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Cubatures of Precision $2k$ and $2k+1$ for Hyperrectangles

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Abstract. It is well known that integration formulas of precision $2k$ $(2k + 1)$ for a region in n-space which is a Cartesian product of intervals can be obtained from one-dimensional Radau (Gauss) rules. The number of function evaluations in these product cubatures is $(k + 1)^n$. In this paper, an algorithm is given for obtaining cubatures for hyperrectangles in n-space of precision $2k$, in many instances $2k + 1$, which uses $(k + 1)(k)^{n-1}$ nodes. The weights and nodes of these new formulas are derived from one-dimensional generalized Radau rules.

1. Introduction. In this paper, we obtain multiple integration formulas exact for polynomials of degree $\leqslant 2k$ or $2k + 1$ which use $(k + 1)(k)^{n-1}$ nodes when the region of integration is a Cartesian product of intervals. The number of function evaluations is less than that of the product Radau or product Gauss rules which use $(k + 1)^n$ nodes. The main results given in Section 3 state explicitly how to obtain the nodes for these new cubatures; the weights in these new formulas are all positive. Examples are given in Section 4 which are constructed from the results of Section 3.

Even though the results are stated for the n-Cube, $I^n = [-1, 1] \times [-1, 1] \times \cdots \times [-1, 1]$, and for a constant weight function, this is done only for convenience of presentation. The development given for cubatures of precision $2k$ remains unaltered if we include in the integral an n-dimensional weight function which is a product of n distinct one-dimensional weight functions. For the $2k + 1$ case, the additional assumption that these weight functions be symmetric is necessary. By restricting our attention to the n-Cube, we need only consider one set of orthogonal polynomials in one variable. It will be apparent how the statement of the theorems must be modified to encompass the more general situation.

The following notation will be used throughout this paper:

$\phi_i(x)$: The normalized Legendre polynomial of degree i.

$\Phi_j(X)$: A polynomial in n variables.

$P_{n,k}$: The real linear space of polynomials in n variables of degree k or less.

$P_k(x)$: The real linear space of polynomials in x of degree k or less.

$W \cdot U$: The set $\{p \cdot q: p \in W \text{ and } q \in U\}$; W and U are sets of polynomials.

Sp W: The real linear span of the set of polynomials W.

$W - U$: The set complement of U relative to W.

For ease of reference, we begin with a statement of those results which are essential to the proof of the main theorems of this paper.

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2. Preliminary Results. For functions of one variable, we have the following lemma which is a restatement, in a slightly different form, of a result given by Boland and Duris [1].

LEMMA 2.1. *Fix an integer* $k \geq 1$ *and a real number* μ_1 *such that* $\phi_k(\mu_1) \neq 0$. *Then the polynomial*

$$\phi_k(\mu_1)\phi_{k+1}(x) - \phi_{k+1}(\mu_1)\phi_k(x)$$

has $k + 1$ *real distinct roots* $\mu_1, \mu_2, \ldots, \mu_{k+1}$ *of which at least* k *lie in the interval* $(-1, 1)$. *Furthermore, these roots can be used as the nodes of a quadrature which is exact for all* $p \in \mathcal{P}_{2k}$.

Observe that if $\mu_1 = -1$, then the quadrature obtained is the Radau rule. Thus, the quadratures of the above lemma can be considered as generalizations of that rule. Also, if μ_1 is such that $\phi_{k+1}(\mu_1) = 0$, then the nodes that are obtained are those of the Gauss quadrature.

The following corollary can be easily derived from Lemma 2.1 and therefore its proof is omitted.

COROLLARY 2.2. *Let* a *be real. The polynomial* $\phi_{k+1}(x) + a\phi_k(x)$ *has* $k + 1$ *real distinct roots of which at least* k *lie in the interval* $(-1, 1)$ *and which can be used as the nodes of a quadrature exact for polynomials of degree* $\leq 2k$.

The construction of the formulas given in the next section are based upon the following theorem.

