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Computation of moderate-degree fully-symmetric cubature rules on the triangle using symmetric polynomials and algebraic solving

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Abstract

A novel method is presented for expressing the moment equations involved in computing fully symmetric cubature rules on the triangle, by using symmetric polynomials to represent the two kinds of invariance inherent in these rules. This method results in a system of polynomial equations that is amenable to solution using algebraic solving techniques; using Gröbner bases, rules of degree up to 15 are computed and presented, some of them new and with all their points inside the triangle.

Since all solutions to the polynomial system are computed, it is for the first time possible to prove whether a given rule type results in specific rules of a given quality; it is thus proved that for degrees up to 14 there are no non-fortuitous rules that can improve on the presented results. For degree 10, an example is also provided showing how the proposed method can be used to exclude the existence of better fortuitous rules as well.

Keywords: Cubature, triangle, fully symmetric rules, symmetric polynomials, Gröbner bases

2000 MSC: Primary 65D32, Secondary 65D30

1. Introduction

The term "cubature" indicates the numerical computation of a multiple integral. This is an important topic in many different disciplines, with a correspondingly large body of literature. A description of the different kinds of cubature rules that exist, as well as of the mathematics used to derive them, is given in the classic book of Stroud [1], with more updated information to be found, among others, in [2] and in chapter 6 of [3]. Stroud [1] also presents a compilation of known (at the time) cubature rules, while newer rules are catalogued in [4, 5] and online at the Encyclopedia of Cubature Formulas [6].

A commonly used method to derive specific cubature rules is based on moment equations and invariant theory (see [7, 2] and [3, pp. 170–182]). This method, which will be used in the present paper, exploits symmetries and invariant theory to set up a non-linear system of equations, whose unknowns are the positions and weights of the integration points. The construction of the system of equations is based on Sobolev's theorem [see e.g. 7]. The use of invariants, together with appropriate algebraic computations, can lead to a significant simplification of the system of equations, which however in most cases still has to be solved numerically using an iterative method.

Although appropriate iterative numerical methods have been successfully used to obtain *individual* numerical solutions to the aforementioned system of equations, obtaining a solution in this way provides no information on its uniqueness. Conversely, inability to obtain a solution does not prove its inexistence (though it is a strong indication, when sufficiently robust numerical methods are employed). It is thus interesting and useful to be able to perform an exhaustive computation that provides all the solutions for a cubature rule.

In this paper we focus on fully symmetric cubature rules on the triangle, for which many specific rules have already been presented in the literature [1, 8, 9, 10, 11, 12, 13, 14, 15]. Extending significantly the results given in analytic form by Lyness and Jespersen [9], we provide results for cubature rules of degree up to 15. Symmetric

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polynomials [16] are used in generating the moment equations, to represent the two kinds of invariance inherent in these rules. This leads to a system of equations which is amenable to algebraic solving, thus allowing all cubature rules of a given type to be computed.

In Section 2 we present concisely the concepts of symmetric polynomials, areal coordinates and polynomial system solving that will be used in the rest of the paper. Section 3 presents the derivation of the moment equations for fully symmetric rules. While the overall derivation follows the one by Lyness and Jespersen [9], symmetric polynomials are used here to express the invariance with respect to permutation of points within an orbit, resulting in expressions that are better suited to algebraic manipulation than those previously reported in the literature.

Instead of using an iterative solver to find a numerical approximation of a single solution of the moment equations, as usually done in the literature, in Section 4 we further transform the moment equations to take into account their invariance with respect to permutations of orbits of the same type (once more, using symmetric polynomials to express the invariance). This invariance (which to the author's knowledge has not been exploited before in the relevant literature) is key in providing a new form of the moment equations that, though not explicitly given as the previous one, is actually amenable to algebraic solving.

Section 5 summarises the cubature rules thus obtained using algebraic solving techniques and comments on the main features of the provided results, among which there are new rules which match (though they do not exceed) existing ones in terms of quality and number of points. Algebraic solving allows (for the first time in the non-trivial cases) the computation of all cubature rules of a given type, thus another important result obtained here is the non-existence of non-fortuitous cubature rules that improve on the ones presented in terms of quality and number of points. The case of fortuitous rules is also considered. Finally, Section 6 concludes by pointing out the main results obtained in the paper.

2. Theoretical background

2.1. Symmetric polynomials

The formulation presented in this paper is based on invariant theory and in particular it uses the theory of symmetric polynomials [16]. As we will see in the following, the use of symmetric polynomials provides an initial concise formulation of the non-linear system of equations, while also leading to simpler computation and presentation of the solution.

A *symmetric polynomial* is a multivariate polynomial in n variables, say x_1, x_2, \ldots, x_n , which is invariant under any permutation of its variables. For example, the polynomial $x_1x_2 + x_2x_3 + x_3x_1$ is a symmetric polynomial of degree 2 in the three variables x_1, x_2 and x_3 , as can be easily seen by swapping any two variables.

We define the *elementary symmetric polynomials* \tilde{x}_k as the sums of all products of k distinct variables x_i , with negative sign when k is odd, that is

$$\tilde{x}_k = (-1)^k \sum_{i_1 < i_2 < \dots < i_k} x_{i_1} x_{i_2} \cdots x_{i_k}$$
(1)

with $\tilde{x}_0 = 1$. The alternating sign $(-1)^k$ in equation (1), which does not appear in the usual definition of the elementary symmetric polynomials, is introduced here as it leads to simpler expressions. While elementary symmetric polynomials are usually denoted using a letter (e.g. Π_k , s_k or e_k) which is different from the variable name, we use here the superimposed tilde over the variable name since we will be dealing with elementary symmetric polynomials of different sets of variables.

The fundamental theorem of symmetric polynomials states that any symmetric polynomial in the variables x_i can be uniquely expressed as a polynomial in the elementary symmetric polynomials \tilde{x}_k [17, p. 118]. This obviously holds true independently of the presence of the alternating sign in equation (1). The proof of the fundamental theorem also provides an algorithm for symmetric reduction, that is for expressing arbitrary symmetric polynomials in terms of the elementary symmetric polynomials.

Equation (1) allows computing the elementary symmetric polynomials \tilde{x}_k in terms of the *n* variables x_i . Conversely, the values x_i can be calculated [17, p. 89] from \tilde{x}_k as the solutions for *x* of the polynomial equation

$$\sum_{i=0}^{n} \tilde{x}_{n-j} x^{j} = 0 \tag{2}$$

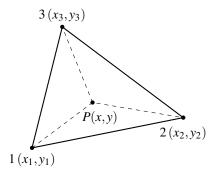


Figure 1: Geometry of a triangle for the definition of areal coordinates

2.2. Areal coordinates

Consider the generic triangle shown in Figure 1, defined through its three vertices with Cartesian coordinates (x_1, y_1) , (x_2, y_2) and (x_3, y_3) . For a point P with Cartesian coordinates x and y, we define the areal coordinates L_1 , L_2 and L_3 [see e.g. 18, pp. 153–156] through the equations

$$x = L_1 x_1 + L_2 x_2 + L_3 x_3 (3a)$$

$$y = L_1 y_1 + L_2 y_2 + L_3 y_3 \tag{3b}$$

$$1 = L_1 + L_2 + L_3 \tag{3c}$$

Note that areal coordinates are also often called barycentric coordinates, even though in the general case barycentric coordinates do not require the normalisation (3c).

Using equations (3) it can be seen that a polynomial of degree d on the triangle can be written using areal coordinates as a linear combination of terms $L_1^i L_2^j L_3^{d-i-j}$, all of which are of total degree d.

2.3. Solution of a system of polynomial equations

Consider a system of m polynomial equations with n variables x_i with $i = 1 \dots n$. The system is *overdetermined* if it has more equations than variables (m > n) and *underdetermined* if it has less equations than variables (m < n).

A solution of the system is any set of values of the variables x_i that satisfies the polynomial equations. If the polynomial coefficients are real, then the values of the x_i in the solution will be in general complex (we ignore solutions with points at infinity). A system is called *inconsistent*, *zero-dimensional* or *positive-dimensional* if it has respectively zero solutions, a finite number of solutions or infinite solutions.

While we have defined above what is a solution of a polynomial system, we must also consider what is *the* solution of the system, i.e. answer the question "what is polynomial system solving" (see Lazard [19] for an answer to this question and an informal overview of the state of the art on algebraic methods for computing the solutions).

For positive-dimensional systems there is not a unique answer to what is the solution (and how it can be expressed). For zero-dimensional systems the solution could be a numerical approximation of all the individual solutions (which, in the general case, cannot be expressed in algebraic form). In algebraic geometry, the *algebraic* solution of the zero-dimensional system consists in expressing the system in a form which is exact (not approximate) and can easily provide the approximate numerical solution; such could be for example the lexicographical Gröbner basis or the rational univariate representation (see again [19] for a more detailed discussion and more references). We prefer here to use the term *analytical solution* for this kind of solution; indeed, considering the computation of the roots of a univariate polynomial as a known function, the analytical solution gives the exact solutions of the polynomial system in terms of known functions.

3. Formulating the system of equations

In the following Section 3.1 the so-called moment equations are derived, following in some main points the classic derivation presented by Lyness and Jespersen [9], while Section 3.2 presents the concept of consistency conditions (see [9, 20, 2]). The specific form of the equations that is obtained is compared in Section 3.3 to existing ones.

