



**1 of 1**

ANL/MCS/CP--81883  
Copy-9308116--1

# A Survey of Numerical Cubature over Triangles\*

J. N. Lyness and Ronald Cools

## Abstract

This survey collects together theoretical results in the area of numerical cubature over triangles and is a vehicle for a current bibliography. We treat first the theory relating to regular integrands and then the corresponding theory for singular integrands with emphasis on the "full corner singularity." Within these two sections we treat successively approaches based on transforming the triangle into a square, formulas based on polynomial moment fitting, and extrapolation techniques. Within each category we quote key theoretical results without proof, and relate other results and references to these. Nearly all the references we have found may be readily placed in one of these categories. This survey is theoretical in character and does not include recent work in adaptive and automatic integration.

*1991 Mathematics Subject Classification:* Primary 41A55, 41A63; Secondary 65B05, 65B15, 65D32.

## 1 Introduction

### 1.1 A Historical Perspective

The numerical calculation of areas has a history that precedes the history of the infinitesimal calculus by several millenia. But the arrival of an analytic method in the late eighteenth century led to a surge in both theoretical and numerical methods for quadrature. The development of numerical methods for cubature (multidimensional integration) came perhaps a century and a half later, following closely the development of computing machines capable of handling these more intensive numerical calculations. Not until the early 1970s did textbooks begin to address cubature.

Undoubtedly, in the early days, cubature was treated as an iterative application of one-dimensional quadrature. But it was quickly realized that it was often more cost-effective

---

\*This work was supported by the Office of Scientific Computing, U.S. Department of Energy, under Contract W-31-109-Eng-38. This article will appear in the proceedings of the Vancouver conference, *Mathematics of Computation 1943-1993*. These proceedings will be published as a volume in the AMS series *Proceedings of Symposia in Applied Mathematics (PSAPOM)*.

January 11, 1994

1

MASTER

The submitted manuscript has been authored by a contractor of the U. S. Government under contract No. W-31-109-ENG-38. Accordingly, the U. S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution, or allow others to do so, for U. S. Government purposes.

to treat cubature over standard regions as a single entity. Two factors inhibiting the development of the theory were the large number of standard regions, each demanding special attention, and the cost of experimentation.

The triangle is simply one of these standard regions; the development of dedicated cubature methods is comparatively recent. Our earliest reference is to Radon's seven-point rule of polynomial degree 5 [Rad48]. A version of this rule is applicable to any planar region. The theory of integration over a triangle has lagged behind the theory for the square, but it has recently been spurred by two particular applications. One is the application to adaptive cubature, where triangles seem to be replacing squares as the basic module. The other application is to the finite element; here integrands with specified singularities may be involved.

The century and a half of development of one-dimensional quadrature has left us with a rich legacy in terms of variety of methods. We have rules involving derivative values, rules with all sorts of weighting functions, equally spaced rules, copy rules, minimum norm rules, equal weight rules, and rules of specified trigonometric degree. There are methods for using the same sets of function values to evaluate sets of integral transforms. We have techniques involving subtracting out singularities, and the method of steepest descent in the complex plane. And we have a wealth of expressions for the discretization error. For an overview of all these, we suggest [DR84].

Compared with all this, the available theory for the triangle is sparse indeed.

## References

[Rad48], [DR84]

## 1.2 Outline and Notation

Throughout this paper,  $\Omega$  denotes a specified triangle, and  $I(\Omega)[f]$  denotes the integral of an integrand function  $f(x, y)$  over this triangle. We refer to

$$Q[f] = \sum_{i=1}^{\nu} w_i f(x_i, y_i), \quad w_i \in \mathbb{R}, \quad (x_i, y_i) \in \mathbb{R}^2 \quad (1.1)$$

as a *cubature rule*, usually some sort of approximation to  $I(\Omega)[f]$ . This rule involves  $\nu = \nu(Q)$  weights and points. It is of *polynomial degree*  $d = d(Q)$  for  $\Omega$  if  $Q[f] = I(\Omega)[f]$  whenever  $f(x, y)$  is a polynomial of degree  $d$  or less. We do not discuss cubature rules requiring derivatives.

In Section 2.1 we introduce the Duffy transformation. This reduces the problem to that of cubature over a square. In Section 3.1 the same transformation is applied to advantage in situations where the integrand has certain singularities.

Section 2.2 is devoted to cubature rules of the form (1.1). Special attention is paid to different approaches to the construction of such rules and to the number of function values

$\nu(Q)$  required to obtain polynomial degree  $d(Q)$ . Because this theory is an immediate generalization of one-dimensional Gaussian quadrature, we refer to these rules generically as GQ. In Section 3.2, the few analogous results known to us involving weight functions are given.

In Section 2.3 we outline the theory of cubature using extrapolation (EQ). It appears that the result of extrapolation is yet another cubature rule, obtained in a somewhat round-about way. This rule turns out to have nontrivial polynomial degree, but is marginally less cost-effective in terms of polynomial degree than the GQ rules. In Section 3.3, extrapolation cubature is discussed in the context of integrand functions having certain algebraic or logarithmic singularities on the edge or at the vertex. This approach to these cubatures has significant advantages in terms of generality and convenience over the corresponding GQ.

In much of the theory, the results are independent of the actual triangle used for the calculation. This is especially true of the polynomial degree of a formula. Any nonsingular linear transformation takes one triangle into another and transforms a cubature formula in an obvious manner. It appears that the polynomial degree of the cubature formula is retained. (But this happens only occasionally when nontrivial weight functions are involved.) Different authors have found it convenient to use several different triangles, some of which are listed below. Originally,

$$\triangle = \{(x, y) : x \geq 0, y \geq 0, x + y \leq 1\}, \quad (1.2)$$

which we refer to as the *standard triangle*, was used almost exclusively. Parts of the theory will involve the *unit square*,

$$\square = [0, 1]^2, \quad (1.3)$$

and what we term the *complementary triangle*,

$$\nabla = \{(x, y) : x \leq 1, y \leq 1, x + y \geq 1\}. \quad (1.4)$$

Clearly,  $\triangle \cup \nabla = \square$ . More recent work has been based on the *equilateral triangle*

$$\triangleleft = \{(x, y) : x \leq \frac{1}{2}, \sqrt{3}y - x \leq 1, -\sqrt{3}y - x \leq 1\}, \quad (1.5)$$

which has vertices at  $(1/2, \pm\sqrt{3}/2)$  and  $(-1, 0)$ . Finally, we have used the triangle

$$\triangleup = \{(x, y) : 0 \leq y \leq x \leq 1\} \quad (1.6)$$

for the Duffy transformation below, simply because this makes the transformation simpler to follow. A consequence of the fact that different authors prefer different triangles is that the same cubature formula can appear in several forms in the literature.

## 2 A Regular Integrand Function

### 2.1 Transformation into a Square

A natural approach to integration over a triangle is to transform the triangle  $\triangle$  into the square  $\square$  as follows:

$$\int_0^1 \left\{ \int_0^x f(x, y) dy \right\} dx = \int_0^1 x \int_0^1 f(x, xt) dt dx.$$

In the days before the formal theory for multidimensional integration, one supposed that a scientist would do this naturally, partly because, in the early days, numerical integration over a square was more familiar. This transformation is now known as the *Duffy transformation* [Duf82].

To integrate over the square, the scientist might use the product of two one-dimensional rules, for example,

$$\sum_{i=1}^{n_t} T_i g(t_i) = \int_0^1 g(t) dt + E_g, \text{ where } E_g = 0 \quad \forall g \in \mathcal{P}_{d_t},$$

and

$$\sum_{j=1}^{n_x} X_j g(x_j) = \int_0^1 x g(x) dx + E_g, \text{ where } E_g = 0 \quad \forall g \in \mathcal{P}_{d_x}.$$

Thus, he would calculate an approximation of the form

$$Q[f] = \sum_{i=1}^{n_t} \sum_{j=1}^{n_x} T_i X_j f(x_j, t_i x_j).$$

A short calculation shows that this is of polynomial degree  $d = \min(d_t, d_x)$ . While, in principle, any pair of one-dimensional quadrature rules can be used, an erudite scientist might choose the Gauss-Legendre rule and the appropriate Gauss-Jacobi rule. The weights and abscissas for these Gaussian rules are often available for moderate to high values of  $n$  (see, e.g., [SS66]). If the scientist also chose  $n_t = n_x$ , he would recover the well-known *Stroud Conical Product rule* [Str71],  $Q_{CP}^{(d)}$ , for which the number of points is

$$\nu_{CP}^{(d)} = \nu(Q_{CP}^{(d)}) = \frac{(d+1)^2}{4} \text{ for all odd } d. \quad (2.1)$$

We note that this is a somewhat indirect way to obtain a rule for a triangle. The rule is not symmetric, and there are three distinct Stroud Conical Product rules for each degree  $d$ , depending on which vertex is the preferred one.

