The state of the art of constructing cubature formulas for multi-variate integrals

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1 Introduction

Given is an integral

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

where $\Omega \subset \mathbb{R}^d$ and $w(x) \geq 0$, $\forall x \in \mathbb{R}^d$.

Search an approximation for $I[f]$

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

with $w_j \in \mathbb{R}$ and $y^{(j)} \in \mathbb{R}^d$.

Webster:
quadrature: the process of finding a square equal in area to a given area.
cubature: the determination of cubic contents.

If $d = 1$ then Q is called a *quadrature formula*.
If $d \geq 2$ then Q is called a *cubature formula*.

Cubature/quadrature formulas are basic integration rules

$\rightarrow$ choose points $y^{(j)}$ and weights w_j independent of integrand f.

$\longrightarrow$ building blocks in many application

and the main topic of this talk.

How should points and weights be chosen?

There are several popular criteria

All demand that

$$I[1] = Q[1].$$

Two major classes:

1. polynomial based methods
   incl. methods exact for algebraic polynomials

2. number theoretic methods
   incl. Monte Carlo and quasi-Monte Carlo methods

Not the topic of this talk...

Repeated quadrature

Given a quadrature rule of degree d

$$\int_0^1 f(x)\mathsf{d}x \approx \sum_{i=1}^{n} w_i f(x_i).$$

Calculate an approximation of the form

$$Q[f] = \sum_{i=1}^{n}\sum_{j=1}^{n} w_i w_j f(x_i, x_j).$$

This is a cubature rule of degree d for

$$\int_0^1 \int_0^1 f(x,y)\mathsf{d}x\mathsf{d}y.$$

Not the topic of this talk...

Copy rules and extrapolation

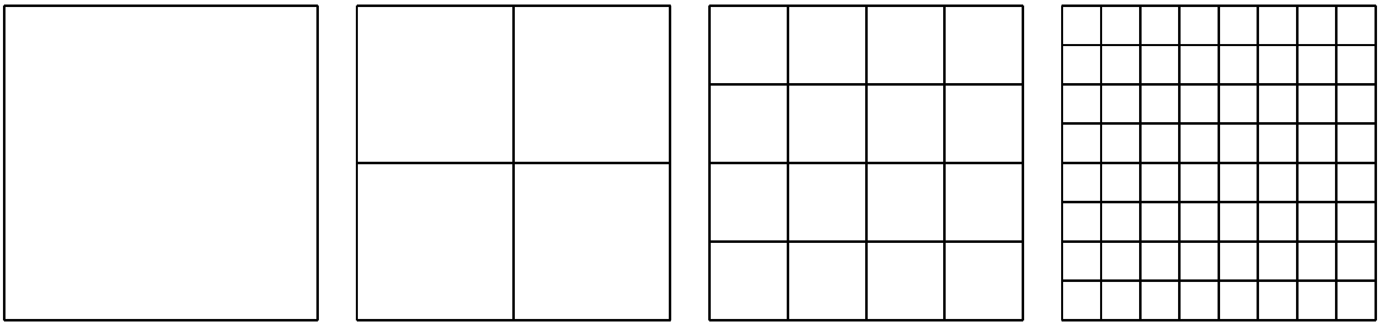
1927: Richardson proposed his deferred approach to the limit.

1955: Romberg integration.

196*: extrapolation used for $\square$

197*: extrapolation used for ◺

$Q^{(m)} := m^2$-copy of Q = divide $\square$ into m^2 small, identical $\square$ s, each of side $1/m$ and apply a properly scaled version of Q to each.



For regular $f(x,y)$, extrapolation is based on the two-dimensional version of the Euler-Maclaurin expansion:

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

This is generalised to singular integrals and other regions.

E.g. $\triangle$:

From a basic result by Lyness & Monegato (1980) follows:

Theorem 1.1 *Let $f_\gamma(x,y)$ be homogeneous of degree γ 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 and g is regular in $\square$.*
Let

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

Then

$$Q^{(m)}(\triangle)[F] - I(\triangle)[F]$$

$$\simeq \sum_{j=0} \frac{A_{2+\gamma+j}}{m^{2+\gamma+j}} + \sum_{j=0} \frac{C_{2+\gamma+j} \ln m}{m^{2+\gamma+j}} + \sum_{s=1} \frac{B_s}{m^s}.$$

Generalisations by
Sidi (1983), Lyness (1992),
Lyness & De Doncker (1993), Verlinden & Haegemans (1993).

2 Polynomial-based methods

Basic criterion = **algebraic degree**

A cubature formula has **algebraic degree** m if it is exact for all polynomials of degree at most m, i.e., $\in \mathcal{P}_m^d$.

The definition of degree is equivalent with

$$Q[f_j] = I[f_j]\ ,\quad j = 1, 2, \ldots, \dim \mathcal{P}_m^d \tag{1}$$

where the f_j form a basis for $\mathcal{P}_m^d$.

If f_j and N are fixed, then (1) form a system of nonlinear equations

$$\sum_{i=1}^{N} w_i f_j(y^{(i)}) = I[f_j]\ ,\quad j = 1, 2, \ldots, \dim \mathcal{P}_m^d. \tag{2}$$

Each equation in (2) is a polynomial equation.
Each point introduces $d + 1$ unknowns.

$\Rightarrow$ A cubature formula of degree (at least) m with N points is determined by $\dim \mathcal{P}_m^d$ nonlinear equations in $N(d + 1)$ unknowns.