THEOREM 2.3. *Let* $B = \{\Phi_1, \Phi_2, \ldots, \Phi_N\}$ *be a set of* N *polynomials in* n *variables, orthornormal with respect to integration over the* n*-Cube. There exists a cubature*

$$\int_{-1}^{1}\int_{-1}^{1}\cdots\int_{-1}^{1} p(x_1, \ldots, x_n)dx_1 \cdots dx_n \cong \sum_{j=1}^{N} w_j p(X_j)$$

which is exact for all polynomials in $\mathrm{Sp}\,B \cdot B$ *if and only if the rows of the matrix*

$$\begin{pmatrix} \Phi_1(X_1) & \Phi_2(X_1) & \cdots & \Phi_N(X_1) \\ \Phi_1(X_2) & \Phi_2(X_2) & \cdots & \Phi_N(X_2) \\ \vdots & \vdots & & \vdots \\ \Phi_1(X_N) & \Phi_2(X_N) & \cdots & \Phi_N(X_N) \end{pmatrix} \tag{2.1}$$

where $X_j = (x_{1,j}, x_{2,j}, \ldots, x_{n,j})$, *form an orthogonal basis for* R^N *with respect to Euclidean inner-product. Furthermore, the weights are given by* $w_j = (\Sigma_{l=1}^N \Phi_l^2(X_j))^{-1}$.

Proof. This result is a generalization of a theorem given by the author [3, Theorem 4.2]. Since the proof of this more general case is essentially the same as that given in [3], it is omitted here and the interested reader is referred to [3].

For one-dimension, if we apply the above theorem with $B = \{\phi_0, \phi_1(x), \ldots, \phi_k(x)\}$ and the Christoffel-Darboux identity, we obtain the converse to Corollary 2.2. With this observation, we state Corollary 2.2 and its converse as

COROLLARY 2.4. *There exists a quadrature*

$$\int_{-1}^{1} p(x)\,dx \cong \sum_{j=1}^{k+1} w_j p(x_j)$$

which is exact for all polynomials in $P_{2k}(x)$ *if and only if the nodes are roots to a polynomial* $\phi_{k+1}(x) + a\phi_k(x)$, *a real. Furthermore, the weights are given by* $w_j = (\Sigma_{l=0}^{k} \phi_l^2(x_j))^{-1}$.

3. Cubatures of Precision $2k$ **and** $2k + 1$. Before giving the results of this paper in their most general form, let us consider the construction of a cubature, exact for all polynomials of degree $2k$ or less, on the square $[-1, 1] \times [-1, 1]$.

If we form the product of two one-dimensional generalized Radau formulas,

$$\int_{-1}^{1} p(x)\,dx \cong \sum_{j=1}^{k+1} A_j p(\mu_j) \quad \text{and} \quad \int_{-1}^{1} q(y)\,dy \cong \sum_{j=1}^{k} B_j q(\lambda_j),$$

then the resulting product cubature

$$\int_{-1}^{1}\int_{-1}^{1} p(x, y)\,dx\,dy \cong \sum_{i=1}^{k+1} \sum_{j=1}^{k} A_i B_j p(\mu_i, \lambda_j) \tag{3.1}$$

is exact for all polynomials in Sp $P_{2k}(x) \cdot P_{2k-2}(y)$. From Corollary 2.4, the nodes of each of the one-dimensional rules, and therefore of (3.1), need only be roots of a polynomial $\phi_{k+1}(x) + a\phi_k(x)$ and $\phi_k(y) + b\phi_{k-1}(y)$, respectively. Therefore, the ordinates, λ_j, $j = 1, 2, \ldots, k$, of the point (μ_i, λ_j) in (3.1) can be obtained independently of the abscissa μ_i. Thus, let us consider a cubature of the form

$$\int_{-1}^{1}\int_{-1}^{1} p(x, y)\,dx\,dy \cong \sum_{i=1}^{k+1} \sum_{j=1}^{k} A_{ij} p(\mu_i, \lambda_{ij}), \tag{3.2}$$

where the μ_i's are roots of a polynomial $\phi_{k+1}(x) + a\phi_k(x)$ and for each $i = 1, 2, \ldots, k + 1$, the λ_{ij}'s are roots of a polynomial $\phi_k(y) + b_i\phi_{k-1}(y)$. The parameters a and b_i, $i = 1, 2, \ldots, k + 1$, shall be determined so that (3.2) is exact for all polynomials in $P_{2,2k}$.