### References

[Duf82],[Str71],[SS66]

## 2.2 Polynomial Moment Fitting

Nearly all the theory of numerical integration over a triangle is related in one way or another to polynomial approximation. In the cubature rule (1.1), the points  $(x_i, y_i)$  and weights  $w_i$  are conventionally chosen so that the formula is exact for all polynomials up to a certain degree  $d$ . If the polynomials  $p_1, p_2, \dots, p_M$  form a basis for the space  $\mathcal{P}_d^2$  of all polynomials in two variables of degree at most  $d$ , then a cubature formula of degree  $d$  is determined by a system of polynomial equations, known as the *moment equations*,

$$Q[p_i] = I(\Omega)[p_i], \quad i = 1, 2, \dots, M = \dim \mathcal{P}_d^2 = \frac{1}{2}(d^2 + 3d + 2). \quad (2.2)$$

Here the *moments*,  $I(\Omega)[p_i]$ , are known, and the unknowns are  $x_i, y_i, w_i; i = 1, 2, \dots, \nu$ , which occur when the left-hand side is replaced by the expression in (1.1). Since a cubature formula of a specified polynomial degree for a specified triangle  $\Omega$  can be scaled onto any other triangle with preservation of its degree, one may choose any convenient triangle  $\Omega$  for this calculation.

One can distinguish between two approaches to construct cubature formulas:

1. one may proceed directly to solve this system of nonlinear equations (most of this section describes this); or
2. one can search for polynomials that vanish at the points of the formula.

This second approach has been very successful in (one-dimensional) quadrature. In cubature, it has turned out to be difficult for the square, and significantly more difficult for the triangle. Radon constructed the first cubature formula for a triangle using the common zeros of three orthogonal polynomials. Schmid [Sch83] used the theory of real polynomial ideals to construct a minimal formula of degree 4 with positive weights. To our knowledge, only very few rules for the triangle have been obtained by using orthogonal polynomials or polynomial ideals. However, this approach did lead to the following important result.

**Theorem 2.1** *The number of points  $\nu(Q)$  in a cubature formula  $Q$  of degree  $d$  for a triangle satisfies  $\nu(Q) \geq \nu_L(d)$ , where*

$$\nu_L(d) = \frac{(d+2)(d+4)}{8} \quad \text{if } d \text{ is even,} \quad (2.3)$$

$$\nu_L(d) = \frac{(d+1)(d+3)}{8} + \left\lfloor \frac{d+1}{4} \right\rfloor \quad \text{if } d \text{ is odd.} \quad (2.4)$$

The first bound can be traced back to the same paper by Radon that contains the first cubature formula for a triangle. In its general form it was probably first published by Stroud in [Str60]. The second bound was obtained by Möller for  $d < 12$  [Möl76] in 1976. This result was generalized by Rasputin in 1983 [Ras83b]. The same bound had been established for centrally symmetric regions, such as a square, in 1973 [Möl73]. It is revealing that it took ten years to modify the theory for a triangle with constant weight function and another ten years for a triangle with a special weight function (see Section 3.2). It is also

Table 1: Known minimal formulas, their properties, and original discoverers

$d$	$\nu_L(d)$	Quality	Reference
2	3	PI(3)	[HS56]
		PI(3)	[Hil77]
3	4	NI	[HS56]
		PI(2)	[Hil77]
4	6	PI	[Cow73]
		PI	[Sch83]
5	7	PI	[Rad48]
6	10	PO	[Ras83a]
7	12	PI	[Gat88, Bec87]
8	15	PO	[CH87]

known that a formula of even degree that attains this lower bound has all weights positive [Mys68, Str71, CH88b]. This property is, however, not guaranteed for formulas of odd degree.

In Table 1 we give an overview of the known minimal formulas. In the third column, P indicates that no negative weights occur and I indicates that there are no abscissas strictly outside the triangle. N and O are the negations of P and I, respectively. The number of distinct formulas (if more than one) is indicated in parentheses.

We now return to the direct approach, item 1 above. This has been fruitful, and an arsenal of cubature formulas now exists. At first, however, progress was painfully slow. In retrospect, it turns out that progress has been governed by the willingness of researchers to appreciate the significance of symmetry and structure and to realize that the detailed application of these is quite different for the triangle than it is for the square.

The term *symmetry* will be familiar to readers. By the symmetry group of a triangle, we mean the group of six linear transformations which take that specific triangle into itself. Any such group is isomorphic with the permutation group  $S_3$ . For the equilateral triangle  $\triangleleft$ , this symmetry group is termed the dihedral group  $D_3$ . The term *structure* is less precise. In cubature it refers to conditions applied to the rule. These take the form of constraints on the solutions of the moment equations. For example, if we look ahead to (2.7), once numerical values for  $K_0, K_1$ , and  $K_2$  have been assigned, the rule has been structured. One may then try to solve the moment equations. It is common experience among those who attempt to solve systems like (2.2) that exploiting the symmetry of the region and imposing a simple structure to the rule form has a simplifying effect on their task. This simplification is a consequence of Sobolev's theorem [Sob62].

**Theorem 2.2** *Let the integral  $I(\Omega)$  and a cubature formula  $Q$  be invariant under the transformations of a group  $\mathcal{G}$ . The cubature formula  $Q$  has polynomial degree  $d$  if  $Q[f] = I(\Omega)[f]$  whenever  $f(x, y)$  is a polynomial of degree  $d$  or less that is invariant with respect to  $\mathcal{G}$ .*



The larger the symmetry group  $\mathcal{G}$ , the lower is the dimension of the space of all  $\mathcal{G}$ -invariant polynomials of degree at most  $d$  and, consequently, the lower is the number of nonlinear equations that determine a  $\mathcal{G}$ -invariant cubature formula.

It is convenient and appropriate to describe these formulas in a partly historic perspective.

- 1a. If no structure is imposed on the cubature formula, one can use the monomials

$$x^i y^j, \quad 0 \leq i + j \leq d,$$

as a basis of  $\mathcal{P}_d^2$ . The number of moment equations in this case is then  $\frac{1}{2}(d^2 + 3d + 2)$ . We have no evidence that any serious attempt was ever made to solve this set of equations directly.

- 1b. In the 1960s, significant progress was made in cubature for the square by exploiting its symmetry. In particular, by imposing a rule structure symmetric under coordinate interchange, one could reduce the number of independent moment equations. It appeared that for the standard triangle  $\triangle$ , a significant reduction was available if one structured the rule to be invariant under coordinate interchange, and fitted only monomials  $x^\alpha y^\beta$  with  $\alpha \geq \beta \geq 0$ . The number of independent moment equations is then  $\lfloor \frac{1}{4}(d^2 + 4d + 4) \rfloor$ . Formulas of degrees 2, 3, 4, 5, and 6 with this symmetry exist with their number of points equal to the lower bound of Theorem 2.1.

In retrospect, one can see that Sobolev's theorem is being applied, in this case with  $\mathcal{G}$  being a group of order 2, whose elements are the unit and a reflection about one median. Later (see 1d below), it was applied using as  $\mathcal{G}$  the full dihedral group  $\mathcal{D}_3$ . Later still (see 1c below), when the overall theory had become more familiar, the same theorem was applied using another subgroup of  $\mathcal{D}_3$ .

- 1c. In the late 1980s, Gatermann [Gat88] and Cools and Haegemans [CH87] searched for minimal formulas for degrees larger than 5, using the subgroup of  $\mathcal{D}_3$  generated by the rotations. This approach led to minimal formulas of degree 7 and 8. It was later established that no formula of degree 6 with 10 points exists with this symmetry [Gat90]. For this symmetry, a basis in polar coordinates using the equilateral triangle  $\triangleleft$  is

$$(r^2)^i (r^3 \cos 3\theta)^j (r^3 \sin 3\theta)^l, \quad 0 \leq 2i + 3(j + l) \leq d, \quad l = 0 \text{ or } 1,$$

and the number of independent moment equations is  $\lfloor \frac{1}{6}(d^2 + 3d + 6) \rfloor$ .