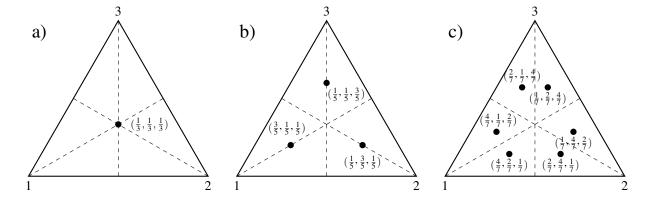


Figure 2: Examples of the three different types of orbits in the case of an equilateral triangle: a) type-0, b) type-1 and c) type-2

3.1. Moment equations

Our objective is to derive a cubature formula (or rule) for the approximate evaluation of the integral of a function f over a triangle Ω with area A,

$$\bar{I}[f] = \sum_{i=1}^{n_K} \bar{w}_i f^{(i)} \approx \frac{1}{A} \int_{\Omega} f \, d\Omega$$
 (4)

where $f^{(i)}$ is the value of f at point i, \bar{w}_i is the corresponding weight and n_K is the number of points used in the cubature. We only consider rules of (polynomial) degree d, that is rules where equation (4) is exact for all polynomials of degree less or equal to d, while it is not exact for at least one polynomial of degree d+1. Note that the issue of the accuracy of the approximation in (4) for a given cubature formula is beyond the focus of this paper (for more details on the underlying theory see e.g. [1, 3]).

Using areal coordinates, the polynomial of degree d can be written as a linear combination of terms $L_1^i L_2^j L_3^{d-i-j}$, therefore the cubature rule can be determined by requiring that equation (4) is exact for each of these terms. The resulting equations are known as the *moment equations*. The number \bar{n}_e of different terms $L_1^i L_2^j L_3^{d-i-j}$, which is the number of equations to be solved, is

$$\bar{n}_e = (d+1)(d+2)/2$$
 (5)

We only consider *fully symmetric* rules where, if a point with areal coordinates $(\Lambda_1, \Lambda_2, \Lambda_3)$ is used in the cubature, then all points resulting from the permutation of the areal coordinates are also used, with the same weight. Integration points in a fully symmetric rule can thus belong to one of three different types of point sets, or *orbits*, depending on the number of areal coordinates which are equal (see figure 2). If all areal coordinates are equal, we get a single "type-0" orbit, with one point (the centroid). If only two areal coordinates are equal, then we get "type-1" orbits with three points which lie on the medians of the triangle. Finally, if all three coordinates are different we get "type-2" orbits with six points. A rule that uses n_0 type-0 orbits, n_1 type-1 orbits and n_2 type-2 orbits is called a rule of type $[n_0, n_1, n_2]$. The number of points for such a rule is

$$n_K = n_0 + 3n_1 + 6n_2 \tag{6}$$

Due to the full symmetry employed, when integrating any of the quantities $L_1^i L_2^j L_3^{d-i-j}$ the sum in equation (4) for the point $(\Lambda_1, \Lambda_2, \Lambda_3)$ and its symmetric points will only contain terms of the form

$$\Lambda_{1}^{i}\Lambda_{2}^{j}\Lambda_{3}^{d-i-j} + \Lambda_{1}^{i}\Lambda_{3}^{j}\Lambda_{2}^{d-i-j} + \Lambda_{2}^{i}\Lambda_{1}^{j}\Lambda_{3}^{d-i-j} + \Lambda_{2}^{i}\Lambda_{3}^{j}\Lambda_{1}^{d-i-j} + \Lambda_{3}^{i}\Lambda_{1}^{j}\Lambda_{2}^{d-i-j} + \Lambda_{3}^{i}\Lambda_{2}^{j}\Lambda_{1}^{d-i-j}$$
 (7)

These terms are symmetric polynomials, and can therefore be written in terms of the elementary polynomials $\tilde{\Lambda}_1 = -(\Lambda_1 + \Lambda_2 + \Lambda_3)$, $\tilde{\Lambda}_2 = \Lambda_1 \Lambda_2 + \Lambda_2 \Lambda_3 + \Lambda_3 \Lambda_1$ and $\tilde{\Lambda}_3 = -\Lambda_1 \Lambda_2 \Lambda_3$. It is easily seen that only terms of the form $\tilde{\Lambda}_1^k \tilde{\Lambda}_2^l \tilde{\Lambda}_3^m$ with k + 2l + 3m = d will be used. Indeed, since $\tilde{\Lambda}_1 = -1$, only terms of the form $\tilde{\Lambda}_2^l \tilde{\Lambda}_3^m$ with $2l + 3m \leq d$ are actually needed.

The cubature rule of order d can therefore be obtained by requiring that equation (4) is exact when the function f is any of the terms $\tilde{\Lambda}_2^l \tilde{\Lambda}_3^m$ with $2l + 3m \le d$. The number of non-negative solutions of $2l + 3m \le d$ for l and m, and therefore the number of equations that must be solved, is given by [21]

$$n_e = 1 + \left| \frac{d^2 + 6d}{12} \right| \tag{8}$$

with $\lfloor x \rfloor$ denoting the largest integer that is less or equal to x. This is a significant reduction in the number of equations, approximately by a factor of 6 for large values of d, compared to the value \bar{n}_e given in equation (5) for the general case.

In Appendix A.1, the computation of a rule of degree 3 with 6 is presented, showing in a simple example the above-described introduction of symmetric polynomials when symmetric rules are considered.

While areal coordinates allow for simple formulations of expressions on a generic triangle, they have the disadvantage of introducing three coordinates, instead of the two independent coordinates needed. For this reason, moment equations have generally been obtained using Cartesian or polar coordinates and referring to a specific triangle (exploiting the fact that all triangles are affine). In the fully symmetric case, however, we see that using areal coordinates we easily end up with only two "coordinates", the symmetric polynomials $\tilde{\Lambda}_2$ and $\tilde{\Lambda}_3$.

As will be seen shortly, the moment equations can be further simplified by using, instead of $\tilde{\Lambda}_2$ and $\tilde{\Lambda}_3$, the quantities

$$p = 1 - 3\tilde{\Lambda}_2$$
 and $q = 1 - \frac{27}{2}\tilde{\Lambda}_3 - \frac{9}{2}\tilde{\Lambda}_2$ (9)

The cubature rule of order d can therefore be obtained by requiring that equation (4) is exact when the function f is any of the terms p^iq^j with $2i+3j \le d$ and $i, j \ge 0$. The moment equations for a fully symmetric rule of degree d and type $[n_0, n_1, n_2]$ can thus be written as

$$\sum_{k=1}^{n_0} \bar{w}_{0,k} p_{0,k}^i q_{0,k}^j + \sum_{k=1}^{n_1} 3\bar{w}_{1,k} p_{1,k}^i q_{1,k}^j + \sum_{k=1}^{n_2} 6\bar{w}_{2,k} p_{2,k}^i q_{2,k}^j = I_{i,j} \quad \text{with} \quad 2i + 3j \le d$$
 (10)

The right hand sides are the integrals

$$I_{i,j} = \frac{1}{A} \int_{\Omega} p^{i} q^{j} d\Omega \tag{11}$$

whose value can be computed by noting that the integrand p^iq^j can be expressed as a polynomial in the areal coordinates L_1 , L_2 and L_3 . Using the well-known formula [18, p. 156] for integration on the triangle

$$\frac{1}{A} \int_{\Omega} L_1^i L_2^j L_3^k d\Omega = \frac{2i! j! k!}{(i+j+k+2)!}$$
 (12)

we can then integrate separately each term of the polynomial and add the results, thus obtaining

$$I_{0,0} = 1$$
, $I_{1,0} = 1/4$, $I_{0,1} = 1/10$, $I_{2,0} = 1/10$, $I_{1,1} = 2/35$, $I_{3,0} = 29/560$, $I_{0,2} = 7/160$, $I_{2,1} = 1/28$,... (13)

The main advantage of using the quantities p and q is that for type-1 orbits we can introduce a new variable u so that $p = u^2$ and $q = u^3$ and therefore $p^i q^j = u^{2i+3j}$, while for the type-0 orbit p = q = 0. Setting $w_0 = \bar{w}_{0,1}$, $v_k = 3\bar{w}_{1,k}$ and $w_k = 6\bar{w}_{2,k}$, after some computations, the moment equations are finally written as

$$w_0 + \sum_{k=1}^{n_1} v_k + \sum_{k=1}^{n_2} w_k = I_{0,0}$$
 (14a)

$$\sum_{k=1}^{n_1} v_k u_k^{2i+3j} + \sum_{k=1}^{n_2} w_k p_k^i q_k^j = I_{i,j} \quad \text{with} \quad 0 < 2i + 3j \le d, j \le 1$$
(14b)

$$\sum_{k=1}^{n_2} w_k (p_k^3 - q_k^2) p_k^i q_k^j = I_{i+3,j} - I_{i,j+2} \quad \text{with} \quad 2i + 3j \le d - 6$$
 (14c)

where in equation (14a) we set $w_0 = 0$ if $n_0 = 0$.

For both d = 0 and d = 1 the only moment equation is (14a). This means that any (fully symmetric) rule exact for d = 0 will also be exact for d = 1, thus there are no rules of degree 0. For this reason in the following we always assume that $d \ge 1$.

3.2. Consistency conditions

To set up the moment equations for a rule of degree d, it is first necessary to determine the type of the rule, i.e. the number of orbits of each type.

