(3/5)}) - E_0^1(0))\mathcal{G}. \tag{6.27}$$

Putting $j = 1$ leads to equations with no real solutions. Thus we set $j = 2$ and write $S_4^{(1)}$ in the form

$$S_4^{(1)} = \eta_0\mathcal{R}(\sqrt{(3/5)}) + \eta_1\mathcal{R}(\gamma_1) + \eta_2\mathcal{R}(\gamma_2) - (\eta_0 + \eta_1 + \eta_2)\mathcal{R}(0). \tag{6.28}$$

Equations (6.18) and (6.20) are valid with $t = 3$. The solutions in terms of η_0 and λ are

$$\begin{aligned} \gamma_1^2 &= 3/5 + A/(\lambda\sqrt{|A|}), \\ \gamma_2^2 &= 3/5 - \lambda\sqrt{|A|}, \end{aligned} \tag{6.29}$$

$$\begin{aligned} \eta_1 &= S_A\lambda^2(1 - \eta_0(9/5))/3(1 + S_A\lambda^2)\gamma_1^2, \\ \eta_2 &= (1 - \eta_0(9/5))/3(1 + S_A\lambda^2)\gamma_2^2, \end{aligned} \tag{6.30}$$

where A and S_A are given by (6.23) and (6.24) above.

The points used by the rule $W_{t+1}^{(n)}$ may be arranged to lie within the hypercube by a suitable choice of the parameters. Once λ has been chosen we may choose η_0 to make A in (6.23) as small as we like. Thus we may make the values of α^2, β^2, γ^2, or of γ_1^2 and γ_2^2 as close to 3/5 as we like, so ensuring that the points for function evaluation lie within the hypercube.

The rule $W_{t+1}^{(n)}$ is a two-parameter system. The number of points $\nu(W_{t+1}^{(n)})$ given below may not be valid if the parameters are chosen to result in a coincidence of points which are in general distinct. In general

$$\nu(W_{t+1}^{(n)}) = \Gamma_{t-3}^{n} + 4\cdot 2\binom{n}{1} + 5\cdot 2^2\binom{n}{2} + \cdots + t2^{t-3}\binom{n}{t-3} + t\cdot 2^{t-2}\binom{n}{t-2} + 2^{t-1}\binom{n}{t-1} + 2^t\binom{n}{t}, \quad n \geqq t-1, t \geqq 4, \tag{6.31}$$

$$\nu(W_4^{(n)}) = 1 + 3\cdot 2\binom{n}{1} + 4\binom{n}{2} + 8\binom{n}{3}, \quad n \geqq 2. \tag{6.32}$$

Here

$$\Gamma_{t-3}^{n} = \nu(E_{t-3}^{n}(G_{t+1})^{t-3}) = 1 + \left[\frac{t+1}{2}\right]2\binom{n}{1} + \left[\frac{t+1}{2}\right]^2 2^2\binom{n}{2} + \cdots + \left[\frac{t+1}{2}\right]^{t-3} 2^{t-3}\binom{n}{t-3} \tag{6.33}$$

and the square brackets indicate the integer part of the enclosed number.

7. The Rule $W_{t+1}^{(n)*}$. There is one very simple adjustment which can be made to $W_{t+1}^{(n)}$ which in some cases results in a more economical rule.

In Section 3 we noted that the null rule

$$S = (E_t^n(\alpha) - E_t^n(0))\mathcal{R}(\alpha)^t \equiv\rangle\ \mathcal{O}^{(t)} \tag{7.1}$$

and in Section 4 we showed that a null rule which projected onto $\mathcal{O}^{(t)}$ was of degree $2t + 1$. It was also stated that any rule formed as a linear combination of rules and null rules of a particular degree was itself of that degree. We define a new rule $W_{t+1}^{(n)*}$ as

$$W_{t+1}^{(n)*} = W_{t+1}^{(n)} + (5/9)^t(E_t^n(\sqrt{(3/5)}) - E_t^n(0))(\mathcal{R}(\sqrt{(3/5)}))^t, n > t, \tag{7.2}$$