- 1d. The full symmetry of a triangle was systematically exploited for the first time in 1975 by Lyness and Jespersen [LJ75], who introduced the equilateral triangle  $\triangleleft$  for this purpose. Since then, this choice has been popular. One of the advantages of  $\triangleleft$  is that it is straightforward to write down a basis for the  $\mathcal{D}_3$ -invariant polynomials of degree  $d$  and less. This is

$$(r^2)^i (r^3 \cos 3\theta)^j, \quad 0 \leq 2i + 3j \leq d,$$

and the number of independent moment equations is

$$E(d) = \left\lfloor \frac{1}{12}(d^2 + 6d + 12) \right\rfloor. \quad (2.5)$$

In the case of the triangle, then, the larger the symmetry group, the smaller the number of independent moment equations  $E(d)$ . We now describe in detail how this theory is applied. We shall employ the equilateral triangle  $\triangleleft$ , denote its area by  $A$ , and work in polar coordinates. We shall apply the convention that  $(r, \theta)$  and  $(-r, \theta + \pi)$  refer to the same point. Since  $Q[f]$  is to have this symmetry, it follows that, if any point  $(r, \alpha)$  appears in  $Q[f]$ , so does any point of the form  $(r, \pm\alpha + \frac{2\pi j}{3})$ , and all distinct points of this set carry the same weight. Such a set of points is sometimes called an *orbit*. A moment's reflection will convince the reader that no orbit has more than six elements; and a basic cubature rule, one that contains only one orbit, can be expressed in the form

$$Q(r, \alpha)[f] = \frac{A}{6} \sum_{j=1}^3 \left\{ f\left(r, \alpha + \frac{2\pi j}{3}\right) + f\left(r, -\alpha + \frac{2\pi j}{3}\right) \right\}, \quad (2.6)$$

where negative values of  $r$  are allowed,  $\alpha \in [0, \pi/6)$ , and  $A$  is the area of the triangle. Moreover, any rule  $Q[f]$  is expressible as a linear combination of these basic rules.

Three geometrically distinct types of orbit occur. The first (type-0), with  $r = 0$ , involves only the centroid. There can be at most one of these in  $Q[f]$ . The type-1 orbits have  $\alpha = 0$  and positive or negative assignments of  $r$ . These have precisely three distinct points all lying on a median of the triangle. All other orbits are termed type-2 orbits and include six distinct points, none of which are on any median.

Let  $K_i$  be the number of orbits of type  $i$  in a  $\mathcal{D}_3$ -invariant cubature formula. These nonnegative integers specify the *structure* of the rule and are known as *structure parameters*. A  $\mathcal{D}_3$ -invariant cubature formula must have the following form:

$$Q[f] = K_0 w_0 f(0, 0) + \sum_{i=1}^{K_1} w_i Q(r_i, 0)[f] + \sum_{i=K_1+1}^{K_1+K_2} w_i Q(r_i, \alpha_i)[f], \quad (2.7)$$

where  $Q(r, \alpha)[f]$  is defined in (2.6) above. The number of points required by this rule is

$$\nu(Q) = K_0 + 3K_1 + 6K_2. \quad (2.8)$$

The process of solving sets of nonlinear equations can be very involved. Some regard it as more of an art than a science. There is a set of inequalities, known as the consistency conditions, that are heuristic but extraordinarily useful. They are based on the inaccurate premise that one may obtain a solution to a set of  $E$  equations in  $N$  unknowns only if  $E \geq N$ . This premise is applied to the set of  $E(d)$  independent moment equations and to any conveniently determined subset of these equations that does not involve some of the unknowns. Some consistency conditions for cubature formula (2.7) have been determined in [LJ75]. These are

$$K_0 + 2K_1 + 3K_2 \geq E(d),$$

$$\begin{aligned} 2K_1 + 3K_2 &\geq E(d) - 1, \\ 3K_2 &\geq E(d - 6), \\ K_0 &\leq 1, \end{aligned} \tag{2.9}$$

where  $E(d)$  is given by (2.5).

A refreshingly well defined problem is that of finding an optimal cubature formula whose structure satisfies these consistency conditions. It is straightforward to show that, when  $Q$  given by (2.7) has polynomial degree  $d$ , then

$$\nu(Q) \geq \nu_{CCL}(d) = \left\lfloor \frac{1}{6}(d^2 + 3d + 2) \right\rfloor. \tag{2.10}$$

In principle, one could use an integer programming routine to determine the set of nonnegative  $K_i$  that, for a given degree  $d$ , satisfies (2.9) and minimizes  $\nu(Q)$  given by (2.8). In practice, this particular set is so simple that it can almost be done by inspection. Then one has to solve the set of nonlinear equations. If no solution can be found, one determines the next best solution of the minimization problem, and iterates. In the end, one is brought to a stop when the system becomes too large for one's computing aids. This search was initiated by Lyness and Jespersen [LJ75], who went as far as  $d = 11$ ; it was continued up to  $d = 20$  by Dunavant [Dun85]. To our knowledge, apart from conical product rules, no rules of higher degree have been determined explicitly.

In the foregoing account we have implicitly assumed that the search has been for all real solutions to the moment equations. As in the theory of one-dimensional quadrature, various additional criteria have been applied in the construction of cubature formulas. For example, a *good* formula (also known as a PI formula in [LJ75]) is one all of whose weights are positive and all points inside the region of integration. Restricting the search to formulas with all weights positive has largely been discontinued. Instead, all rules are found, and, when of interest, the value of a *condition number*

$$\sigma(Q) = \frac{\sum_{i=1}^{\nu} |w_i|}{\sum_{i=1}^{\nu} w_i} \tag{2.11}$$

is reported. Rules having some points outside the triangle are also reported. A different cost criterion, the *cytolic* point count (conventionally termed  $\bar{\nu}$ ), is occasionally used. Its justification is set in a context in which a large triangular region is subdivided into  $m^2$  small triangular regions of equal area, and the cubature rule is applied to each smaller triangle. This reflects the average number of points per cell by discounting appropriately the corner and edge point count. These variations have added little to the theory.

On the other hand, Silvester [Sil70], by means of a somewhat elegant use of homogeneous coordinates, introduced the theory necessary to construct analogues of the open and the closed type of one-dimensional Newton-Cotes rules. The closed type uses all points on  $\triangle$  of the form  $(j/m, k/m)$  except the three vertices when  $m$  is even, is of degree  $d = m$ , and has  $\mathcal{D}_3$  symmetry. Like the one-dimensional Newton-Cotes rules, the weights are rationals, and the value of  $\sigma$ , ((2.11) above), increases indefinitely with increasing  $m$ . For these the

point count is

$$\nu_{NCC}(d) = \frac{1}{2}(d+1)(d+2) - \frac{3}{2}(1+(-1)^d). \quad (2.12)$$

*Embedded formulas* are pairs (or longer sequences) of cubature formulas where some or all of the points of a less precise formula are also used by a more precise formula. In contrast with the one-dimensional situation, where the gap between the degree of a Gaussian quadrature formula and its Kronrod extension is large, in two dimensions one can construct embedded formulas of successive degrees.

For constructing such embedded formulas, the approach using orthogonal polynomials has been more successful. Although published results are scarce, the highest-degree embedded sequences available have been constructed by using this approach.

**Theorem 2.3** [CH90] *Let a set of  $\nu$  distinct points support two distinct cubature formulas of respective degrees  $2k-1$  and  $2k+m$ ,  $m \in \mathbb{N}$ , in such a way that, for every point, the two assigned weights are different from each other. Then  $\nu \geq (k+1)^2$ .*

The lower bound of Theorem 2.3 is known to be sharp for pairs of degrees (1,3) and (5,7). The confirming rules appeared in references [GM78, CH88a]. Simpler, but less effective, embedded formulas are obtained naturally by extrapolation (which is treated in the following section).

Nearly all the cubature formulas for the triangle that were known before 1971 are collected in Stroud's standard work on multiple integration [Str71]. A list of more recent references to available rules, together with information about the quality of these rules, has been compiled by Cools and Rabinowitz [CR93].