The moment equations (14) form a system of n_e equations in n_v variables, where n_e is given in equation (8) while $n_v = n_0 + 2n_1 + 3n_2$. Similarly, the subsystem (14c) has $n_e - d$ equations and $3n_2$ variables.

We assume that both the system (14) and its subsystem (14c) are inconsistent if and only if they are overdetermined. This assumption, together with the fact that there may be at most one type 0 orbit, yields the following consistency conditions [9]

$$3n_2 \ge n_e - d \tag{15a}$$

$$3n_2 + 2n_1 + n_0 \ge n_e \tag{15b}$$

$$n_0 \le 1 \tag{15c}$$

which must be satisfied to obtain a solution of the moment equations, and thus they restrict the choice of the rule type. For a given degree d, a minimal-point rule is sought, that is a rule that satisfies the consistency conditions with the lowest total number of points, as given by equation (6). This yields

$$n_2 = \lfloor (n_e - d + 2)/3 \rfloor, \qquad n_1 = \lfloor (n_e - 3n_2)/2 \rfloor, \qquad n_0 = n_e - 3n_2 - 2n_1$$
 (16)

It is conceivable that a rule that violates the consistency conditions may lead to a system of moment equations that, although overdetermined, has solutions. These so-called *fortuitous* rules have great theoretical interest, as well as practical interest in the case where they have fewer integration points compared to the minimal-point rules described above. No fortuitous rules are encountered in the present paper, however, nor in the available literature on cubature rules on the triangle. As will be mentioned in Section 5, the use of analytical solutions means that starting from rules that respect the consistency conditions does not preclude the identification of fortuitous rules with fewer points.

The polynomial system of moment equations (14) can be inconsistent, zero-dimensional or positive-dimensional. We use here the same terms to identify the corresponding rule types and individual rules, thus we have inconsistent rule types, which yield no rules, zero-dimensional rule types, which yield a finite number of zero-dimensional rules, and positive-dimensional rule types which yield an infinite number of positive dimensional rules. In the case of positive-dimensional rule types, the analytical solution can be expressed using a number of the unknowns as free parameters.

3.3. Advantages of the suggested form of the moment equations

As already mentioned, the development of the method given in Sections 3.1 and 3.2 to formulate the moment equations using symmetric polynomials follows in some main points the classic one presented by Lyness and Jespersen [9]. It provides, however, polynomial moment equations, while [9] also uses cosines. In this, the present method is similar to the one presented by Wandzura and Xiao [13], but with equations that can be written in the simple form (14) and which are of lower degree.

All three methods are equivalent, in that they yield the same rules. Indeed, it is relatively easy to pass from one method to the other: setting $p_i = r_i^2$, $q_i = r_i^3 \cos 3\alpha_i$ and $u_i = r_i$ in equations (14) yields after some calculations the moment equations in [9], while it is easily seen that, for the triangle used in [13], p and q are equal to the invariants $x^2 + y^2$ and $x^3 - 3xy^2$.

In the author's opinion, the present method is simpler and more intuitive in its formulation, is elegantly formulated without reference to a specific triangle and it provides simpler formulas. From a practical point of view, however, the main advantage is that the resulting polynomial equations are of significantly lower degree than those provided by the other methods, for example the maximum degree of equations (14c) is $\lfloor d/2 \rfloor + 1$ instead of d+1. This is especially important when solving the equations analytically.

4. Analytical solution of the moment equations

4.1. The usefulness of analytical solutions

Except for some trivial low-degree rules, the moment equations are generally solved numerically, e.g. using a multivariate Newton-Raphson solver. The cubature rule is then given as a table of integration point coordinates and weights, expressed as floating point approximations of a given precision. This numerical approximation of the cubature rule is the one actually required when using the rule in applications.

Iterative numerical methods have the advantage of being able to provide cubature rules of high degree [see e.g. 15]. Convergence of the method to a solution is not guaranteed, however, as it most often depends on the selection of an appropriate "initial guess" required by the solver. This means that inability to obtain a solution does not prove that the solution does not exist. Additionally, when a numerical solution is obtained iteratively, no information is obtained regarding the existence of other solutions. For this reason, in this paper we investigate the analytical solution of the moment equations, in order to obtain a definitive answer regarding the different cubature rules for a given degree and type.

There exist algorithms for solving analytically arbitrary systems of polynomial equations, for example using Gröbner bases (see [19] for an informal overview of the state of the art). Unfortunately, when applied directly to the moment equations as presented in equation (14) or in similar forms in the literature, the requirements of these algorithms in both computer memory and computation time are such that in practice they fail to provide a solution even for rules of relatively low degree. Analytical solutions for higher degrees cannot therefore be obtained just by applying algebraic solving techniques to the moment equations as presented in the literature or even as obtained here in equation (14); it is necessary to exploit as much as possible the structure of the moment equations, as will be presented in Section 4.3.

An interesting alternative to the analytical solution of the moment equations is to use homotopy continuation methods to compute *numerically* all the solutions of the system [22]. The use of homotopy continuation is however clearly beyond the scope of the present paper.

4.2. Solution strategy

The subsystems (14a), (14b) and (14c) have respectively 1, d-1 and n_e-d equations. The weight w_0 (if it is non-zero) appears only in equation (14a) while the variables v_k and u_k appear only in equations (14a) and (14b).

Consider first the case of a rule with a type-0 orbit ($n_0 = 1$). Equation (14a) is then just used to determine w_0 when all other weights have been calculated. The weights v_k of type-1 orbits can be eliminated from equations (14b), as described in [23, pp. 771–773] for cubature rules on other regions, to obtain the (linear in the symmetric polynomials \tilde{u}_k) system of equations

$$\sum_{k=0}^{n_1} J_{i-k} \tilde{u}_k = 0, \qquad i = n_1 + 2, \dots, d$$
 (17)

where

$$J_{i} = \begin{cases} I_{j,0} - \sum_{k=1}^{n_{2}} w_{k} p_{k}^{j} & \text{if } i = 2j \\ I_{j,1} - \sum_{k=1}^{n_{2}} w_{k} p_{k}^{j} q_{k} & \text{if } i = 2j + 3 \end{cases}$$

$$(18)$$

The system (17) has n_1 unknowns \tilde{u}_k (since $\tilde{u}_0 = 1$) and $d - n_1 - 1$ equations. If $n_1 = (d-1)/2$ then equations (14c) are sufficient to evaluate the variables w_k , p_k and q_k of type-2 orbits, and then equations (17), (14b) and (14a) yield in turn the values of \tilde{u}_k , v_k and w_0 . The same happens if $n_1 > (d-1)/2$, but in this case the system is positive-dimensional and some of the \tilde{u}_k remain as free parameters in the solution. Finally, if $n_1 < (d-1)/2$ then obtaining a solution is more difficult, since to evaluate w_k , p_k and q_k we need not only equations (14c) but also the equations that remain after eliminating \tilde{u}_k from (17).

When the type-0 orbit is not used $(n_0 = 0)$, it is generally easier to introduce an additional equation

$$\sum_{k=1}^{n_1} v_k u_k = J_1 \tag{19}$$

where J_1 is an unknown quantity, which is not defined by (18). Eliminating the weights v_k from equations (14a), (14b) and (19) leads to a system of equations like (17), only that the index i is now in the range $i = n_1, \ldots, d$ and J_1 is an additional unknown that must be eliminated.

In all cases, equations (14c) must be solved, possibly together with the equations that remain after eliminating \tilde{u}_k from (17). Unfortunately, no easy way has been found to simplify these equations as we did to derive the system (17). The use of symmetric polynomials can, however, again lead to somehow simpler expressions.

4.3. Permutation invariance of the orbits

In Section 3 we exploited the fact that the cubature rule is invariant with respect to a permutation of the integration points within a given orbit, and expressed this invariance using symmetric polynomials.

Another obvious property of the cubature rules, which however has received much less attention in the literature and has not up to now been exploited, is their invariance with respect to permutation of orbits of the same type. This is reflected in the fact that the moment equations (14) are polynomials which are "symmetric" (i.e. invariant with respect to permutation) in the pairs (u_k, v_k) and in the triplets (p_k, q_k, w_k) . This can be seen from the system (17) where, having eliminated the v_k , the resulting polynomials are symmetric in the u_k and have thus been expressed in terms of the elementary symmetric polynomials \tilde{u}_k . In a similar way, eliminating q_k and w_k allows us to express the moment equations in terms of the symmetric polynomials \tilde{p}_k .

The system that results by eliminating the v_k , q_k and w_k from the moment equations (14) and expressing the results in terms of the \tilde{u}_k and \tilde{p}_k is generally much longer to write out than the moment equations (14). It has however fewer variables, and it leads to a much simpler expression for the solution, when such a solution is actually found.

Indeed, one important advantage of expressing the moment equations in terms of symmetric polynomials is that the number of solutions of the system is equal to the number of different cubature rules that can be obtained. Consider for example the degree-4 [0, 2, 0] rule, for which Lyness and Jespersen [9] mention that, in the present notation, u_1 and u_2 are the roots of $15x^4 + 20x^3 - 30x^2 + 4$. This does not mean, however, than any combination of the roots is a valid solution for u_1 and u_2 , indeed only two pairs of solutions give a cubature rule. In terms of symmetric polynomials, on the other hand, the solution is obtained by solving the equations $3\tilde{u}_1^2 - 4\tilde{u}_1 - 2 = 0$ and $5\tilde{u}_2 + 2\tilde{u}_1 + 2 = 0$, where it is seen that two different rules are obtained, one for each solution of the system.