Define

$$\overline{W} = \{\phi_i(x)\phi_j(y) \colon 0 \leqslant i \leqslant k \text{ and } 0 \leqslant j \leqslant k - 1\}.$$

Since the sum in (3.2) will integrate each polynomial in Sp $P_{2k}(x) \cdot P_{2k-2}(y)$ and since Sp $\overline{W} \cdot \overline{W} =$ Sp $P_{2k}(x) \cdot P_{2k-2}(y)$, we have from Theorem 2.3 that for two distinct nodes (μ_r, λ_{rs}) and (μ_t, λ_{tw})

$$\sum_{i=0}^{k} \phi_i(\mu_r)\phi_i(\mu_t) \sum_{i=0}^{k-1} \phi_i(\lambda_{rs})\phi_i(\lambda_{tw}) = 0. \tag{3.3}$$

In order to apply Theorem 2.3 so that (3.2) is exact for $p \in P_{2,2k}$, we need a set W of $(k + 1)(k)$ orthonormal polynomials for which Sp $W \cdot W$ contains $P_{2,2k}$. Thus, define $W = (\overline{W} \cup \{\phi_0\phi_k(y)\}) - \{\phi_k(x)\phi_{k-1}(y)\}$.

For the cubature (3.2) to be exact for each polynomial in Sp $W \cdot W$, it is necessary that for two distinct nodes (μ_r, λ_{rs}) and (μ_t, λ_{tw})

$$\sum_{i=0}^{k-2} \phi_i(\lambda_{rs})\phi_i(\lambda_{tw}) \sum_{i=0}^{k} \phi_i(\mu_r)\phi_i(\mu_t) + \phi_{k-1}(\lambda_{rs})\phi_{k-1}(\lambda_{tw}) \sum_{i=0}^{k-1} \phi_i(\mu_r)\phi_i(\mu_t) + \phi_0^2\phi_k(\lambda_{rs})\phi_k(\lambda_{tw}) = 0. \tag{3.4}$$

Comparing (3.4) to (3.3), we see that (3.4) will be satisfied if the node (μ_i, λ_{ij}) is chosen so that μ_i is a root of a polynomial $\phi_{k+1}(x) + a\phi_k(x)$ and λ_{ij} is a root of the polynomial $\phi_0\phi_k(y) - \phi_k(\mu_i)\phi_{k-1}(y)$.

The sufficient condition just indicated for $n = 2$ generalizes to arbitrary n and this result is given in the following theorem.

THEOREM 3.1. *Let $n \geqslant 2$ and $k \geqslant 2$ be fixed integers. Also, let μ_1 be real and fixed and such that $\phi_k(\mu_1) \neq 0$ and let $\mu_2, \mu_3, \ldots, \mu_{k+1}$ be the remaining roots of the polynomial $\phi_k(\mu_1)\phi_{k+1}(x) - \phi_{k+1}(\mu_1)\phi_k(x)$. For each $i = 1, 2, \ldots, k+1$, let λ_{ij}, $j = 1, 2, \ldots, k$, be the roots of the polynomial*

$$\phi_0\phi_k(x) - \phi_k(\mu_i)\phi_{k-1}(x). \tag{3.5}$$

Then the cubature

$$\int_{-1}^{1}\int_{-1}^{1} \cdots \int_{-1}^{1} p(x_1, x_2, \ldots, x_n)\, dx_n \cdots dx_2 dx_1 \cong \sum_{j_1=1}^{k+1} \sum_{j_2=1}^{k} \cdots \sum_{j_n=1}^{k} A_{j_1} B_{j_1 j_2} \cdots B_{j_1 j_n} p(\mu_{j_1}, \lambda_{j_1 j_2}, \ldots, \lambda_{j_1 j_n}), \tag{3.6}$$

where

$$A_{j_1} = \left(\sum_{l=0}^{k} \phi_l^2(\mu_{j_1}) \right)^{-1}$$

and

$$B_{j_1 j_i} = \left(\sum_{l=0}^{k-1} \phi_l^2(\lambda_{j_1 j_i}) \right)^{-1}$$

is exact for all $p \in P_{n,2k}$.

