An Encyclopaedia of Cubature Formulas [1]

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In memory of Arthur H. Stroud
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Abstract

About 13 years ago we started collecting published cubature formulas for the approximation of multivariate integrals over some standard regions. In this paper we describe how we make this information available to a larger audience via the World Wide Web.

1 Prologue

About three decades ago, Arthur H. Stroud published his encyclopedic work on multiple numerical integration, Approximate Calculation of Multiple Integrals [10]. In this book, Stroud presented a complete summary of the theoretical and practical aspects of multiple numerical integration, a comprehensive bibliography and a listing of almost all *multiple integration rules* (also called *cubature rules* or *cubature formulas*) known at that time for a variety of regions. A similar work was published by Mysovskikh [8] about two decades ago. Both books have proved useful to workers in the field and most papers concerned with multiple numerical integration refer to at least one of these books.

In 1993, Cools and Rabinowitz [5] published a paper, continuing the work of Stroud in one specific area, namely the compilation of all so-called *monomial cubature rules* which appeared since the publication of [10]. The paper [5] does not contain any table with points and weights of cubature formulas, but only references to about 100 papers. This work, and its sequel published in 1999 [4], is well known among people working in the area. It is however not well known to people who need cubature formulas to solve their particular problem. Furthermore, results that appear in the (e.g.) numerical analysis literature are not very accessible for (e.g.) physicists. And as time goes by, these results become less and less accessible. The fact that they are scattered around in more than 100 publications only increases the problem.

A similar situation arises in many fields and modern technology such as the World Wide Web creates opportunities to make results available easier for a broader audience. The Handbook of Mathematical Functions [1] contains only a few pages with cubature rules, including Radon's cubature rule of degree 5 with 7 points [9]. This probably explains the widespread use of Radon's rule.

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The Digital Mathematical Library is a large project aiming at developing a new (digital) version of the widespread Handbook of Mathematical Functions. (See [6] and `http://dlmf.nist.gov/` for more about this project.) It is not expected to include tables of cubature rules however and there is room and need for another initiative in this specialised area. This article describes our initiative in this area, but first we give some background.

2 Background on cubature formulas

In our encyclopaedia we consider various approximations of an integral

$$I[f] := \int_\Omega w(\mathbf{x}) f(\mathbf{x}) \mathsf{d}\mathbf{x}$$

where $\Omega \subset \mathrm{I\!R}^n$, $I[1] < \infty$ and $w(\mathbf{x}) \geq 0$, $\forall \mathbf{x} \in \mathrm{I\!R}^n$, $n \geq 2$, by *cubature formulas* of the form

$$Q[f] := \sum_{j=1}^{N} w_j f(\mathbf{y}^{(j)})$$

with $w_j \in \mathrm{I\!R}$ and $\mathbf{y}^{(j)} \in \mathrm{I\!R}^n$. If the remainder R in

$$I[f] = Q[f] + R[f]$$

has the property that $R[f] = 0$ if f is an arbitrary linear combination of algebraic monomials of the form

$$\prod_{j=1}^{n} x_j^{i_j} \quad \text{with} \quad \sum_{j=1}^{n} i_j \leq d \tag{1}$$

and $R[f] \neq 0$ for some such monomial with $\sum_{j=1}^{n} i_j = d + 1$ then the cubature formula is said to have *degree d*. The monomials (1) form a basis for the vector space of all polynomials in n variables of degree at most d, denoted by $\mathcal{P}_d^n$. In the encyclopaedia we only consider basic cubature rules (as opposed to composite cubature rules) with a relatively low number of points N to achieve a certain degree d.

The minimal number of points N^* needed by a cubature formula to achieve a certain degree d, does not only depend on this degree and the dimension, but also on the shape of the region and the weight function:

$$N^* := F(n, d, \Omega, w(.)).$$

The major problem is that in general this function F is not known! In virtually all cases lower and upper bounds are known, and occasionally a cubature formula is known that attains the lower bound. The current status on lower bounds and known minimal formulas is presented in [3].

The N points and weights of a cubature formula of degree d are a solution of a system of polynomial equations

$$\sum_{j=1}^{N} w_j f_k(\mathbf{y}^{(j)}) = I[f_k] \ , \quad k = 1, \ldots, \dim \mathcal{P}_d^n$$

where the f_k form a basis for $\mathcal{P}_d^n$, e.g., the monomial basis (1). This system is fully determined if the region and weight function are given and N and d are fixed. Observe that the number of equations in this system ($= \dim \mathcal{P}_d^n$) is not necessarily equal to the number of unknowns ($= N(d+1)$). Furthermore this system becomes very large for increasing N and d.

Only in rare cases the monomial basis (1) is used as the basis for the calculation. Many known cubature formulas have a symmetry corresponding to the symmetry of the region. In most cases this symmetry was introduced while searching for them, to simplify their construction. Imposing symmetry on a cubature formula indeed reduces the number of free parameters in the problem. The disadvantage is that such a cubature formula cannot be expected to have the lowest possible number of points. In general we need a basis for the space of polynomials invariant with respect to the symmetry group under consideration, see [3] §5 and §10 for details.