It is worth considering that even when solving the moment equations numerically, considering the invariance with respect to permutation of orbits of the same type can have a significant effect on the solution method. As an example, there is only one degree-15 [1,7,4] rule. The system (14c) however has 4! = 24 solutions, while if we were to solve all equations (14) together we would have 7!4! = 120960 solutions. It is thus conceivable that an iterative numerical solution algorithm may fail to converge by being "attracted" in turn by different solutions.

4.4. Solution quality

Once a cubature rule is determined by solving the moment equations, the sign of the weights and the position of the integration points is examined, to determine the *quality* of the solution. The quality is described using a two-letter label: the first letter is P if all weights are positive and N if at least one weight is negative, while the second letter is I if all points are inside the triangle, O if there is at least one point outside the triangle, and B if no points are outside the triangle but at least one is on the boundary of the triangle. The following qualities are therefore encountered: PI, NI, PB, NB, PO, NO.

In all the above cases, the coordinates and weights of the integration points are considered to be real. Though it is well-known that complex solutions may exist, these are not taken into account, since a cubature rule with complex-valued coordinates of the integration points would be of little, if any, use. Moreover, the moment equations are usually solved using numerical methods that only return real solutions, as these methods perform significantly better than methods that could return complex solutions.

On the other hand, when obtaining the solutions analytically it is easy to also consider complex solutions. For this reason, we expand the above definition of the quality of cubature rules by setting the first letter of the label to C if at least one weight is complex-valued and by setting the second letter of the label to C if at least one integration point has complex coordinates. Interestingly, while it is not possible to have complex weights without complex coordinates, it is possible to have real weights with complex coordinates. The following three additional qualities are therefore obtained: CC, PC, NC.

Including complex solutions allows us to make the distinction between moment equations that have no solution and those that have solutions, even though they may all be complex. Considering as an example a degree-15 rule, there are no solutions for type [0,7,4] (which does not satisfy the consistency conditions), while there is a single complex (NC) solution for type [1,7,4] (which satisfies the consistency conditions). It is generally expected that all types satisfying the consistency conditions will yield at least one solution, but with complex solutions appearing with increasing frequency as the degree of the rule increases.

Although we compute all solutions, independently of their quality, in most applications we need rules of PI (or at most NI) quality. For this reason, if a minimal-point rule does not yield any PI rules, we investigate rules with increasingly more points until a rule is found that has a PI solution. When considering rules with additional points, it is possible to have rules with the same degree and number of points, but different type and different number of free parameters appearing in the solution.

Consider for example the degree-7 rules. The minimal-point rule [1, 2, 1] has 13 points and the best quality achievable with it is NI. Increasing the number of points, we get either a [0, 3, 1] or a [0, 1, 2] rule, both with 15 points, where the first has one free parameter while the second has none. In this case, where both types can yield PI rules, we would generally prefer the zero-dimensional one as it has more type-2 orbits, so less integration points are restricted to be located on the medians.

In general, among rules with the same number of points and the same quality, we would prefer those with more type-2 orbits and thus less free parameters. The presence of free parameters in the solution of the moment equations, on the other hand, allows for much greater flexibility in obtaining a rule of PI quality. Moreover, the use of more type-1 orbits leads to simpler moment equations, which are easier to solve analytically.

Note that the numerical, iterative solution of the moment equations for positive-dimensional rules [see e.g. 13] yields only one of the infinite solutions. Though it is possible to consider numerically the variation of the solution with the variation of a parameter [see e.g. 12], analytical solutions are much more powerful in studying parametrically positive-dimensional cubature rules and their quality. The study and presentation of such rules, however, requires a much more extensive discussion which goes well beyond the scope of the present paper. For this reason, in Section 5 we only present results for zero-dimensional cubature rules.

5. Results and discussion

Using the method described in Sections 3 and 4 we compute here analytically cubature rules for degree up to 15. As described in Section 4.3, the permutation invariance of the orbits should be exploited to express the moment equations (14) in a form more suitable for analytical solution, for example in terms of the symmetric polynomials \tilde{u}_k and \tilde{p}_k . This has been achieved for each degree and rule type in a heuristic way, which involved (for higher degrees) extensive calculations until the initial system was transformed into a new one, solvable (on the available hardware and software) using Gröbner bases.

The actual calculations performed in each case (using the MapleTM computer algebra system) are obviously too lengthy to be written out here. Indeed, in the non-trivial cases, the analytical solution itself becomes too long, as is already apparent in Appendix B for the degree-6 rule. An overview of the computations for the [0, 5, 2] rule of degree 11 is given as an example in Appendix A.2.

Table 1 gives a summary of the properties of all cubature rules thus computed. As already mentioned, we only consider zero-dimensional rules. We calculate for each degree the minimal-point rules and, if none of these are of quality PI, we calculate additional rule types with more points until a rule with PI quality is found (except for d = 15 where additional rules were not computed). Appendix B provides analytical expressions for evaluating some of the cubature rules, while Appendix C provides numerical values for new rules of PI or NI quality.

The only case where three rule types must be computed to obtain PI quality is d = 11. This is therefore the only case (for d < 15) where a positive-dimensional rule of PI quality (type [1,5,2] with 28 points) has less points than the best possible zero-dimensional rule of the same quality (type [0,2,4] with 30 points). Where NI rules are acceptable,

¹A type [1,5,2] fully symmetric PI rule is given by Zhang et al. [24], while Lyness and Jespersen [9] had already presented a [1,5,2] PB rule. As [1,5,2] rules are positive-dimensional, there are actually infinite rules obtainable, depending in this case on a single parameter. These can be obtained using the method presented in this paper, however as already mentioned we focus here only on zero-dimensional rules.

Table 1: Summary of the properties of all computed rules

degree	type	points	solutions	PI	NI	PB	РО	NO	PC	NC	CC
1	[1,0,0]	1	1	1	_	_	_	_	_	_	_
2	[0, 1, 0]	3	2	1	_	1	_	_	_	_	_
3	[1, 1, 0]	4	1	_	1	_	_	_	_	_	_
	[0, 0, 1]	6	1	1	_	-	_	_	_	_	-
4	[0, 2, 0]	6	2	1	_	-	1	_	_	_	-
5	[1, 2, 0]	7	1	1	_	-	_	_	_	_	-
6	[0, 2, 1]	12	6	2	_	-	2	_	_	_	2
7	[1, 2, 1]	13	4	-	1	-	1	_	_	_	2
	[0, 1, 2]	15	4	2	_	-	_	_	_	_	2
8	[1, 3, 1]	16	2	1	1	-	_	_	_	_	-
9	[1, 4, 1]	19	1	1	_	-	_	_	_	_	-
10	[0, 4, 2]	24	14	-	_	-	4	1	_	_	9
	[1, 2, 3]	25	15	4	_	_	_	2	_	3	6
11	[0, 5, 2]	27	6	_	_	_	1	_	_	2	3
	[1, 3, 3]	28	23	_	2	_	5	3	2	4	7
	[0, 2, 4]	30	34	4	_	_	1	1	4	2	22
12	[0, 5, 3]	33	24	2	1	-	_	_	_	_	21
13	[0, 6, 3]	36	8	_	_	_	_	1	_	1	6
	[1, 4, 4]	37	54	2	3	_	4	5	2	8	30
14	[0, 6, 4]	42	38	1	_	_	3	3	_	3	28
15	[1, 7, 4]	46	1	-	-	-	-	-	-	1	_

the two (newly computed) [1,3,3] rules can be used. The first [1,3,3] NI rule given in Appendix C is then to be preferred as it has a small negative weight for a single point, while the second one has a large negative weight for three points. Additionally, as shown in Figure 3, the first rule has a much more uniform distribution of points. Figure 3 also shows that the first [1,3,3] NI rule has a more uniform distribution of points than the [1,5,2] PI rule in [24] (which has the same number of points).

The results summarised in Table 1 confirm the general expectation that as the rule degree increases the number of solutions will increase, though with most solutions being complex ones. This is not always the case, however, as evidenced by the existence of a single [1,7,4] rule for d=15. It is thus clear that it is not possible to detect in these results a specific pattern in the number of solutions, the number of real solutions or the number of PI (or NI) solutions.

The results obtained here, answer (for the first time when considering non-trivial cases) questions such as "how many degree-10 PI rules of type [1, 2, 3] exist?" and, more importantly, questions such as "is there a degree-10 PI rule with 24 points?" Indeed, a very important result obtained through the analytical computation of all the solutions for a given rule type is that we can prove the non-existence of better fully symmetric rules for a given degree. Considering for example rules of degree d=10, Table 1 shows that there exist no non-fortuitous PI rules with 24 points and therefore any such rule will have at least 25 points. Indeed, taking into account the results summarised in Table 1 and the fact that there exist positive-dimensional PI rules of degree 11 with 28 points, the minimum number of points for non-fortuitous rules of PI (or PI and NI) quality is given in Table 2.