## References

[Bec87], [CH87], [CH88b], [CH88a], [CH90], [Cow73], [CR93], [Dun85], [Gat88], [Gat90], [GM78], [Hil77], [HS56], [LJ75], [Möl73], [Möl76], [Mys68], [Rad48], [Ras83a], [Ras83b], [Sch83], [Sil70], [Sob62], [Str60], [Str71]

## Additional reference material for this section

[BE90], [dD79], [Eng70], [Eng80], [Fra71], [Gat92], [Gün75], [Hem73], [HMS56], [Lau55], [Lau82], [LG78], [Moa74], [Ras86], [SF73], [Str61], [Str64], [Str66], [Str69]

## 2.3 Extrapolation

In 1927, Richardson [Ric27] proposed his deferred approach to the limit. Possibly the first application of this in one-dimensional quadrature became known as Romberg integration [Rom55]. In the mid-1960s, extrapolation was applied by several authors to integration

over a square. In the 1970s the techniques used to construct this theory were modified to provide corresponding results for the triangle. We describe first the theory for the square and then the significantly more difficult theory for the triangle.

We define a one-point rule

$$Q_{\alpha,\beta}[f] = f(\alpha, \beta). \tag{2.13}$$

The  $m^2$ -copy version of this rule for integration over the square  $\square$  is

$$Q_{\alpha,\beta}^{(m)}(\square)[f] = \frac{1}{m^2} \sum_{j=0}^{m-1} \sum_{k=0}^{m-1} f\left(\frac{j+\alpha}{m}, \frac{k+\beta}{m}\right). \tag{2.14}$$

Using (2.13), we may express a general cubature formula (1.1) as

$$Q[f] = \sum_{i=1}^{\nu} w_i Q_{\alpha_i, \beta_i}[f]. \tag{2.15}$$

$Q$  is *centrally symmetric* for the square  $\square$  if it may be re-expressed in the form

$$Q(\square)[f] = \sum_{j=1}^{\mu} \frac{w_j}{2} (Q_{\alpha_j, \beta_j}[f] + Q_{1-\alpha_j, 1-\beta_j}[f]).$$

The  $m^2$  copy of (2.15) is defined as

$$Q^{(m)}(\square)[f] = \sum_{i=1}^{\nu} w_i Q_{\alpha_i, \beta_i}^{(m)}(\square)[f]. \tag{2.16}$$

This rule is an approximation to  $I(\square)[f]$  obtained by subdividing the square  $\square$  into  $m^2$  identical squares, each of side  $1/m$ , and applying a properly scaled version of  $Q[f]$  to each. If  $Q$  is centrally symmetric, then  $Q^{(m)}(\square)[f]$  is also centrally symmetric.

For regular  $f(x, y)$ , extrapolation is based on the two-dimensional version of the *Euler-Maclaurin expansion*. When  $f \in C^p(\square)$ ,  $p \in \mathbb{N}$ , the almost self-evident extension of the standard one-dimensional expansion may be expressed in the form

$$Q^{(m)}(\square)[f] - I(\square)[f] = \sum_{q=1}^{p-1} \frac{B_q(\square; Q; f)}{m^q} + O(m^{-p}). \tag{2.17}$$

The coefficients in this expansion have the form

$$B_q(\square; Q; f) = \sum_{\substack{q_1 + q_2 = q \\ q_i \geq 0}} c_{q_1, q_2}(Q) \int_{\square} f^{(q_1, q_2)}(x, y) dx dy, \tag{2.18}$$

where  $c_{q_1, q_2}(Q)$  is obtained by applying the rule  $Q$  to

$$\frac{B_{q_1}(x)B_{q_2}(y)}{q_1!q_2!},$$

$B_q(t)$  being the Bernoulli polynomial of degree  $q$  in  $t$ . Integral representations for the remainder term of the expansion (2.17) have been given in [LM70].

These coefficients have several properties that are useful in constructing individual extrapolation procedures and in assessing them.

1. If  $Q$  is centrally symmetric, then

$$B_q(\square; Q; f) = 0 \quad \forall \text{ odd } q, \quad (2.19)$$

and so the Euler-Maclaurin expansion (2.17) is an even expansion.

2. If  $Q$  is of polynomial degree  $d$ , then

$$B_q(\square; Q; f) = 0, \quad q = 1, 2, \dots, d. \quad (2.20)$$

3. If  $f(x, y)$  is a polynomial of degree  $d(f)$ , then the asymptotic expansion (2.17) reduces to a finite sum, and

$$B_q(\square; Q; f) = 0 \quad \forall q > d(f). \quad (2.21)$$

There are curiosities in the theory. For example, when  $f(x, y)$  is periodic with unit period, one finds that all coefficients  $B_q$  are zero, but  $Q^{(m)}[f] - I[f]$  need not be zero. The vanishing of the remainder term is a stronger result than, and is not implied by, the vanishing of all individual terms.

Romberg integration over the square is conventionally based on the product trapezoidal rule

$$Q^{(m)}(\square)[f] = \frac{1}{4} \sum_{\alpha=0}^1 \sum_{\beta=0}^1 Q_{\alpha,\beta}^{(m)}(\square)[f]$$

and occasionally on the mid-square rule  $Q_{1/2,1/2}^{(m)}(\square)[f]$ .

The extrapolation process will be familiar to the reader. The numerical result, conventionally denoted by  $T_{k,p}$ , is a linear combination of  $p + 1$  distinct approximations to  $I[f]$ , namely,  $Q^{(m_i)}[f]$  with  $i = k, k + 1, \dots, k + p$ . This combination is constructed so that the first  $p$  nonzero terms on the right of (2.17) disappear from the corresponding expansion of  $T_{k,p} - I[f]$ . When  $f(x, y)$  is a polynomial of degree  $p$ , the result in item 3 assures us that other terms also disappear. In fact, the remainder term vanishes too, leaving the result that  $T_{k,p}$  is exact, and so the implied rule is of polynomial degree  $p$ . More familiar is the case of an even expansion when the extrapolation is designed to recognize only even terms, and the result  $T_{k,p}$  is of polynomial degree  $2p + 1$ .

We refer to these generalizations of Romberg integration collectively as *extrapolation quadrature* (EQ). The reader should note that there are many parameters to be set. These include the rule  $Q$  to be used, the mesh ratio sequence  $m_i$ , and, of course, for an individual result, the values of  $k$  and  $p$ .

The theory given above for the square is extraordinarily simple to establish. Only integral representations for the remainder term pose any serious difficulty at all. In contrast, development of the corresponding theory for the standard triangle  $\triangle$  has not been

straightforward. When one subdivides the standard triangle  $\triangle$  into  $m^2$  equal triangles using lines parallel to  $x = 0, y = 0$  and  $x + y = 0$ , one finds  $m(m + 1)/2$  identical triangles oriented in the same way as  $\triangle$  together with  $m(m - 1)/2$  identical triangles oriented in the same way as  $\nabla$ . If one proceeds on a cell-by-cell basis, it is clear how to assign points to the first set of triangles, but not the second set. In [Lyn78] this incongruity was resolved by introducing a *rule pair*. The resulting theory is complicated.

**Definition 2.1** A rule pair  $(Q(\triangle), Q(\nabla))$  comprises two cubature rule operators

$$\begin{aligned} Q^{(1)}(\triangle)[f] &= \sum_{i=1}^{\nu} w_i f(\alpha_i, \beta_i), \text{ and} \\ Q^{(1)}(\nabla)[f] &= \sum_{i=1}^{\bar{\nu}} \bar{w}_i f(\bar{\alpha}_i, \bar{\beta}_i) \end{aligned} \quad (2.22)$$

where  $\sum_{i=1}^{\nu} w_i + \sum_{i=1}^{\bar{\nu}} \bar{w}_i = 1$ .

These are two quite independent rules, pertaining to the two different triangles. To construct the  $m$ -copy, one requires both rules. Then we have the following definition.

**Definition 2.2**

$$\begin{aligned} Q^{(m)}(\triangle)[f] &= \frac{1}{m^2} \sum_{i=1}^{\nu} w_i \sum_{j=0}^{m-1} \sum_{k=0}^{m-1-j} f\left(\frac{\alpha_i + j}{m}, \frac{\beta_i + k}{m}\right) \\ &+ \frac{1}{m^2} \sum_{i=1}^{\bar{\nu}} \bar{w}_i \sum_{j=0}^{m-2} \sum_{k=0}^{m-2-j} f\left(\frac{\bar{\alpha}_i + j}{m}, \frac{\bar{\beta}_i + k}{m}\right). \end{aligned} \quad (2.23)$$

Note that when  $m = 1$ ,  $Q^{(m)}(\triangle)[f]$  may be zero, but in an extrapolation technique, this zero value may be used as a meaningful result.