$W_{t+1}^{(n)*}$ uses the same points as $W_{t+1}^{(n)}$ with the important exception that it replaces points used by the basic rule $\mathcal{R}(0)^{n-t} * \mathcal{R}(\sqrt{(3/5)})^t$ by points used by $\mathcal{R}(\sqrt{(3/5)})^n$. Thus

$$\nu(W_{t+1}^{(n)*}) = \nu(W_{t+1}^{(n)}) - 2^t\binom{n}{t} + 2^n. \tag{7.3}$$

TABLE 1

It is only possible to choose λ so that the integration rules $\bar{W}_{t+1}^{(n)}$ (or $\bar{W}_{t+1}^{(n)*}$) require only function evaluations within the hypercube of integration for certain values of n and t. Some of these values are indicated by a $\times$ (or $*$) in this table. The absence of a $\times$ (or $*$) indicates that for the corresponding values of n and t no such choice of λ is possible.

$n =$	3	4	5	6	7	8	9	10	≧11
$t = 3$			× *	× *	× *	× *	× *	× *	× *
4	×	×	×	× *	× *	× *	× *	× *	× *
5		×	×	×	× *	× *	× *	× *	× *
6			×		*	× *	× *	× *	× *
7						*	× *	× *	× *
8							*	*	× *

TABLE 2

The number of function evaluations required by certain n-dimensional integration rules of degree 9.

n	$(G_5)^n$	$E_4^n(0)(G_5)^4$	$\bar{G}_5^{(n)}$	$W_5^{(n)}$	$\bar{W}_5^{(n)}$	$W_5^{(n)*}$	$\bar{W}_5^{(n)*}$	Bound†
6	15,625	5,385	1,735	713	653	537	*477*	344
10	9.8×10^6	62,201	11,801	5,161	4,981	2,825	*2,645*	2,344
15	3.1×10^{12}	380,301	52,701	27,341	*26,921*	38,269	37,849	26,320

† The final column is a lower bound on the number of points required by any rule of degree 9 of hypercubic symmetry (see Lyness [3, equation (4.5)]).

For sufficiently large n, 2^n exceeds $2^t\binom{n}{t}$ and the rule $W_{t+1}^{(n)}$ is more economical than the rule $W_{t+1}^{(n)*}$. However, there is a range of values of n and t for which the reverse is true. Table 2 illustrates this situation.

The rule $W_{t+1}^{(n)*}$ may be generated directly using the recursion relation of Section 5, namely,

$$W_{t+1}^{(m)*} = E_{m-1}^{m}(0)W_{t+1}^{(m-1)*} + S_{t+1}^{(m)}. \tag{7.4}$$

Here we set

$$W_{t+1}^{(t)*} = W_{t+1}^{(t)} \tag{7.5}$$

and

$$S_{t+1}^{(m)} = (5/9)^t(E_{m-1}^m(\sqrt{(3/5)}) - E_{m-1}^m(0))(\mathcal{R}(\sqrt{(3/5)}))^{m-1}, \qquad m > t. \tag{7.6}$$

This rule is not the only rule which may be considered as an adjustment of $W_{t+1}^{(n)}$. In fact, any n-dimensional rule $R_{t+1}^{(n)}$ may be obtained from $W_{t+1}^{(n)}$ by adding the null rule $R_{t+1}^{(n)} - W_{t+1}^{(n)}$ and so may be considered as an adjustment. However, this adjustment of $W_{t+1}^{(n)}$ to $W_{t+1}^{(n)*}$ is a simple adjustment and in some cases results in a considerable reduction in the number of function evaluations required. Other adjustments are not considered here.

8. The Choice of Parameters λ, η_0. Besides altering the rule, we may try to reduce the number of points by a suitable choice of the parameters η_0 and λ. We may attempt to choose the parameters λ and η_0 in such a way that the coefficient of some basic rule is zero. The principal terms in (6.31) are usually those involving the highest powers of n. The terms n^t and n^{t-1} arise from the basic rules $\mathcal{R}(0)^{n-t}*\mathcal{R}(\sqrt{(3/5)})^t$ and $\mathcal{R}(0)^{n-t+1}*\mathcal{R}(\sqrt{(3/5)})^{t-1}$ and the coefficients of these terms are independent of λ and η_0.