3 Towards an encyclopaedia of cubature formulas

3.1 The pre-electronic era

The compilation of cubature formulas presented in [5] was restricted to the following regions:

C_n: the n-dimensional cube (hypercube)

$$\Omega := \{(x_1, \ldots, x_n) : -1 \le x_i \le 1, i = 1, \ldots, n\}$$

with weight function $w(\mathbf{x}) := 1$,

S_n: the hypersphere (n-dimensional ball)

$$\Omega := \left\{ (x_1, \ldots, x_n) : \sum_{j=1}^{n} x_i^2 \le 1 \right\}$$

with weight function $w(\mathbf{x}) := 1$,

T_n: the n-dimensional simplex

$$\Omega := \left\{ (x_1, \ldots, x_n) : \sum_{j=1}^{n} x_i \le 1 \text{ and } x_i \ge 0, i = 1, \ldots, n \right\}$$

with weight function $w(\mathbf{x}) := 1$,

$E_n^{r^2}$: the entire n-dimensional space $\Omega := \mathbb{R}^n$ with weight function

$$w(\mathbf{x}) := e^{-r^2} \quad \text{with} \quad r^2 := \sum_{j=1}^{n} x_j^2,$$

E_n^r: the entire n-dimensional space $\Omega := \mathbb{R}^n$ with weight function

$$w(\mathbf{x}) := e^{-r}.$$

In his book, Stroud [10] included cubature formulas for several regions that were not treated in [5, 4]: the hexagon, the octahedron, the cubical and spherical shell, parabolic regions, cones, torus, pyramid and last but not least, the surface of the sphere.

A cubature formula of a certain degree for a finite region and constant weight function preserves its degree after an affine transformation. Different cubature formulas constructors prefer, e.g., different cubes ($[0,1]^n$ or $[-1,1]^n$) and triangles (T_2 or an equilateral triangle). Also the symmetries of the region and the cubature formula play a role. A different cubature formula for the same region can be obtained by an isometry. For example, a cubature formula for the square can be transformed into a possibly different formula by rotating all points through an angle $\pi/2$. We do not distinguish between geometrically equivalent cubature formulas.

In [5] individual tables are given with information about cubature formulas for the following regions of particular dimension: C_n, T_n, $n = 2,3,4$; S_n, E_n^r, $n = 2,3$; $E_n^{r^2}$, $n = 2,3,5$; and one additional table for C_n, S_n, T_n and $E_n^{r^2}$ of general dimension. In most cases, a separate table of embedded sequences of cubature rules was added.

In the tables in [5] a reference to the first article or book that includes a cubature formula is given. If a formula appears in several publications, in principle all of them are listed. In addition to references some information about each cubature formula is given: its degree d, the corresponding number of integration points N, and a quality indicator giving some information about the location of the points and the sign of the weights. A $*$ is added to N for each cubature formula that is known to use the lowest possible number of points. A reference to Stroud's book [10] is included only to avoid gaps in the tables.

In December 1999 an updated version of [5], containing new results and some corrections, was published in [4].

3.2 The electronic era

In 1997 we started to make the tables with references available on the World Wide Web. In a window which resembles Figure 1, a visitor of our web site can select a region. Selecting, e.g., triangle will show something like Figure 2. The abbreviated reference is a hyperlink to the full reference, shown in a sub-window below.

The added value, apart from its better availability, was initially very limited. All cubature formulas included in [10] were added to the tables and some Javascript was added so that users could see the number of points used by a cubature formula derived for general dimensions, for a user-specified dimension. The online-encyclopaedia of cubature formulas was born.

Since then, two features were added:

1. Most of the references now contain hyperlinks to a small index card with information about each author. (This helps visitors to contact the authors.)

2. For many cubature formulas, the points and weights are electronically

Figure 1: Overview of available tables

Tables

- Cubature formulas for the cube

square cube four-cube n-cube

- Cubature formulas for the sphere

circle sphere four-sphere n-sphere

- Cubature formulas for the space with weight function $\exp(-r^2)$

plane space four-space five-space n-space

- Cubature formulas for the space with weight function $\exp(-r)$

plane space four-space n-space

- Cubature formulas for the simplex

triangle tetrahedron four-simplex five-simplex n-simplex

available. (Visitors to these web pages started to ask for copies of some of the articles, because they did not have easy access to them.)

We did not want to copy all points and weights manually from the original publications. That could increase the number of errors! The convenient solution to this problem was that all cubature rules must be recomputed and files must be computer-generated.

This implies a validation of the published results. Published results indeed require validation. Several types of errors can occur. Misprints are the most prevalent. Even Stroud's book [10] contains some of this; some are listed in Table 1. In addition, one has to fear inaccurate results, i.e., not all published digits are necessarily correct. Furthermore, some published results are simply wrong, e.g., because the authors solved the wrong system of nonlinear equations.