When  $f \in C^p(\triangle)$ ,  $p \in \mathbb{N}$ , the Euler-Maclaurin expansion for the triangle may be written in the form

$$Q^{(m)}(\triangle)[f] - I[f] = \sum_{q=1}^{p-1} \frac{B_q(\triangle; Q; f)}{m^q} + O(m^{-p}). \quad (2.24)$$

This was established in [Lyn78]. The coefficients  $B_q(\triangle; Q; f)$  have a more complicated structure than those for the square in (2.18). Clearly

$$B_q(\triangle; Q; f) = \sum_{i=1}^{\nu} w_i B_q(\triangle; Q_{\alpha_i, \beta_i}; f) + \sum_{i=1}^{\bar{\nu}} \bar{w}_i B_q(\triangle; Q_{\bar{\alpha}_i, \bar{\beta}_i}; f).$$

It may be shown that

$$B_q(\triangle; Q_{\alpha, \beta}; f) = \sum_{\substack{q_1 + q_2 = q \\ q_i \geq 0}} B_{q_1, q_2}(\triangle; Q_{\alpha, \beta}; f),$$

where, so long as  $\alpha, \beta \in (0, 1)$  and  $\alpha + \beta \neq 1$ ,

$$B_{q_1, q_2}(\triangle; Q_{\alpha, \beta}; f) = \frac{B_{q_1}(\alpha)B_{q_2}(\{\alpha + \beta\})}{q_1!q_2!} \int_0^1 \frac{\partial^{q_1}}{\partial x^{q_1}} f^{(0, q_2-1)}(x, 1-x) dx \\ - \frac{B_{q_1}(\alpha)B_{q_2}(\beta)}{q_1!q_2!} \int_0^1 \frac{\partial^{q_1}}{\partial x^{q_1}} f^{(0, q_2-1)}(x, 0) dx.$$

Here  $\{x\}$  means the fractional part of  $x$ . Moreover, when  $Q$  includes abscissas on the edges and even outside its triangle, the expansion (2.24) remains valid, and the coefficients may be obtained from those given above by using analytic continuation.

Clearly an associated rule for the square is

$$Q(\square) = Q(\triangle) + Q(\nabla).$$

This rule  $Q(\square)$  is centrally symmetric if  $\nu = \bar{\nu}$ ,  $w_i = \bar{w}_i$  and  $\alpha_i + \bar{\alpha}_i = \beta_i + \bar{\beta}_i = 1$ .

Results analogous to (2.19), (2.20), and (2.21) hold, namely,

1. if  $Q(\square)$  is centrally symmetric, then  $B_q(\triangle; Q; f) = 0 \forall$  odd  $q$ ;
2. if both  $Q^{(1)}(\triangle)$  and  $Q^{(1)}(\nabla)$  have polynomial degree  $d$  for their respective triangles, then  $B_q(\triangle; Q; f) = 0$ ,  $q = 1, 2, \dots, d$ ; and
3. if  $f(x, y)$  is a polynomial of degree  $d(f)$ , then the asymptotic expansion (2.24) reduces to a finite sum, and

$$B_q(\triangle; Q; f) = 0 \forall q > d(f) + 1. \quad (2.25)$$

These results were obtained earlier using an entirely different approach [LP73] involving product integration. This equally complicated theory was generalized in 1979 by de Doncker [dD79]. Let  $\mu$  be half an odd integer,  $f \in C^p(\triangle)$ ,  $p \in \mathbb{N}$  and

$$Q^{(\mu)}[f] = \frac{1}{\mu^2} \sum_{j=1}^{\mu+1/2} \sum_{k=1}^{\mu-j+1/2} f\left(\frac{j-1/2}{\mu}, \frac{k-1/2}{\mu}\right).$$

Then

$$Q^{(\mu)}[f] = I[f] + \sum_{\substack{q \text{ even} \\ q < p}} \frac{B_q}{\mu^q} + O(m^{-p}).$$

In any extrapolation procedure based on this expansion, one is allowed to employ only values of  $\mu$  for which  $2\mu$  is an odd integer. De Doncker has shown that when  $f$  is a polynomial of degree  $d(f)$ , then  $B_q = 0 \forall q > d(f)$ . This means that an extrapolation procedure that eliminates  $B_q$ ,  $q \leq d(f)$ , leaves an exact result. This circumstance may be used to generate rules of specified degree. Grundmann and Möller [GM78], in an independent approach, established a set of rules of the form

$$Q_t[f] = \sum_{j=1}^t a_{t,j} Q^{(j-1/2)}[f] \quad (2.26)$$



of degree  $2t - 1$ . These rules are identical with rules obtained later by De Doncker using extrapolation. (For larger  $t$ , the rule (2.26) has unduly high condition number; see (2.11) above. An alternative is to extrapolate using only a selection of the approximations  $Q^{(j-1/2)}[f]$ . This reduces the conditioning error at a cost in extra function values.) So far as we are aware, this approach to integration over the triangle has not been developed further, nor has the corresponding theory for squares.

## References

[dD79], [GM78] [LM70], [LP73], [Lyn78] [Ric27] [Rom55]

## 3 Specified Singularities

### 3.1 Transformation into a Square

The Duffy transformation, introduced in Section 2.1, may be used to advantage in the case where the integrand function has a full corner singularity and a line singularity along the opposite edge. In particular, for the triangle  $\triangle$ , when the integrand is of the form

$$f(x, y) = y^\lambda(x - y)^\mu(1 - x)^\nu r_\rho(x, y)g(x, y),$$

where  $r_\rho(x, y) = (x^2 + y^2)^{\rho/2}$  and  $g(x, y)$  is regular in the triangle of integration, one finds readily that

$$\int_0^1 \left\{ \int_0^x f(x, y) dy \right\} dx = \int_0^1 \int_0^1 x^{1+\lambda+\mu+\rho} (1-x)^\nu (1-t)^\mu r_\rho(1, t) g(x, tx) dt dx. \quad (3.1)$$

Note that, while  $r_\rho(x, xt)$  has a singularity at  $x = 0$ , this has been extracted, leaving the innocuous function  $r_\rho(1, t)$  which is regular for all  $t$ . This integral may be approximated by the product of a pair of Gauss-Jacobi formulas, just as described in Section 2.1.

This transformation is correct as written when  $r_\rho(x, y)$  is replaced by any other function homogeneous of degree  $\rho$  in the triangle of integration, as defined in Definition 3.1 below.

### 3.2 Polynomial Moment Fitting

In this section we discuss cubature rules with a nonconstant weight function for the triangle. This weight function  $w(x, y)$  is given, and its moments are known, usually in analytic form. The rule  $Q[f]$  is of the same form as in preceding sections, but it is designed to approximate the integral

$$I(\Omega; w(x, y))[f] = \int_\Omega \int w(x, y) f(x, y) dx dy. \quad (3.2)$$

As before, when this approximation is exact for all polynomials of degree  $d$  or less, the rule  $Q[f]$  is said to be of degree  $d$ .

The major difference between this theory and the special case with unit weight function is that, in general, one cannot transform the triangle into another of different shape and retain both the nature of the singularity and the polynomial degree. What happens is that the affine transformation alters the weight function too. When  $w(x, y) = 1$ , this is no problem. But, in general, one finds a rule of the original polynomial degree for a new triangle and a new weight function.

The shape of the triangle and the weight function are now important, and, for a fixed type of weight function like  $1/r$ , one needs a new rule for each differently shaped triangle. For reasons unknown to us, only one triangle has been treated, this having sides in the ratio  $\sqrt{5}, \sqrt{5}, 2$ . One set of rules has a radial weight function  $1/r$ ,  $r$  being measured from the mid-point of the shorter side. The other is similar, except that  $r$  is now measured from the vertex opposite the shorter side. Only results for low degrees (1, 2, 3, 5, and 7) are published [CL78, Hae93, PFB81]. Most of them were constructed by solving the nonlinear equations that define them and imposing symmetry with respect to one median (the only symmetry available). The highest-degree results were obtained using the common zeros of three orthogonal polynomials, a variant of the method used by Radon.

The narrowness of the scope for possible application of these numerical results is manifest. If one has an equilateral triangle, or a right-angled triangle, these weights and abscissas are useless. They are of value for triangles of one specified shape only. Unfortunately, the authors do not make this clear. The casual reader could easily retain the impression that these results are of wider application.