Proof. For the case $n = 2$, the proof has been indicated in the discussion given prior to the statement of the theorem.

In general, for $n \geqslant 2$, we define

$$\begin{aligned} W_{n,k} = (&\{\Phi(x_1, x_2, \ldots, x_{n-1})\phi_j(x_n): \\ &j = 0, 1, \ldots, k-1 \text{ and } \Phi \in W_{n-1,k}\} \cup \{\phi_0^{n-1}\phi_k(x_n)\}) \\ &- \{\phi_0^{n-2}\phi_k(x_1)\phi_{k-1}(x_n)\}, \end{aligned}$$

where $W_{1,k} = \{\phi_j(x_1): j = 0, 1, \ldots, k\}$.

It follows from an induction on n that $P_{n,k}$ is a subspace of Sp $W_{n,k}$ and therefore, since $P_{n,2k} = \text{Sp}\, P_{n,k} \cdot P_{n,k}$, $P_{n,2k}$ is a subspace of Sp $W_{n,k} \cdot W_{n,k}$. Furthermore, $W_{n,k}$ contains $(k+1)(k)^{n-1}$ orthonormal polynomials

Again by an induction on n, it follows that for two nodes $(\mu_r, \lambda_{rs_2}, \lambda_{rs_3}, \cdots, \lambda_{rs_n})$ and $(\mu_t, \lambda_{tw_2}, \lambda_{tw_3}, \cdots, \lambda_{tw_n})$, chosen as described, the Euclidean product of the two rows of the matrix (2.1) with the polynomials given in $W_{n,k}$ can be written as

$$\left(\sum_{i=0}^{k} \phi_i(\mu_r)\phi_i(\mu_t)\right) \prod_{j=2}^{n} \sum_{i=0}^{k-1} \phi_i(\lambda_{rs_j})\phi_i(\lambda_{tw_j}). \tag{3.7}$$

If the two nodes are distinct, we have that (3.7) is equal to zero and therefore, from Theorem 2.3 the cubature (3.6) is exact for all polynomials in Sp $W_{n,k} \cdot W_{n,k}$ which in turn gives us that it is exact for $p \in P_{n,2k}$.

Furthermore, setting $(\mu_r, \lambda_{rs_2}, \cdots, \lambda_{rs_n}) = (\mu_t, \lambda_{tw_2}, \cdots, \lambda_{tw_n})$ in (3.7), we obtain the reciprocal of the corresponding weight. This completes the proof of the theorem.

We see that in the above theorem there is some freedom in the choice of μ_1. By restricting μ_1 to be a root of the Legendre polynomial of degree $k + 1$, then for certain values of k the cubature (3.6) will be exact for all polynomials in $P_{n,2k+1}$. This result is given as

THEOREM 3.2. *In Theorem* 3.1, *if k is odd and μ_1 is chosen so that* $\phi_{k+1}(\mu_1) = 0$, *then the cubature formula* (3.6) *is exact for all* $p \in P_{n,2k+1}$.

Proof. Since we have that (3.6) is exact for $p \in P_{n,2k}$, with the additional assumptions it suffices to show that the cubature sum applied to each orthogonal polynomial $\Pi_{l=1}^{n}\phi_{i_l}(x_l)$, with $\Sigma_{l=1}^{n} i_l = 2k + 1$, is zero in order to obtain the desired conclusion.

Since k is assumed odd, by letting $2m = k + 1$, we can order the roots of $\phi_{k+1}(x)$ so that $\mu_{2m-i+1} = -\mu_i$, $i = 1, 2, \ldots, m$. Therefore, for any l, $\phi_l(\mu_{2m-i+1}) = (-1)^l\phi_l(\mu_i)$. Also, since symmetric nodes in Gauss quadrature have equal weights, $A_{2m-i+1} = A_i$. Lastly, for $i = 1, 2, \ldots, m$ and for $j = 1, 2, \ldots, k$, we can set $\lambda_{2m-i+1,j} = -\lambda_{ij}$ since $-\lambda_{ij}$ is a root to the polynomial $\phi_0\phi_k(x) - \phi_k(\mu_{2m-i+1}) \cdot \phi_{k-1}(x)$. Thus, we see also that for any l, $\phi_l(\lambda_{2m-i+1,j}) = (-1)^l\phi_l(\lambda_{ij})$. Having $\lambda_{2m-i+1,j} = -\lambda_{ij}$ gives us that the two weights $B_{2m-i+1,j}$ and B_{ij} are equal.