Another important result is that, using the analytical computation of the cubature rules, we can also prove the non-existence of specific fortuitous rules. Consider for example again the case of degree-10 rules where we compute the 24-point [0,4,2] rule. If there were a fortuitous rule with two type-2 orbits and less than 24 points, then the [0,4,2] rule should be positive-dimensional in order to depend on some parameters which, for specific values, would yield the fortuitous rule. Computing analytically the [0,4,2] rule, however, shows that it is zero-dimensional, as expected. Similarly, since the [1,2,3] rule is zero-dimensional, there exist no fortuitous rules with three type-2 orbits and less than 25 points. Since it is easily shown that for degree 10 no rules exist with one or zero type-2 orbits and also that no [0,0,4] rules exist (which would have 24 points) we see that there are no fortuitous degree-10 rules with 24 points or

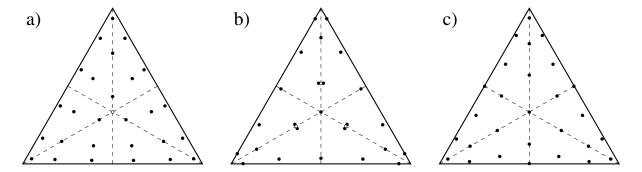


Figure 3: Distribution of points for cubature rules of degree 11 with 28 points (white dots indicate points with negative weight): a) zero-dimensional [1,3,3] NI rule with 1 negative weight, b) zero-dimensional [1,3,3] NI rule with 3 negative weights, c) positive-dimensional [1,5,2] PI rule as computed by Zhang et al. [24]

Table 2: Minimum number of points for non fortuitous rules of degree up to 14 for a given rule quality

	degree													
quality	1	2	3	4	5	6	7	8	9	10	11	12	13	14
any	1	3	4	6	7	12	13	16	19	24	27	33	36	42
PI or NI	1	3	4	6	7	12	13	16	19	25	28	33	37	42
PI	1	3	6	6	7	12	15	16	19	25	28	33	37	42

less. Similar tests could be performed for all other rule degrees considered here.

A list of numerical values for all computed rules, independently of their quality, can be found at the address http://arxiv.org/src/1111.3827v1/anc/allrules.pdf as ancillary material for the arXiv preprint of this paper [25]. This list includes the zero-dimensional rules found in [1, 8, 9, 10, 11]. An interesting property of some rules of bad quality (i.e. neither PI nor NI) is that the orbits that have points outside the triangle or with complex coordinates have a much smaller weight (in absolute value). This is the case for example for d = 11 and the fourth [1, 3, 3] NC rule, or for d = 15 and the [1, 7, 4] NC rule. These rules, together with a node elimination algorithm [15], could possibly be used to derive cubature rules that are not fully symmetric with fewer points than the fully symmetric ones.

6. Conclusions

In this paper we have used symmetric polynomials to express the double invariance inherent in fully symmetric cubature rules in the triangle (invariance with respect to permutation of points within an orbit and with respect to permutation of orbits of the same type). This has allowed us to formulate the moment equations in such a way that analytical solutions have been derived for zero-dimensional rules of degree up to 15.

A few new rules with all points inside the triangle have been thus derived and are given in Appendix C. Additionally, the analytical solutions ensure that all possible rules of a given type and degree were computed, independently of their quality. This allows us, for example, to prove that indeed no rules of PI or even NI quality exist for some cases where no such rules were encountered in the literature.

Though only zero-dimensional rules have been computed here, the proposed analytical approach is also well-suited for the thorough study of positive-dimensional rules. In this case, however, an additional difficulty lies in finding intuitive and useful ways to present the (infinite) solutions and their properties.

In all cases, starting from the formulation presented in this paper and combining a better understanding of the structure of the moment equations together with better-performing algorithms, software implementations and hardware platforms, should allow determining rules of increasingly high degree.

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Appendix A. Two simple examples

A.1. Rule of degree 3 with 6 points

Consider a rule of degree d=3 with $n_K=6$ points. From equation (5) there are 10 linearly independent polynomials of degree up to 3. In Cartesian coordinates these could be for example the monomials

$$[1, x, y, x^2, y^2, xy, x^3, y^3, x^2y, xy^2]$$
(A.1)

while in areal coordinates the linearly independent polynomials, expressed as $L_1^i L_2^j L_3^{d-i-j}$, are the monomials

$$[L_1^3, L_2^3, L_3^3, L_1^2L_2, L_2^2L_3, L_3^2L_1, L_1^2L_3, L_2^2L_1, L_3^2L_2, L_1L_2L_3]$$
(A.2)

For the fully symmetric case, we consider the case of a single type-2 orbit, so that there is a single weight \bar{w} and the areal coordinates of the six points are given by $(\Lambda_1, \Lambda_2, \Lambda_3)$, $(\Lambda_2, \Lambda_3, \Lambda_1)$, $(\Lambda_3, \Lambda_1, \Lambda_2)$, $(\Lambda_1, \Lambda_3, \Lambda_2)$, $(\Lambda_2, \Lambda_1, \Lambda_3)$ and $(\Lambda_3, \Lambda_2, \Lambda_1)$ where Λ_1, Λ_2 and Λ_3 are all different. To obtain the cubature rule, we want equation (4) to be exact when f is any of the monomials in (A.2), with the right-hand integrals easily calculated using equation (12). For the monomials L_1^3 , $L_1^2L_2$ and $L_1L_2L_3$ we thus obtain the equations

$$\bar{I}[L_1^3] = 2\bar{w}(\Lambda_1^3 + \Lambda_2^3 + \Lambda_3^3) = 1/10 \tag{A.3a}$$

$$\bar{I}[L_1^2 L_2] = \bar{w}(\Lambda_1^2 \Lambda_2 + \Lambda_2^2 \Lambda_3 + \Lambda_3^2 \Lambda_1 + \Lambda_1^2 \Lambda_3 + \Lambda_2^2 \Lambda_3 + \Lambda_3^2 \Lambda_2) = 1/30$$
(A.3b)

$$\bar{I}[L_1 L_2 L_3] = 6\bar{w}(\Lambda_1 \Lambda_2 \Lambda_3) = 1/60$$
 (A.3c)

while for the remaining seven monomials we don't get any additional equations. Using a fully symmetric rule we have thus reduced the 10 initial equations to just 3, as given by equation (8).

The quantities in parentheses in equations (A.3) are symmetric polynomials in the variables Λ_1 , Λ_2 and Λ_3 , so equations (A.3) can be rewritten, using symmetric reduction and taking into account that $\tilde{\Lambda}_1 = -1$, as

$$2\bar{w}(1 - 3\tilde{\Lambda}_2 - 3\tilde{\Lambda}_3) = 1/10 \tag{A.4a}$$

$$\bar{w}(\tilde{\Lambda}_2 + 3\tilde{\Lambda}_3) = 1/30 \tag{A.4b}$$

$$6\bar{w}(-\tilde{\Lambda}_3) = 1/60\tag{A.4c}$$

which yield the solution

$$\bar{w} = 1/6, \tilde{\Lambda}_2 = 1/4, \tilde{\Lambda}_3 = -1/60$$
 (A.5)

The actual values of Λ_1 , Λ_2 and Λ_3 are computed by solving the polynomial equation $\Lambda^3 + \tilde{\Lambda}_1 \Lambda^2 + \tilde{\Lambda}_2 \Lambda + \tilde{\Lambda}_3 = 0$ with $\tilde{\Lambda}_1 = -1$, $\tilde{\Lambda}_2 = 1/4$ and $\tilde{\Lambda}_3 = -1/60$ to obtain the approximate solution $\Lambda_1 = 0.1090390091$, $\Lambda_2 = 0.2319333686$ and $\Lambda_3 = 0.6590276224$ (or, obviously, any permutation of these values).

The same solution can easily be obtained directly, using the moment equations (14) which in this case can be written as

$$w_1 = 1, \quad w_1 p_1 = 1/4, \quad w_1 q_1 = 1/10$$
 (A.6)

Considering that $w_1 = 6\bar{w}$ and using the definitions (9) we thus obtain again the solution (A.5).

A.2. Rule of degree 11 and type [0,5,2]

We show here the computations needed to obtain an analytical solution for the rule of degree d = 11 and type [0, 5, 2]. This rule has been selected as its computation is clearly not trivial, yet is still simple enough to allow the main points of the computation to be presented in a relatively concise way.

We start with the moment equations in the form given in equation (14), and specifically with equations (14c) which for this rule are written explicitly as

$$w_1(p_1^3 - q_1^2) + w_2(p_2^3 - q_2^2) = 9/1120$$
 (A.7a)

$$p_1 w_1 (p_1^3 - q_1^2) + p_2 w_2 (p_2^3 - q_2^2) = 9/2800$$
 (A.7b)

$$q_1 w_1(p_1^3 - q_1^2) + q_2 w_2(p_2^3 - q_2^2) = 9/6160$$
 (A.7c)

$$p_1^2 w_1(p_1^3 - q_1^2) + p_2^2 w_2(p_2^3 - q_2^2) = 9/6160$$
(A.7d)

$$p_1 q_1 w_1 (p_1^3 - q_1^2) + p_2 q_2 w_2 (p_2^3 - q_2^2) = 9/11440$$
 (A.7e)

Solving equations (A.7a) and (A.7b) for w_1 and w_2 yields

$$w_1 = \frac{9}{5600} \frac{5p_2 - 2}{(p_1^3 - q_1^2)(p_2 - p_1)}, \quad w_2 = \frac{9}{5600} \frac{5p_1 - 2}{(p_2^3 - q_2^2)(p_1 - p_2)}$$
(A.8)

while replacing (A.8) into equations (A.7c) and (A.7e) and solving for q_1 and q_2 yields

$$q_1 = \frac{10}{143} \frac{13p_2 - 7}{5p_2 - 2}, \quad q_2 = \frac{10}{143} \frac{13p_1 - 7}{5p_1 - 2}$$
 (A.9)