Lyness and Gatteschi [LG82] have treated a variant problem. They use a general triangle and an integrand function  $w(x, y)f(x, y)$  closely related to that in the preceding subsection. In terms of the triangle  $\triangle$ , the weight function is

$$w(x, y) = y^\lambda(x - y)^\mu(1 - x)^\nu r^\beta, \quad (3.3)$$

and the rest of the integrand function is of the form  $f(x, y) = h(r)g(x, y)$ . The cubature rule is of *joint polynomial degree*  $d$  if it is exact for all functions  $h(r)g(x, y)$ , where  $g$  and  $h$  are polynomials of degree  $\gamma$  and  $\delta$ , respectively, and  $\gamma + \delta \leq d$ . The authors provide the specifications for a product rule of the same type as in the preceding subsection. However, one of the product rule components is a one-dimensional *quasi-degree* quadrature rule.

The only theoretical results known to us about formulas for triangles with weight function are the following. First, the lower bound for the number of points presented in Theorem 2.1 is valid for even degrees whenever the integral has a positive weight function. Recently, Berens and Schmid [BS92] proved that Theorem 2.1 is valid for the integral

$$I[g] = \int_0^1 \int_0^x y^\lambda(x - y)^\mu(1 - x)^\nu g(x, y) dy dx \quad (3.4)$$

for odd degrees also.

## References

[BS92] [CL78], [Hae93], [LG82] [PFB81]

### 3.3 Extrapolation

A powerful method of handling integration over a triangle of an integrand having certain boundary singularities is by extrapolation. The results resemble closely corresponding results for integration over a square, and much of this theory may be established as a minor corollary to the theory for the square.

The theory is based on homogeneous functions:

**Definition 3.1** *The function  $f(x, y)$  is homogeneous of degree  $\gamma$  about the origin in a region  $\mathcal{R}$  if  $f(kx, ky) = k^\gamma f(x, y)$  for all  $k > 0$  and  $(x, y) \in \mathcal{R} \setminus \vec{0}$ .*

This is in fact an  $n$ -dimensional definition. In one dimension the only homogeneous functions of degree  $\gamma$  are of the form  $kx^\gamma$ . In higher dimensions more sophisticated functions may be homogeneous. Two-dimensional examples include  $r^\gamma = (x^2 + y^2)^{\gamma/2}$ ,  $x^\gamma$ ,  $(x - 3y + r)^\gamma$ , and  $(x^5 + 6y^5)^{\gamma/5}$  which are homogeneous of degree  $\gamma$ , while any function of  $y/x$ , such as  $\theta = \arctan(y/x)$ , is of degree zero. The singularities that can be handled through extrapolation are closely related to homogeneous functions.

Two early and fundamental papers [LM80, Sid83] establish error functional expansions for singular integrals over triangles. The basic result in [LM80] is as follows.

**Theorem 3.1** *Let  $f_\gamma(x, y)$  be homogeneous of degree  $\gamma$  about the origin in the first quadrant  $x \geq 0, y \geq 0$  and be  $C^p$ ,  $p \in \mathbb{N}$ , there except possibly at the origin. Then*

$$Q^{(m)}(\triangle)[f_\gamma] - I(\triangle)[f_\gamma] = \frac{A_{2+\gamma}(\triangle; Q; f_\gamma)}{m^{2+\gamma}} + \frac{C_{2+\gamma}(\triangle; Q; f_\gamma)(\ln m)}{m^{2+\gamma}} + \sum_{s=1}^{p-1} \frac{B_s(\triangle; Q; f_\gamma)}{m^s} + O(m^{-p}), \quad (3.5)$$

where  $C_{2+\gamma} = 0$  unless  $\gamma \in \mathbb{N}$ .

The identical expansion had been previously established for the square. The proof in the case of the square is not easy. However, once established for the square, it can be established for the triangle almost trivially. One notes that  $\square = \triangle \cup \nabla$ . Then, since

$$Q^{(m)}(\triangle) + Q^{(m)}(\nabla) = Q^{(m)}(\square),$$

any expansion for  $\triangle$  is simply the difference of the corresponding expansion for  $\square$  and for  $\nabla$ . However,  $f_\gamma(x, y)$  is regular within  $\nabla$ , and so  $Q^{(m)}(\nabla)[f_\gamma]$  has an expansion of the same type as (2.24). Taking this difference then simply alters the coefficients in some of the existing terms and does not introduce any additional terms.

Detailed expressions for the coefficients in the case of the square are given in [Lyn76]. The coefficients in (3.5) have the following properties:

1. if both  $Q^{(1)}(\triangle)$  has polynomial degree  $d$  for  $\triangle$  and  $Q$  has polynomial degree  $d$  for  $\square$ , then

$$C_s = B_s = 0 \text{ for all odd } s; \quad (3.6)$$

2. if  $Q$  is of polynomial degree  $d$ , then

$$C_s = B_s = 0 \text{ for } s = 1, 2, \dots, d. \quad (3.7)$$

The result as stated applies only to  $f_\gamma(x, y)$ , which is homogeneous of degree  $\gamma$ . A natural extension to

$$F(x, y) = f_\gamma(x, y)g(x, y),$$

where  $g$  is regular in  $\square$ , follows by expanding  $g(x, y)$  as a Taylor series about the origin and noting that each term  $f_\gamma(x, y)g^{(r,s)}(0, 0)x^r y^s / r!s!$  is itself homogeneous of degree  $\gamma + r + s$ , and so the theorem applies also to this term in its own right. Taking care to handle the remainder term properly, we are led to an expansion of the form

$$Q^{(m)}(\triangle)[F] - I(\Delta)[F] \simeq \sum_{j=0}^d \frac{A_{2+\gamma+j}}{m^{2+\gamma+j}} + \sum_{j=0}^d \frac{C_{2+\gamma+j} \ln m}{m^{2+\gamma+j}} + \sum_{s=1}^d \frac{B_s}{m^s}.$$

Sidi's result for  $F(x, y) = x^{\gamma+1} \ln x g(x, y)$  [Sid83] has the same form as this.

A standard result from classical analysis allows differentiation of any asymptotic expansion with respect to an incidental parameter so long as the coefficients are differentiable. The proof (not given here) of Theorem 3.1 above indicates that the coefficients are analytic functions of  $\gamma$  in any region not including integer  $\gamma$ .

Setting  $\Phi(x) = \frac{\partial}{\partial \gamma} f_\gamma(x, y) = f_\gamma(x, y) \ln f_\gamma(x, y)$ , we find

$$Q^{(m)}(\triangle)[\Phi] - I(\Delta)[\Phi] \simeq \frac{\partial A_{2+\gamma} / \partial \gamma}{m^{2+\gamma}} - \frac{A_{2+\gamma} \ln m}{m^{2+\gamma}} + \sum_{s=1}^d \frac{\partial B_s / \partial \gamma}{m^s}, \quad \gamma \notin \mathbb{Z}, \quad (3.8)$$

where  $A_{2+\gamma}$  and  $B_s$  are the coefficients in (3.5). In the case that  $\gamma \in \mathbb{Z}$ , a serious calculation is required. This yields an expansion of the same form as one would have obtained if one had ignored the fact that the coefficients are discontinuous. This effect is to include in (3.8) an additional term in  $(\ln m)^2 m^{-(2+\gamma)}$ .

Several generalizations of this result extend or alter the singularity structure of the integrand in a way that is quite infeasible for Gaussian quadrature. For example, let

$$\Phi(x, y) = (f_1(x, y) + f_2(x, y) + f_3(x, y))g(x, y),$$

where  $f_1$  and  $f_2$  are homogeneous of degree  $\gamma_1$  and  $\gamma_2$  about the origin and  $f_3$  is homogeneous of degree  $\gamma_3$  about another vertex. Then the expansion for  $Q(\triangle)[\Phi] - I(\Delta)[\Phi]$  is simply a concatenation of three expansions, each having the same form. The justification for concatenating the first two is obvious. We have to appeal to the Darboux theorem to establish the theoretical basis for including the third; see [LM80].

Another generalisation is established in [Lyn92]. One may apply the same expansion to any differently shaped triangle so long as it has the same singular behavior at the vertex. The point here is that an affine transformation, besides transforming the triangle, transforms the singularity. In the case of GQ, this means that one must start anew to calculate a rule. However, a singularity of homogeneous degree  $\gamma$  is transformed into another of the same

degree; and if the technique depends only on this degree, then it is invariant under the transformation. We consider this to be perhaps the most important attribute of EQ.