Applying the cubature sum in (3.6) to $\Pi_{l=1}^{n}\phi_{i_l}(x_l)$, where $\Sigma_{l=1}^{m} i_l = 2k + 1$, we have

$$\sum_{j_1=1}^{m}\Bigg(A_{j_1}\phi_{i_1}(\mu_{j_1})\prod_{l=2}^{n}\sum_{j_l=1}^{k} B_{j_1j_l}\phi_{i_l}(\lambda_{j_1j_l}) + A_{2m-j_1+1}\phi_{i_1}(\mu_{2m-j_1+1})\prod_{l=2}^{n}\sum_{j_l=1}^{k} B_{2m-j_1+1,j_l}\phi_{i_l}(\lambda_{2m-j_1+1,j_l})\Bigg),$$

which is equal to

$$\sum_{j_1=1}^{m}\Bigg(A_{j_1}\phi_{i_1}(\mu_{j_1})\prod_{l=2}^{n}\sum_{j_l=1}^{k} B_{j_1j_l}\phi_{i_l}(\lambda_{j_1j_l}) + (-1)^{2k+1}A_{j_1}\phi_{i_1}(\mu_{j_1})\prod_{l=2}^{n}\sum_{j_l=1}^{k} B_{j_1j_l}\phi_{i_l}(\lambda_{j_1j_l})\Bigg).$$

and which we see is zero, This completes the proof of the theorem.

4. Numerical Examples. The algorithm indicated by Theorem 3.2 was programmed and examples were computed for several values of k. Since the examples were obtained for illustration, the computations were done in single precision, seven significant figures. The Gauss nodes and weights were entered, using the tables given in Stroud and Secrest [4]. The Newton-Raphson procedure was used to find the roots λ_{ij}; however, they were obtained only to 5 decimal places. The values for λ_{ij} and B_{ij} are given only for $i = 1, 2, \ldots, (k + 1)/2$ since $\lambda_{2m-i+1,j} = -\lambda_{i,j}$ and $B_{2m-i+1,j} = B_{i,j}$.

TABLE I

$k = 3$	precision: 7	
	λ_{ij}	B_{ij}
$\mu_1 = 0.861136$	0.905324	0.326846
	0.212374	0.966221
	−0.708838	0.706934
$\mu_2 = 0.339981$	0.694138	0.742512
	−0.272274	1.011006
	−0.974255	0.246482

It is shown by Franke [2] that for a cubature, for a symmetric planar region, to be of precision 7, one must use at least 12 nodes. Thus, this cubature is a minimum point formula for $n = 2$.

TABLE II

$k = 5$	precision: 11	
	λ_{ij}	B_{ij}
$\mu_1 = 0.932469$	0.944096	0.156115
	0.647156	0.435729
	0.114424	0.596903
	−0.471752	0.537090
	−0.891065	0.274168
$\mu_2 = 0.661209$	0.887200	0.283882
	0.453135	0.555783
	−0.152812	0.616007
	−0.699427	0.441015
	−0.978752	0.103319
$\mu_3 = 0.238619$	1.000772	0.079262
	0.721144	0.446380
	0.167629	0.623893
	−0.446102	0.562927
	−0.885745	0.287544

We should observe that in the last example some of the nodes lie outside of the n-Cube. The cubature of Theorem 3.2 was computed for $k = 7$. For the Gauss node $\mu_1 = 0.183434$, one of the roots, λ_{ij}, is -1.006044. Therefore, from these examples, we see that all the nodes need not lie within the n-Cube.

We finally note that Theorem 3.1 does not include the case $k = 1$. However, it is not difficult to obtain directly from Theorem 2.3 cubatures of precision 2 which use $n + 1$ nodes. These cubatures will be minimum point formulas.

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