Finally, replacing (A.8) into equation (A.7d) yields

$$55p_1p_2 - 22(p_1 + p_2) + 10 = 0 (A.10)$$

which is a symmetric polynomial and can be easily expressed in terms of the elementary symmetric polynomials as

$$55\tilde{p}_2 + 22\tilde{p}_1 + 10 = 0 \tag{A.11}$$

so that

$$\tilde{p}_2 = -(2/5)\tilde{p}_1 - 2/11 \tag{A.12}$$

It is easy to verify that if any of the denominators in equations (A.8) and (A.9) were equal to zero, then the system (A.7) would be inconsistent. Defining the quantity δ as

$$\delta = -(52270200125/36)(p_1^3 - q_1^2)(p_2^3 - q_2^2) \tag{A.13}$$

we therefore have $\delta \neq 0$. Substituting equations (A.9) into (A.13), expressing the resulting symmetric polynomial in p_1 and p_2 in terms of the elementary symmetric polynomials \tilde{p}_1 and \tilde{p}_2 and using equation (A.12), the value of δ can be expressed, after a few simple calculations, as

$$\delta = 44926453\tilde{p}_1^3 + 115639095\tilde{p}_1^2 + 104579475\tilde{p}_1 + 31726625 \tag{A.14}$$

Instead of using the remaining moment equations (14a) and (14b), we use the form given in (17), that is

$$\sum_{k=0}^{5} J_{i-k} \tilde{u}_k = 0, \qquad i = 5, \dots, 11$$
(A.15)

where the range for i starts from n_1 and not from $n_1 + 2$ since $n_0 = 0$. The values of J_i are obtained by substituting (A.8) and (A.9) into (18), expressing the resulting symmetric polynomial in p_1 and p_2 in terms of the elementary symmetric

polynomials \tilde{p}_1 and \tilde{p}_2 and using equation (A.12) to obtain

```
896\delta J_0 = 29800061863\tilde{p}_1^3 + 77149680465\tilde{p}_1^2 + 70346443596\tilde{p}_1 + 21618970430
448\delta J_2 = 2940954731\tilde{p}_1^3 + 7544944836\tilde{p}_1^2 + 6844096545\tilde{p}_1 + 2097413200
1120\delta J_4 = 2940954731\tilde{p}_1^3 + 7430900763\tilde{p}_1^2 + 6640424505\tilde{p}_1 + 2006089825
560\delta J_6 = 884705536\tilde{p}_1^3 + 2226589365\tilde{p}_1^2 + 1971919950\tilde{p}_1 + 589170125
2800\delta J_8 = 3117204662\tilde{p}_1^3 + 7898788755\tilde{p}_1^2 + 7004540400\tilde{p}_1 + 2088628375
6160\delta J_{10} = 5055953903\tilde{p}_1^3 + 12947897820\tilde{p}_1^2 + 11564885475\tilde{p}_1 + 3462657250
2240\delta J_3 = 5311689097\tilde{p}_1^3 + 13216597680\tilde{p}_1^2 + 11669947575\tilde{p}_1 + 3467843000
1120\delta J_5 = 1924925717\tilde{p}_1^3 + 4811751945\tilde{p}_1^2 + 4244987175\tilde{p}_1 + 1263326875
112\delta J_7 = 141691121\tilde{p}_1^3 + 356916846\tilde{p}_1^2 + 315385785\tilde{p}_1 + 93825400
6160\delta J_9 = 5812791842\tilde{p}_1^3 + 14800883955\tilde{p}_1^2 + 13161333900\tilde{p}_1 + 3928363375
80080\delta J_{11} = 56562404327\tilde{p}_1^3 + 145598683230\tilde{p}_1^2 + 130613972775\tilde{p}_1 + 39228386500
```

Substituting the above expressions into equations (A.15) and multiplying by δ we obtain a polynomial system of seven equations with seven unknowns $(\tilde{p}_1, \tilde{u}_1, \tilde{u}_2, \tilde{u}_3, \tilde{u}_4, \tilde{u}_5, J_1)$, where each equation is of degree 3 in \tilde{p}_1 , of degree 1 in $\tilde{u}_1 \dots \tilde{u}_5$ and of degree 0 or 1 in J_1 . We have therefore transformed the initial moment equations (14) into a new polynomial system which is invariant with respect to permutation of orbits of the same type.

Since the new system has resulted from multiplication of (A.15) by δ , it must be solved under the constraint $\delta \neq 0$ to compute the Gröbner basis for a lexicographical ordering. The analytical solution can then be written in terms of univariate polynomials, for example in \tilde{p}_1 , so that the values of \tilde{p}_1 are the roots of

$$9470888994525673\tilde{p}_{1}^{6} + 226562700234548964\tilde{p}_{1}^{5} + 1593701306680736682\tilde{p}_{1}^{4} + 2874813231904110640\tilde{p}_{1}^{3}$$

$$+ 2110043534402532300\tilde{p}_{1}^{2} + 656107531431066000\tilde{p}_{1} + 65822515401595000 = 0 \quad (A.16)$$

with \tilde{u}_1 given by

$$\begin{split} \tilde{u}_1 &= \frac{2247158968823382227008437555667297}{901112086802069498690105557296000} \tilde{p}_1^5 + \frac{390885591544102806213623935828597}{6758340651015521240175791679720} \tilde{p}_1^4 \\ &\quad + \frac{51024046646868800588472413534238157}{135166813020310424803515833594400} \tilde{p}_1^3 + \frac{9054475913093892568756717300904137}{18773168475043114556043865777000} \tilde{p}_1^2 \\ &\quad + \frac{28055470659132049424051721082649239}{135166813020310424803515833594400} \tilde{p}_1 + \frac{1083108239119841307303070737374777}{43929214231600888061142645918180} \end{split}$$

and the values of $\tilde{u}_2 \dots \tilde{u}_5$ similarly given by univariate polynomials in \tilde{p}_1 of degree 5.

For a given value of \tilde{p}_1 , i.e. a single numerical solution of the equation (A.16), we can then compute the numerical values of $\tilde{u}_1 \dots \tilde{u}_5$ and, from equation (A.12 of \tilde{p}_2 . From \tilde{p}_1 and \tilde{p}_2 we calculate the values of p_1 and p_2 , from which equations (A.8) and (A.9) give also the values of w_1, w_2, q_1, q_2 . Similarly, from the values $\tilde{u}_1 \dots \tilde{u}_5$ we calculate $u_1 \dots u_5$ and, using (14a) and (14b), the values of $v_1 \dots v_5$.

Appendix B. Analytical expressions for the cubature rules

This appendix lists analytical expressions for some of the rule types considered in this paper. For each rule type we list the degree d, the rule type and a list of expressions. Using these expressions, it is easy to obtain the coordinates and weights of the integration points for all rules of the given type.

```
• d = 1 [1, 0, 0]: w_0 = 1
```