Recently, in the case of the square, an expansion has been developed for the full corner singularity [LdD93, VH93]

$$F(x, y) = x^\lambda y^\mu f_\gamma(x, y)g(x, y).$$

It is beyond the scope of this article to pursue this further. The situation seems to be that for many algebraic or logarithmic singularities that occur at a vertex or along a side, an extrapolation expansion exists.

## References

[LdD93], [LM80], [Lyn76], [Lyn92], [Sid83], [VH93]

## 4 Concluding Remarks

The prevailing situation for regular integrands seems to be qualitatively different from that for singular integrands.

For regular integrands, so far as rules of specified polynomial degree are concerned, recent progress has been less than spectacular. Fifty years ago, what are now called conical product rules were available, allowing a result of polynomial degree  $d$  based on  $(d + 1)^2/4$  function values. Present theory reveals that the minimal formulas require more than half this number; these formulas are available only up to  $d = 8$ . The intermediate  $\mathcal{D}_3$  formulas, using approximately  $(d + 1)^2/6$ , are available up to  $d = 20$ . The general development of extrapolation quadrature (a set of methods based on Richardson's deferred approach to the limit) has been slow. The theory is complicated. Many variant and potentially interesting formulas exist; but so far as polynomial degree is concerned, the number of points required increases at best like  $d^3/48$ .

For singular integrands, the situation is not the same. Gaussian rules of specified polynomial degree are difficult to construct, and very few are available in the literature. Compounding this scarcity is the circumstance that with the same weighting function, a different rule is required for each differently shaped triangle. On the other hand, progress on extrapolation quadrature for singular integrands has been significant and a wide class of algebraic and logarithmic singularities is now within the reach of this theory. Moreover, for these, while possibly expensive, the integration can be carried out effectively in an iterative manner without the need for tables of weights and abscissas. The theory is to a significant extent independent of the shape of the triangle.

However, different parts of the theory are connected and may be useful in a single application. For example, suppose one requires a Gaussian formula for an integrand function having an extensive but known singularity structure of the type encountered in Section 3.3. To construct any Gaussian formula, one needs accurate numerical values of the moments.

These might be determined by using extrapolation based on expansions of Section 3.3, using for  $Q$  one of the minimal formulas of Section 2.2. In this context, one might bear in mind that the expansions of Section 3.3 require, in their proof, the expansions of Section 2.3. The reader may find the description above somewhat artificial and self-serving. However, calculations of this general nature are habitually used to construct special finite elements. Thus, all four principal parts of the theory may be said to have contributed to this application in a cooperative manner.

The ever-present problem of constructing minimal formulas remains, and we are convinced that the more courageous and idealistic of us will continue to find the time to face this daunting set of successively harder challenges. We are particularly gratified that these formulas have found a role, albeit minor, in the related area of extrapolation quadrature.

The scope of this article has been limited to a review of the theory of integration over the triangle. We refer the reader interested in the important application to adaptive quadrature over the triangle to [HK85] and to [Kea92]. In [Lyn83], he will find a somewhat dated but detailed practical guide to handling applications. In [Sid79] a general framework is presented for all sorts of extrapolation, linear and nonlinear. The cogent problems of convergence and stability in extrapolation are treated in [Sid90]. A useful list of references about cubature over all standard regions has recently appeared in [CR93]. This provides a welcome update to the reference list contained in the standard works on this topic, namely, [Str71, Mys81]. Some very recent work in integration over curved surfaces and in the integration of expressions containing derivatives is not treated here. Our hope is that this synopsis of the theory, with its linked bibliography, will be helpful to individuals interested in further research in this and related areas.

## References

[CR93], [HK85] [Kea92], [Lyn83], [Mys81], [Sid79], [Sid90], [Str71]

## References

- [BE90] J. Berntsen and T.O. Espelid. Degree 13 symmetric quadrature rules for the triangle. Reports in Informatics 44, Dept. of Informatics, University of Bergen. 1990.
- [Bec87] T. Becker. *Konstruktion von interpolatorischen Kubaturformeln mit Anwendungen in der Finit-Element-Methode*. Ph.D. thesis, Technische Hochschule Darmstadt, 1987.
- [BS92] H. Berens and H.J. Schmid. On the number of nodes of odd degree cubature formulae for integrals with Jacobi weights on a simplex. In T.O. Espelid and A. Genz, editors, *Numerical Integration - Recent Developments, Software and Applications*, volume 357 of *NATO ASI Series C: Math. and Phys. Sciences*, pages 37-44, Dordrecht, 1992. Kluwer Academic Publishers.

- [CH87] R. Cools and A. Haegemans. Construction of minimal cubature formulae for the square and the triangle using invariant theory. Report TW 96, Dept. of Computer Science, K.U. Leuven, 1987.
- [CH88a] R. Cools and A. Haegemans. An embedded pair of cubature formulae of degree 5 and 7 for the triangle. *BIT*, 28:357–359, 1988.
- [CH88b] R. Cools and A. Haegemans. Why do so many cubature formulae have so many positive weights? *BIT*, 28:792–802, 1988.
- [CH90] R. Cools and A. Haegemans. A lower bound for the number of function evaluations in an error estimate for numerical integration. *Constr. Approx.*, 6:353–361, 1990.
- [CL78] M. Critescu and G. Loubignac. Gaussian quadrature formulas for functions with singularities in  $1/r$  over triangles and quadrangles. In C.A. Brebbia, editor, *Recent Advances in Boundary Element Methods*. Pentech. Press, 1978.
- [Cow73] G.R. Cowper. Gaussian quadrature formulas for triangles. *Internat. J. Numer. Methods Engrg.*, 7:405–408, 1973.
- [CR93] R. Cools and P. Rabinowitz. Monomial cubature rules since “Stroud”: A compilation. *J. Comput. Appl. Math.*, 48:309–326, 1993.
- [dD79] E. de Doncker. New Euler Maciaurin Expansions and Their Application to Quadrature Over the s-Dimensional Simplex. *Math. Comp.*, 33:1003–1018, 1979.
- [DR84] P.J. Davis and P. Rabinowitz. *Methods of Numerical Integration*. Academic Press, London, 1984.
- [Duf82] M.G. Duffy. Quadrature over a pyramid or cube of integrands with a singularity at a vertex. *SIAM J. Numer. Anal.*, 19:1260–1262, 1982.
- [Dun85] D.A. Dunavant. High degree efficient symmetrical Gaussian quadrature rules for the triangle. *Internat. J. Numer. Methods Engrg.*, 21:1129–1148, 1985.
- [Eng70] H. Engels. Über gleichgewichtete Kubaturformeln für ein Dreiecksgebiet. *Elek. Daten.*, 12:535–539, 1970.
- [Eng80] H. Engels. *Numerical Quadrature and Cubature*. Academic Press, London, 1980.
- [Fra71] R. Franke. Obtaining cubatures for rectangles and other planar regions by using orthogonal polynomials. *Math. Comp.*, 25:803–813, 1971.
- [Gat88] K. Gatermann. The construction of symmetric cubature formulas for the square and the triangle. *Computing*, 40:229–240, 1988.
- [Gat90] K. Gatermann. Gruppentheoretische Konstruktion von symmetrischen Kubaturformeln. Technical Report TR 90-1, Konrad-Zuse-Zentrum für Informationstechnik Berlin. 1990.