Solving a system of nonlinear (polynomial) equations related to cubature formulas is a non trivial problem. For recomputing, the published results are however very suitable since they can be used as starting values for an iterative zero-finder.

Our codes were developed in Fortran 90. The iterative zero-finder is based on HYBRJ1 from MINPACK [7]. One of the advantages of Fortran 90 is that one can overload operators. With a package available that overloads the basic arithmetic operators by their multi-precision analogue [2], it becomes almost trivial to write the code that does all its computations in extended precision. This is also very helpful to monitor quadratic convergence of the iterative zero-finder.

Figure 2: Screenview: top part of the table for T_2

Cubature formulae for the triangle

Degree	N	Quality	References
1	1	PI	[str71]
	3	PB	[str71]
2	3*	PB	[str71]
		PI	[str71]
		PI	[hil77]
		PI	[hil77]
		PB	[hil77]
	4	EI	[eng70a][eng80]
		EI	[hil77]
		NB	[dd79]
	6	PB	[str71]
3	4*	NI	[str71]
		PI	[hil77]
		PI	[hil77]
	5	EI	[eng70a][eng80]
		PI	[hil77]

References

This window will jump to the reference of your interest.

Because we aim at computer generated files, we had to specify the file structure. Each cubature formula has a separate file for each of the offered precisions. At the moment each cubature formula is available in two precisions: 16 and 32 correct digits. Each file consists of 3 parts, illustrated in Figure 3 by Radon's cubature formula for C_2 [9]:

1. The first part contains the description of the cubature formula: region, dimension, degree, number of points and a description of its symmetry. This is the information needed to set up the system of equations. This part is not changed by our program.

2. The second part can contain background information. It can contain, e.g., historical notes, a picture of the location of the zeros, the orthogonal polynomials that vanish in the points of the cubature formula. This part is ignored by the program.

3. The third part contains the points and weights. On input these are the starting values. On output these are the recomputed values. Actually not all points are listed but only generators of the different orbits involved.

Figure 3: Screenview: cubature formula of degree 5 with 7 points for C_2

Region: Cube
Dimension: 2
Degree: 5
Points: 7
Structure: Symmetric
Rule struct: 1 1 0 1

Orthogonal polynomials
The points are the common zeros of the orthogonal polynomials
$p_0 = p_{3,0}$
$p_1 = p_{3,2}$
$p_2 = p_{3,1} + p_{3,3}$
where
$p_{3,0} = x^3 - (3/5)x$
$p_{3,1} = x^2y - (1/3)y$
$p_{3,2} = xy^2 - (1/3)x$
$p_{3,3} = y^3 - (3/5)y$

```
Generator: [ Origin ]
( 0., 0., )
Corresponding weight:
1.1428571428571428,

Generator: [ Central symmetry ]
( 0.96609178307929590, 0., )
Corresponding weight:
0.31746031746031746,

Generator: [ Rectangular symmetry ]
( 0.57735026918962576, 0.77459666924148337, )
Corresponding weight:
0.55555555555555555,
```

Table 1: Misprints in points or weights listed in [10]

Region	number	wrong	correct
C_n	3-1	$r_{i,n} = \frac{(-1)i}{\sqrt{3}}$	$\frac{(-1)^i}{\sqrt{3}}$
C_2	3-1	$(\pm r, \pm r)$	$(\pm\sqrt{r}, \pm\sqrt{r})$
C_2	7-3	$\frac{31}{649}$	$\frac{31}{648}$
S_2	5-1	$(\pm s, t)$	$(\pm s, \pm t)$
U_n	7-1	$(t, t, t, \ldots, t)_{FS}$	$(t, t, 0, \ldots, 0)_{FS}$
T_n	3-6	$(r, s, t, \ldots, t; t)$	$(r, \ldots, r, s; t)$
E_3^r	7-1	$D = \frac{4239+373\sqrt{130}}{917568}V$	$D = \frac{4239+373\sqrt{130}}{197568}V$

The relation between a generator and a set of points is explained in the online documentation as part of a detailed description of the file structure.

For each cubature formula, a file must be created containing a complete description in the first part and the published points and weights in the third part. The program takes this file and replaces it with a file with the recomputed formula with as many correct digits as specified. It must be verified that the iterative zero-finder converges to the published cubature formula.

4 Epilogue

Arthur H. Stroud is best known in the numerical analysis community for his books on quadrature [11] and on cubature [10]. His death in 1998 was not noticed in our community. The above mentioned books are both encyclopedic but now out of date, both in their presentation and contents. The project described in this paper is a simple continuation of what Stroud started, adapted to the current state of technology.

In some aspects this project it still in its infancy, but in other aspects it is very mature. To our knowledge the overview tables of known cubature formulas are presently complete, and we commit ourselves to keep them up to date. This project can be continued in several directions. Comments and suggestions from the users are very welcome. What is currently available in our encyclopaedia may be useful for many people. At the moment access is free through `www.cs.kuleuven.ac.be/~nines/ecf/`.

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