•
$$d = 2$$
 [0, 1, 0]: $u_1^2 = 1/4$, $v_1 = 1$

```
d = 3 [0, 0, 1]: p_1 = 1/4, q_1 = 1/10, w_1 = 1
• d = 4 [0, 2, 0]: 3\tilde{u}_1^2 - 4\tilde{u}_1 - 2 = 0, \tilde{u}_2 = -2/5(\tilde{u}_1 + 1), v_i = ((81/248)\tilde{u}_1 - 6/31)u_i + (15/124)\tilde{u}_1 + 151/248
• d = 5 [1,2,0]: \tilde{u}_1 = -2/7, \tilde{u}_2 = -2/7, v_i = -(7/400)u_i + 39/100, w_0 = 9/40
• d = 6 [0, 2, 1]:
        p_1^6 - \tfrac{2943}{896}p_1^5 + \tfrac{12577377}{3211264}p_1^4 - \tfrac{6335029}{2809856}p_1^3 + \tfrac{211997025}{314703872}p_1^2 - \tfrac{7914723}{78675968}p_1 + \tfrac{14953009}{2517630976} = 0,
        q_1 = \frac{6773849}{1180960} - \frac{17597477}{258335} p_1 + \frac{618894079}{2066680} p_1^2 - \frac{2009158}{3355} p_1^3 + \frac{20120576}{36905} p_1^4 - \frac{6422528}{36905} p_1^5,
w_1 = \frac{88271353265388941906672}{1552328339949698669325} - \frac{2093018886005051378041487}{3104656679899397338650} p_1 + \frac{4677969412268735483683874}{1552328339949698669325} p_1^2
       \begin{array}{l} w_1 = \frac{60252328339949698669325}{1552328339949698669325} - \frac{203104656679899397338650}{3104656679899397338650} p_1 + \frac{7152328339949698669325}{1552328339949698669325} p_1^2 \\ - \frac{874483029603676756153618}{141120758177245333575} p_1^3 + \frac{8938712246012353125723136}{1552328339949698669325} p_1^4 - \frac{2885760563751222732259328}{1552328339949698669325} p_1^5, \\ \tilde{u}_1 = -\frac{5647577278829}{5843759130} + \frac{219725386019839}{17838843660} p_1 - \frac{4934508553334726}{84734507385} p_1^2 + \frac{965776421126167}{7703137035} p_1^3 - \frac{538505362157056}{4459710915} p_1^4 + \frac{3379769853673472}{84734507385} p_1^5, \\ \tilde{u}_2 = \frac{15104616525664}{20453156955} - \frac{581971572152849}{62435952810} p_1 + \frac{3683852401439816}{84734507385} p_1^2 - \frac{709365733908202}{77703137035} p_1^3 + \frac{389416992756736}{4459710915} p_1^4 - \frac{2417750126231552}{84734507385} p_1^5, \\ v_i = \left(\frac{409434268039529549940720811615256576}{158205456880303475487279097255725} p_1^5 - \frac{410497105230467053184700451899528704}{52735152293434491829093032418575} p_1^4 + \frac{114666485932207310484775951381500251}{14382314261845770498843554295975} p_1^3 - \frac{1141034063408380347314793772529581321}{14382314261845770498843554295975} p_1^3 - \frac{1141034063408380347314793772529581321}{12094060917373379673163721296743300} p_1 - \frac{68148358857994347902974327222077377}{126563212121447897302836415981834} p_1^4 + \frac{153804297816157841896911608744616331}{660151175786603354357391177225} p_1^5 + \frac{17884598780372115712297691281128448}{5455360582079430189216520595025} p_1^4 - \frac{600366862842903249663697383981056}{54554003354357391177225} p_1^5 + \frac{17884598780372115712297691281128448}{5455360582079430189216520595025} p_1^4 - \frac{1600804293851424897302836415981834}{5455360582079430189216520595025} p_1^4 - \frac{1600804293851424897302836415981834}{5455360582079430189216520595025} p_1^4 - \frac{1600804293851424897302836415981834}{5455360582079430189216520595025} p_1^4 - \frac{1600804293851424897302836415981834}{5455360582079430189216520595025} p_1^4 - \frac{1600804293851424897302836415981834}{545536058207943018921652059502
                            -\frac{\frac{1660804293851424897302836415981834}{64059941871098130017201501872275}p_1^3+\frac{2716663212121457459566848039780239}{1818453527359810063072173531675}p_1^2\\ -\frac{\frac{3169975113118311937146770957038031}{10910721164158860378433041190050}p_1+\frac{220460485921384140338311776720617}{10910721164158860378433041190050}
• d = 7 [1, 2, 1]:
         p_1^4 - \frac{23}{12}p_1^3 + \frac{655}{448}p_1^2 - \frac{85}{196}p_1 + \frac{1619}{37632} = 0,
        q_1 = \tfrac{73}{160} - \tfrac{63}{20}p_1 + \tfrac{273}{40}p_1^2 - \tfrac{21}{5}p_1^3, w_1 = \tfrac{5559373039}{1374543450} - \tfrac{4035503891}{196363350}p_1 + \tfrac{3029805464}{98181675}p_1^2 - \tfrac{577446688}{32727225}p_1^3,
        \tilde{u}_1 = \frac{204779}{4630} - \frac{616196}{2315} p_1 + \frac{978558}{2315} p_1^2 - \frac{585648}{2315} p_1^3, \ \tilde{u}_2 = -\frac{86623}{2315} + \frac{511579}{2315} p_1 - \frac{811132}{2315} p_1^2 + \frac{484512}{2315} p_1^3, \\ v_i = \left( -\frac{637366793665532978264}{9952562883613960471} p_1^3 + \frac{3156091037460298906045}{27157688650841881413} p_1^2 - \frac{9803429487627684799252}{135788443254209407065} p_1 + \frac{14666951220214040085227}{1267358803705954465940} \right) u_i
        +\frac{7823399076093706515424}{135788443254209407065}p_1^3-\frac{39124895515170463542614}{407365329762628221195}p_1^2+\frac{98256377831808794616331}{1629461319050512884780}p_1-\frac{109198370776069008639239}{114062292333553590193460} w_0=-\frac{3660769728}{100486445}p_1^3+\frac{4347049032}{703405115}+\frac{6057843876}{100486445}p_1^2-\frac{752902776}{20097289}p_1
• d = 7 [0, 1, 2]:
        u_1^4 - (4/9)u_1^3 - (1/3)u_1^2 + (1/36), v_1 = \frac{156673}{8817780} + \frac{2159752}{2204445}u_1 + \frac{5368006}{2204445}u_1^2 - \frac{3133452}{734815}u_1^3,
        \tilde{p}_1 = -\frac{1079}{1281} - \frac{310}{1281} u_1 - \frac{128}{427} u_1^2 + \frac{720}{427} u_1^3, \, \tilde{p}_2 = \frac{1493}{11956} + \frac{1130}{8967} u_1 + \frac{2116}{8967} u_1^2 - \frac{2046}{2989} u_1^3,
        q_i = \left(\tfrac{489}{427} + \tfrac{465}{854}u_1 + \tfrac{288}{427}u_1^2 - \tfrac{1620}{427}u_1^3\right)p_i - \tfrac{653}{2989} - \tfrac{1695}{5978}u_1 - \tfrac{1587}{2989}u_1^2 + \tfrac{9207}{5978}u_1^3,
        w_i = \left(-\frac{21117033567}{4098798070}u_1^3 + \frac{34215330023}{8197596140}u_1^2 + \frac{676519529}{409879807}u_1 - \frac{22884360891}{16395192280}\right)p_i
                            +\frac{7377613908}{2049399035}u_1^3-\frac{123702006967}{49185576840}u_1^2-\frac{10640567105}{9837115368}u_1+\frac{103431908839}{98371153680}u_2^2
• d = 8 [1, 3, 1]:
        p_1 = 2/5, \, q_1^2 - \tfrac{116}{355}q_1 + \tfrac{443}{17750}, \, w_1 = \tfrac{1286875}{529326}q_1 - \tfrac{561275}{4234608}, \, w_0 = \tfrac{197671347}{256973920} - \tfrac{32981985}{6424348}q_1,
       \tilde{u}_1 = \frac{181760}{50289} q_1 - \frac{70340}{50289}, \quad \tilde{u}_2 = -\frac{124960}{50289} q_1 + \frac{10642}{50289}, \quad \tilde{u}_3 = -\frac{50410}{50289} q_1 + \frac{14008}{50289}, \quad \tilde{u}_4 = \left(-\frac{18610928498796911607672845}{2275833709245992090597766} u_i^2 + \frac{19252524428004364259122223}{4551667418491984181195532} u_i + \frac{12430296145585635931273841}{4551667418491984181195532}\right) q_1
```

• d = 3 [1, 1, 0]: $u_1 = 2/5$, $v_1 = 25/16$, $w_0 = -9/16$

• d = 9 [1, 4, 1]:

 $p_1 = 2/5, \, q_1 = 2/11, \, w_1 = \frac{3025}{11648}, \, w_0 = \frac{85293}{878080} \, \tilde{u}_1 = -\frac{212}{407}, \, \tilde{u}_2 = -\frac{1002}{2035}, \, \tilde{u}_3 = \frac{212}{2035}, \, \tilde{u}_4 = \frac{112}{2035}, \, \tilde{u}_4 = \frac{112}{2035}, \, \tilde{u}_5 = \frac{506023048885425107}{1503746382262924800} + \frac{11465050245708013}{334165862725094400} u_i - \frac{10064998401780383}{12531219852191040} u_i^2 + \frac{52676213406614851}{109363373255485440} u_i^3$

Appendix C. Numerical values for new cubature rules of PI or NI quality

This appendix lists all the computed cubature rules of quality PI and NI that are *not* listed in the Encyclopedia of Cubature Formulas [6]. Since only zero-dimensional rules are considered in this paper, there is a finite number of solutions and it is thus possible to list approximate numerical values for all individual solutions; this of course would not be possible for positive-dimensional rules where an infinite number of solutions exists.

For each rule we first list the degree d, the number of points n_K , the rule type, the rule quality, the maximum integration error e and (for NI rules) the condition number σ . We then provide a list of the orbits, where the first column is the number of points in the orbit, the second is the weight for each integration point and the last three columns are the areal coordinates defining a point in the orbit.

The condition number σ is defined as

$$\sigma = \sum_{i}^{n_{K}} |\bar{w}_{i}| / \sum_{i}^{n_{K}} \bar{w}_{1} = \sum_{i}^{n_{K}} |\bar{w}_{i}|$$
 (C.1)

therefore $\sigma = 1$ for PI rules and $\sigma > 1$ for NI rules.