The term $t\cdot 2^{t-2}\binom{n}{t-2}$ arises from the basic rules $\mathcal{R}(0)^{n-t+2}*R^{(t-2)}$, where $R^{(t-2)}$ may be $\mathcal{R}(\alpha)^{t-3}*\mathcal{R}(\beta)$, $\mathcal{R}(\gamma)^{t-2}$ or $\mathcal{R}(\sqrt{(3/5)})^{t-2}$. It appears that neither of the coefficients of the first two of these may be set to zero. However, the coefficient of $\mathcal{R}(0)^{n-t+2}*\mathcal{R}(\sqrt{(3/5)})^{t-2}$ is zero if we set $\eta_0 = \bar{\eta}_0$, where

$$\bar{\eta}_0 = -(\tfrac{5}{9})^{t-2}(n - t + 2)\{\tfrac{5}{18}(n - t + 1) - 1\}. \tag{8.1}$$

The corresponding coefficient in $W_{t+1}^{(n)*}$ is zero if we set $\eta_0 = \bar{\eta}_0^*$, where

$$\bar{\eta}_0^* = (\tfrac{5}{9})^t(\tfrac{4}{5}(n - t) + \tfrac{13}{5}). \tag{8.2}$$

This choice defines the rules $\bar{W}_{t+1}^{(n)}$ and $\bar{W}_{t+1}^{(n)*}$, respectively, the bar indicating that the parameter η_0 has been set to the value $\bar{\eta}_0$ and $\bar{\eta}_0^*$, respectively.

It remains to ensure that the rules $\bar{W}_{t+1}^{(n)}$ and $\bar{W}_{t+1}^{(n)*}$ exist. That is to see that with the above choice of parameter η_0 it is still possible to choose λ so that α, β, γ or γ_1 and γ_2 are real. An examination of the various equations leads to the conclusion that it is always possible to choose λ so that $\bar{W}_{t+1}^{(n)}$ and $\bar{W}_{t+1}^{(n)*}$ exist, but it is not always possible to choose λ so that all the points for function evaluation lie within the hypercube. Values of n and t for which this is also possible are indicated in Table 1.

The number of points required by these rules is given simply in terms of expressions (6.31) and (7.3) for $\nu(W_{t+1}^{(n)}$ and $\nu(W_{t+1}^{(n)*})$. Thus

$$(8.3) \qquad \nu(\bar{W}_{t+1}^{(n)}) = \nu(W_{t+1}^{(n)}) - 2^{t-2}\binom{n}{2},$$

$$(8.4) \qquad \nu(\bar{W}_{t+1}^{(n)*}) = \nu(W_{t+1}^{(n)*}) - 2^{t-2}\binom{n}{2}.$$

Further adjustments to these rules are possible. The most obvious is to replace the term $E_{t-3}^{n}(0)(G_{t+1})^{t-3}$ by a different term which uses points already used by the other terms in the rule $W_{t+1}^{(n)}$. Or alternatively we might choose the remaining parameter λ so that one of α, β, γ coincides with one of the coordinates used by G_{t+1}. This would result in a reduction in the number of points. However, either procedure would need an inconvenient amount of analytical work, in terms of the relative gain in economy of function evaluations. In the case of $\bar{W}_5^{(15)}$ (see Table 2) the number of points required by this rule as it stands is 26,921. The term $E_1^{15}(0)G_5$ accounts for only 60 of these points. Thus we would at the outside manage to reduce the number of points to 26,861, a reduction of one third of one percent in the number of function evaluations. From the point of view of the practice of integration such a reduction is not worthwhile. From a theoretical point of view, it would be interesting to do this if it were to result in a minimal rule, i.e., one of the set of rules of this degree which is most economical in function evaluations. The investigation of minimal rules is in progress at the present time.

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