- [Gat92] K. Gatermann. Linear representations of finite groups and the ideal theoretical construction of  $G$ -invariant cubature formulas. In T.O. Espelid and A. Genz, editors, *Numerical Integration - Recent Developments, Software and Applications*, volume 357 of *NATO ASI Series C: Math. and Phys. Sciences*, pages 25-35. Dordrecht, 1992. Kluwer Academic Publishers.
- [GM78] A. Grundmann and H.M. Möller. Invariant integration formulas for the  $n$ -simplex by combinatorial methods. *SIAM J. Numer. Anal.*, 15:282-290, 1978.
- [Gün75] C. Günther. Zweidimensionale Quadraturformeln vom Grad 7 mit 14 Punkten. *Numer. Math.*, 24:309-316, 1975.
- [Hae93] A. Haegemans. Cubature formulas for triangles and squares with a  $1/r$  singularity. Report TW 192, Dept. of Computer Science, K.U. Leuven, 1993.
- [Hem73] P.W. Hemker. A sequence of nested cubature rules. NW 3/73, Stichting mathematisch centrum, 1973.
- [Hil77] P. Hillion. Numerical integration on a triangle. *Internat. J. Numer. Methods Engrg.*, 11:797-815, 1977.
- [HK85] M. Hollosi and P. Keast. Numerical integration of singular functions over a triangle. Technical Report 1985CS-3, Computing Science Division, Dalhousie University, 1985.
- [HMS56] P.C. Hammer, O.J. Marlowe, and A.H. Stroud. Numerical integration over simplexes and cones. *Math. Tables Aids Comput.*, 10:130-137, 1956.
- [HS56] P.C. Hammer and A.H. Stroud. Numerical integration over simplexes. *Math. Tables Aids Comput.*, 10:137-139, 1956.
- [Kea92] P. Keast. Software for integration over triangles and general simplices. In T.O. Espelid and A. Genz, editors, *Numerical Integration - Recent Developments, Software and Applications*, volume 357 of *NATO ASI Series C: Math. and Phys. Sciences*, pages 283-294, Dordrecht, 1992. Kluwer Academic Publishers.
- [Lau55] R. Lauffer. Interpolation mehrfacher Integrale. *Arch. Math.*, 6:159-164, 1955.
- [Lau82] D.P. Laurie. CUBTRI - automatic cubature over a triangle. *ACM Trans. Math. Software*, 8:210-218, 1982.
- [LdD93] J.N. Lyness and E. de Doncker. Quadrature error expansions. II. The full corner singularity. *Numer. Math.*, 64:355-370, 1993.
- [LG78] M.E. Laursen and M. Gellert. Some criteria for numerically integrated matrices and quadrature formulas for triangles. *Internat. J. Numer. Methods Engrg.*, 12:67-76, 1978.
- [LG82] J.N. Lyness and L. Gatteschi. A note on cubature over a triangle of a function having specified singularities. In G. Hämmerlin, editor, *Numerical Integration*, volume 57 of *ISNM*, pages 164-169, Basel, 1982. Birkhäuser Verlag.



- [LJ75] J.N. Lyness and D. Jespersen. Moderate degree symmetric quadrature rules for the triangle. *J. Inst. Math. Appl.*, 15:19–32, 1975.
- [LM70] J.N. Lyness and B.J.J. McHugh. On the remainder term in the  $N$ -dimensional Euler-Maclaurin expansion. *Numer. Math.*, 15:333–344, 1970.
- [LM80] J.N. Lyness and G. Monegato. Quadrature error functional expansion for the simplex when the integrand has singularities at vertices. *Math. Comp.*, 34:213–225, 1980.
- [LP73] J.N. Lyness and K.K. Puri. The Euler-Maclaurin expansion for the simplex. *Math. Comp.*, 27:273–293, 1973.
- [Lyn76] J.N. Lyness. An error functional expansion for  $N$ -dimensional quadrature with an integrand function singular at a point. *Math. Comp.*, 30:1–23, 1976.
- [Lyn78] J.N. Lyness. Quadrature over a simplex. *SIAM J. Numer. Anal.*, 15:122–133 and 870–877, 1978.
- [Lyn83] J.N. Lyness. QUG2 - integration over a triangle. ANL/MCS-TM- 13, Mathematics and Computer Science Division, Argonne National Laboratory, 1983.
- [Lyn92] J.N. Lyness. On handling singularities in finite elements. In T.O. Espelid and A. Genz, editors, *Numerical Integration - Recent Developments, Software and Applications*, volume 357 of *NATO ASI Series C: Math. and Phys. Sciences*, pages 219–233, Dordrecht, 1992. Kluwer Academic Publishers.
- [Moa74] T. Moan. Experiences with orthogonal polynomials and “best” numerical integration formulas on a triangle; with particular reference to finite element approximations. *ZAMM*, 54:501–508, 1974.
- [Möl73] H.M. Möller. *Polynomideale und Kubaturformeln*. Ph.D. thesis, Universität Dortmund, 1973.
- [Möl76] H.M. Möller. Kubaturformeln mit minimaler Knotenzahl. *Numer. Math.*, 25:185–200, 1976.
- [Mys68] I.P. Mysovskikh. On the construction of cubature formulas with fewest nodes. *Dokl. Akad. Nauk SSSR*, 178, 1968, (Russian). *Soviet Math. Dokl.* 9: 277–280, 1968 (English).
- [Mys81] I.P. Mysovskikh. *Interpolatory Cubature Formulas*. Ized. ‘Nauka’, Moscow-Leningrad, 1981. (Russian).
- [PFB81] H.L.G. Pina, J.L.M. Fernandes, and C.A. Brebbia. Some numerical integration formulae over triangles and squares with a  $1/r$  singularity. *Appl. Math. Modelling*, 5:209–211, 1981.
- [Rad48] J. Radon. Zur mechanischen Kubatur. *Monatsh. Math.*, 52:286–300, 1948.

- [Ras83a] G.G. Rasputin. On the construction of cubature formulas containing preassigned knots. *Metody Vychisl.*, 13:122–128, 1983, (Russian).
- [Ras83b] G.G. Rasputin. On the question of numerical characteristics for orthogonal polynomials of two variables. *Metody Vychisl.*, 13:145–154, 1983, (Russian).
- [Ras86] G.G. Rasputin. Construction of cubature formulas containing preassigned nodes. *Izv. Vyssh. Uchebn. Zaved. Mat.*, 11:44–51, 1986, (Russian). *Soviet Math. (Iz. VUZ)* 30: 58–67, 1986 (English).
- [Ric27] L.F. Richardson. The deferred approach to the limit. *Trans. Phil. Roy. Soc.*, 226:261–299, 1927.
- [Rom55] W. Romberg. Vereinfachte numerische Integration. *Norske Vid. Selsk. Forh. (Trondheim)*, 28:30–36, 1955.
- [Sch83] H.J. Schmid. Interpolatorische Kubaturformeln. *Dissertationes Math.*, CCXX, 1983.
- [SF73] G. Strang and G.J. Fix. *An Analysis of the Finite Element Method*. Series in Automatic Computation. Prentice-Hall, London, 1973.
- [Sid79] A. Sidi. Some properties of a generalization of the Richardson extrapolation process. *J. Inst. Math. Applics.*, 24:327–346, 1979.
- [Sid83] A. Sidi. Euler-Maclaurin expansions for integrals over triangles and squares of functions having algebraic/logarithmic singularities along an edge. *J. Approx. Theory*, 39:39–53, 1983.
- [Sid90] A. Sidi. On a generalization of the Richardson extrapolation process. *Numer. Math.*, 57:365–377, 1990.
- [Sil70] P. Silvester. Symmetric quadrature formulae for simplexes. *Math. Comp.*, 24:95–100, 1970.
- [Sob62] S.L. Sobolev. Cubature formulas on the sphere invariant under finite groups of rotations. *Dokl. Akad. Nauk SSSR*, 146:310–313, 1962, (Russian). *Soviet Math. Dokl.* 3: 1307–1310, 1962 (English).
- [SS66] A.H. Stroud and D. Secrest. *Gaussian Quadrature Formulas*. Prentice-Hall, Englewood Cliffs, N.J., 1966.
- [Str60] A.H. Stroud. Quadrature methods for functions of more than one variable. *New York Acad. Sci.*, 86:776–791, 1960.
- [Str61] A.H. Stroud. Numerical integration formulas of degree 3 for product regions and cones. *Math. Comp.*, 15:143–150, 1961.
- [Str64] A.H. Stroud. Approximate integration formulas of degree 3 for simplexes. *Math. Comp.*, 18:590–597, 1964.

- [Str66] A.H. Stroud. Some approximate integration formulas of degree 3 for an  $n$ -dimensional simplex. *Numer. Math.*, 9:38–45, 1966.
- [Str69] A.H. Stroud. A fifth degree integration formula for the  $n$ -simplex. *SIAM J. Numer. Anal.*, 6:90–98, 1969.
- [Str71] A.H. Stroud. *Approximate calculation of multiple integrals*. Prentice-Hall, Englewood Cliffs, N.J., 1971.
- [VH93] P. Verlinden and A. Haegemans. An error expansion for cubature with an integrand with homogeneous boundary singularities. *Numer. Math.*, 65:383–406, 1993.

Mathematics and Computer Science Division, Argonne National Laboratory,  
9700 South Cass Avenue, Argonne, IL 60439, U.S.A.  
*E-mail address:* lyness@mcs.anl.gov

Department of Computer Science, Katholieke Universiteit Leuven,  
Celestijnenlaan 200A, B-3001, Heverlee, Belgium  
*E-mail address:* ronald.cools@cs.kuleuven.ac.be

#### DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

**DATE  
FILMED**

3 / 23 / 94

**END**