The integration error is computed by comparing numerical (double-precision) and exact values for the integration of all the monomials $x^i y^j$ with $i + j \le d$ on a reference triangle with vertices (0,0), (0,1) and (1,0) in the Cartesian plane. More specifically, the scaled error e is computed as

$$e = \max_{\substack{i,j \ge 0\\i+j \le d}} \left| \frac{\bar{I}[x^i y^j]}{\frac{1}{A} \int_{\Omega} x^i y^j d\Omega} - 1 \right| / \epsilon$$
 (C.2)

where ϵ is the so-called machine epsilon value ($\epsilon = 2^{-52}$ for double precision arithmetic).

```
d = 7, n_K = 15, type [0, 1, 2], quality PI, e = 2
3
     1.2539360744930307e-01
                              5.1348172032878493e-01
                                                        2.4325913983560754e-01
                                                                                 2.4325913983560754e-01
6
     7.6306338340541706e-02
                              5.0714384307207043e-02
                                                        3.1864418984753705e-01
                                                                                 6.3064142584525590e-01
     2.7663524601473427e-02
                              4.5720829846320324e-02
                                                        8.6636631341749002e-02
                                                                                 8.6764253881193067e-01
                                 d = 10, n_K = 25, type [1, 2, 3], quality PI, e = 1
     8.3219736986450142e-02
                              3.333333333333333e-01
                                                        3.33333333333333e-01
                                                                                 3.33333333333333e-01
3
     5.2651949468244594e-02
                              6.7417376425181049e-01
                                                        1.6291311787409476e-01
                                                                                 1.6291311787409476e-01
3
     1.0951288340268411e-02
                              9.4299299942322433e-01
                                                        2.8503500288387836e-02
                                                                                 2.8503500288387836e-02
6
     5.6277279710811180e-02
                              1.4681150539393041e-01
                                                        3.3669587527823165e-01
                                                                                 5.1649261932783794e-01
                              2.9307604504579472e-02
6
     3.5394947791538391e-02
                                                        3.6336261699457053e-01
                                                                                 6.0732977850085000e-01
6
     2.9322864095652236e-02
                              3.3685698680610287e-02
                                                        1.5330305516956137e-01
                                                                                 8.1301124614982834e-01
                            d=11, n_K=28, type [1, 3, 3], quality NI, e=2, \sigma=1.125
                              3.33333333333333e-01
    -6.2401629433482428e-02
                                                        3.33333333333333e-01
                                                                                 3.33333333333333e-01
                              4.3271289449998075e-01
                                                        2.8364355275000962e-01
3
     8.1727170838649564e-02
                                                                                 2.8364355275000962e-01
3
     4.8964652505867335e-02
                              7.1120974700789952e-01
                                                        1.4439512649605024e-01
                                                                                 1.4439512649605024e-01
     1.3801353886270255e-02
                              9.3453870606708818e-01
                                                        3.2730646966455908e-02
                                                                                 3.2730646966455908e-02
     5.3402351795938245e-02
                              1.1639641340049335e-01
                                                        3.3535007852506066e-01
                                                                                 5.4825350807444599e-01
     2.6325058735312046e-02
                              2.2611513300388206e-02
                                                        3.7249492189107103e-01
                                                                                 6.0489356480854077e-01
     2.5092939092269870e-02
                              2.7990225682080982e-02
                                                        1.6490131047191468e-01
                                                                                 8.0710846384600434e-01
```

```
d = 11, n_K = 28, type [1, 3, 3], quality NI, e = 16, \sigma = 24.81
                              3.333333333333333e-01
                                                        3.33333333333333e-01
1
     1.9188748901448341e-01
                                                                                  3.33333333333333e-01
3
     4.4946736418864346e-02
                              3.6186335127135712e-02
                                                        4.8190683243643214e-01
                                                                                  4.8190683243643214e-01
3
     4.1100128875197643e-02
                              8.1104704303693675e-01
                                                        9.4476478481531623e-02
                                                                                  9.4476478481531623e-02
3
    -3.9689908345461279e+00
                                                                                  2.4162811001152990e-01
                              5.1674377997694020e-01
                                                        2.4162811001152990e-01
6
     2.0349375070302612e+00
                              2.2731189719293939e-01
                                                        2.5397442939188326e-01
                                                                                  5.1871367341517734e-01
6
     3.4015193574745321e-02
                              3.0655038923840410e-02
                                                        2.5125205566042453e-01
                                                                                  7.1809290541573506e-01
6
     7.2047025186125795e-03
                              1.5009373287576387e-03
                                                        6.5611553303429522e-02
                                                                                  9.3288750936781284e-01
                                 d = 11, n_K = 30, type [0, 2, 4], quality PI, e = 2.5
3
     5.6231659174681110e-02
                              4.4705870171202569e-01
                                                                                  2.7647064914398715e-01
                                                        2.7647064914398715e-01
3
     4.7761405533085872e-02
                              7.1603550041918619e-01
                                                        1.4198224979040690e-01
                                                                                  1.4198224979040690e-01
6
     5.4734256165112738e-02
                              1.2302303722598859e-01
                                                        3.3224127181415769e-01
                                                                                  5.4473569095985372e-01
6
     2.8014058918038700e-02
                              2.4403997190791452e-02
                                                        3.7269746079157825e-01
                                                                                  6.0289854201763030e-01
     2.4798737818199088e-02
6
                              2.7853864808466097e-02
                                                        1.6711516327952143e-01
                                                                                  8.0503097191201248e-01
6
     7.1230814114326493e-03
                              2 7150941709503694e-02
                                                        3 9345094696029689e-02
                                                                                  9.3350396359446662e-01
                                  d = 11, n_K = 30, type [0, 2, 4], quality PI, e = 2
3
                              2.1289840740104060e-01
    7.2178042397209270e-02
                                                        3.9355079629947970e-01
                                                                                  3.9355079629947970e-01
3
                              4.0418683822051027e-02
                                                        4.7979065808897449e-01
     4.3215435615360841e-02
                                                                                  4.7979065808897449e-01
6
                              1.2539956353662088e-01
                                                                                  6.0862423456007753e-01
     5.8173710322163019e-02
                                                        2.6597620190330159e-01
6
     1.6975848322983403e-02
                              1.2409970153698532e-02
                                                        2.8536418538696462e-01
                                                                                  7.0222584445933685e-01
6
     2.7591464156449593e-02
                              5.2792057988217709e-02
                                                        1.3723536747817085e-01
                                                                                  8.0997257453361144e-01
6
     6.2289048587855958e-03
                                                        5.6817155788572447e-02
                              5.1003445645828061e-03
                                                                                  9.3808249964684475e-01
                                  d = 11, n_K = 30, type [0, 2, 4], quality PI, e = 2
3
                                                        2.7477281791211699e-01
     5.8325662127449619e-02
                              4.5045436417576603e-01
                                                                                  2.7477281791211699e-01
3
                                                                                  3.2841872644105845e-02
     1.3875995631494550e-02
                              9.3431625471178831e-01
                                                        3.2841872644105845e-02
6
     5.3363542393340484e-02
                              1.2142499385875732e-01
                                                        3.3479535924927089e-01
                                                                                  5.4377964689197179e-01
6
     2.7812320904551124e-02
                              2.4000467625830910e-02
                                                        3.7185999509036796e-01
                                                                                  6.0413953728380113e-01
6
     2.5253412629931399e-02
                              1.2700068887578271e-01
                                                        1.5804000955235862e-01
                                                                                  7.1495930157185867e-01
6
     2.4136561859371575e-02
                              2.7039712564819973e-02
                                                        1.6492234326164145e-01
                                                                                  8.0803794417353858e-01
                                 d = 11, n_K = 30, type [0, 2, 4], quality PI, e = 2.5
                              7.1187870201519159e-01
                                                        1.4406064899240421e-01
3
     4.8883135862392292e-02
                                                                                  1.4406064899240421e-01
3
                              9.3450946869957339e-01
                                                        3.2745265650213304e-02
     1.3814368459654939e-02
                                                                                  3.2745265650213304e-02
6
     3.5111950829892619e-02
                              2.4046986824731959e-01
                                                        3.0207587109553998e-01
                                                                                  4.5745426065714043e-01
6
     5.0153096874909698e-02
                              1.1000518620988445e-01
                                                        3.3722210801729928e-01
                                                                                  5.5277270577281628e-01
6
     2.5039771321642791e-02
                              2.1520759771076191e-02
                                                        3.7311327681727726e-01
                                                                                  6.0536596341164655e-01
6
                              2.7875756416958290e-02
                                                        1.6500707013095728e-01
     2.5013095479197943e-02
                                                                                  8.0711717345208443e-01
                                  d = 12, n_K = 33, type [0, 5, 3], quality PI, e = 2
                              4.5707498597014783e-01
                                                        2.7146250701492608e-01
                                                                                  2.7146250701492608e-01
3
     6.2541213195902760e-02
3
     4.9918334928060942e-02
                              1.1977670268281378e-01
                                                        4.4011164865859311e-01
                                                                                  4.4011164865859311e-01
3
     2.4266838081452033e-02
                              2.3592498108916896e-02
                                                        4.8820375094554155e-01
                                                                                  4.8820375094554155e-01
3
     2.8486052068877545e-02
                              7.8148434468129142e-01
                                                        1.0925782765935429e-01
                                                                                  1.0925782765935429e-01
3
     7.9316425099736385e-03
                              9.5070727312732881e-01
                                                        2.4646363436335595e-02
                                                                                  2.4646363436335595e-02
6
     4.3227363659414211e-02
                              1.1629601967792659e-01
                                                        2.5545422863851735e-01
                                                                                  6.2824975168355607e-01
6
     2.1783585038607558e-02
                              2.3034156355267139e-02
                                                        2.9165567973834096e-01
                                                                                  6.8531016390639190e-01
6
     1.5083677576511439e-02
                              2.1382490256170590e-02
                                                        1.2727971723358937e-01
                                                                                  8.5133779251024004e-01
```

```
d = 12, n_K = 33, type [0, 5, 3], quality NI, e = 2.5, \sigma = 1.637
3
     5.9921579300409806e-02
                              4.5297113890586446e-01
                                                        2.7351443054706777e-01
                                                                                 2.7351443054706777e-01
3
     2.8078756439547521e-02
                              2.3689177706651337e-02
                                                        4.8815541114667433e-01
                                                                                  4.8815541114667433e-01
3
     5.2528996017723132e-02
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     5.5601967530453329e-02
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3
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3
6
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