One can distinguish between 2 approaches to construct cubature formulas:

1. solve the system of nonlinear equations

$$\sum_{i=1}^{N} w_i f_j(y^{(i)}) = I[f_j] \ , \quad j = 1, 2, \ldots, \dim \mathcal{P}_m^d .$$

   directly
   → **invariant theoretical approach**

2. search for polynomials that vanish at the points of the formula
   → **ideal theoretical approach**.

This 2nd approach has been very successful in quadrature. In cubature, it has turned out to be difficult for □ , significantly more difficult for ◺ and even more difficult for $n > 2$.

Students are advised strongly not to use the 1st approach to construct quadrature formulas.

↕ ↕ ↕

Most cubature formulas available are constructed using the 1st approach! (Ill conditioned? Who cares!)

2.1 The first century in a nutshell

1877: J.C. Maxwell constructed the first cubature formulas.
Fully symmetric, degree 7 for C_2 and C_3 .

1890: P. Appell : orthogonal polynomials $\leftrightarrow$ cubature formulas

1948: J. Radon : cubature formula of degree 5 using the common zeros of 3 orthogonal polynomials of degree 3.

196* : A. Stroud and И.П. Мысовских : orthogonal polynomials $\leftrightarrow$ cubature formulas for n-dimensional regions.

196*-197*: Two groups of researchers:

The *first*: attacked the system of nonlinear equations.
$\rightarrow$ consistency conditions
(P. Rabinowitz, N. Richter and F. Mantel)

The *second*: used the relation between orthogonal polynomials and cubature formulas.
(A. Stroud, И.П. Мысовских, Г. Распутин, R. Franke, R. Piessens and A. Haegemans)
$\rightarrow$ introduction of polynomial ideals in 1973 (H.M. Möller).
$\rightarrow$ introduction of real ideals in 1978 (H.J. Schmid).

2.2 Bounds for number of points

How many points are needed in a cubature formula
to obtain a specified degree of precision?

A very general upper and lower bound is given in

Theorem:

The number of points N in a cubature formula of degree m satisfies

$$\dim \mathcal{P}^d_{\lfloor m/2 \rfloor} \leq N \leq \dim \mathcal{P}^d_m.$$

For 'standard' space of algebraic polynomials this means

$$\binom{d + \lfloor m/2 \rfloor}{d} \leq N \leq \binom{d+m}{d}$$

Remark: the lower bound is equal for degree $2k$ and $2k+1$.

$f \in \mathcal{P}^d$ of degree k for which $I[fg] = 0$, $\forall g \in \mathcal{P}^d_{k-1}$
is called an **orthogonal polynomial** for I.

There exist $(\dim \mathcal{P}^d_k - \dim \mathcal{P}^d_{k-1})$ unique orthogonal polynomials of degree k of the form

$$P^{a_1,a_2,\ldots,a_d} := x_1^{a_1} x_2^{a_2} \ldots x_d^{a_d} + Q \qquad (3)$$

with $a_i \in \mathbb{N}$, $\sum_{i=1}^{d} a_i = k$ and $Q \in \mathcal{P}^d_{k-1}$.

$\longrightarrow$ ***basic orthogonal polynomials***.

Each basic orthogonal polynomial of degree k has only one term of degree k, with constant 1.

Illustration:
generalisation of a property of Gauss quadrature formulas.

Theorem:

A necessary condition for the existence of a cubature formula of degree $2k+1$ with $N = \dim \mathcal{P}^d_k$ points is that the basic orthogonal polynomials of degree $k+1$ have N common zeros.

The condition of this theorem does not hold for regions Ω such as a □ or ◺ with $w(x) = 1$.

2.3 Connection with ideal theory, and better bounds

If a set of points is given,
then the set of all polynomials
that vanish at these points is an ideal.

Theorem:

Let I be an integral over a d-dimensional region.
Let $\{y^{(1)}, \ldots, y^{(N)}\} \subset \mathbb{C}^d$
and $\mathfrak{A} := \{f \in \mathcal{P}^d : f(y^{(i)}) = 0, i = 1, \ldots, N\}$.
Then the following statements are equivalent.

- $f \in \mathfrak{A} \cap \mathcal{P}^d_m$ implies $I[f] = 0$.
- There exists a cubature formula Q such that $I[f] = Q[f]$, $\forall\ f \in \mathcal{P}^d_m$, with at most $\dim \mathcal{P}^d_m - \dim(\mathfrak{A} \cap \mathcal{P}^d_m)$ (complex) weights different from zero.

For degree $m = 2k - 1$

$$N_{hmm} = \frac{k(k+1)}{2} + \left\lfloor \frac{k}{2} \right\rfloor = \dim \mathcal{P}^2_{k-1} + \left\lfloor \frac{k}{2} \right\rfloor$$

- **1973**: for □ with central symmetric weight function
- **1976**: for ◺ $1 \leq k \leq 6$ ($m \leq 11$) (Möller)
- **1983**: for ◺ $\forall k$ (Распутин)
- **1992**: for ◺ with weight function $y^\lambda (x-y)^\mu (1-x)^\nu$ (Berens and Schmid)

Cubature formulas with N_{hmm} points do *not* always exist.

But N_{hmm} is the best possible
if one only takes into account the central symmetry.

Overview of known bounds and formulas

degree	N_{min}	$\tilde{N}_{min}$	□	◺
1	1	1	1	1
2	3		3	3
3	3	4	4	4
4	6		6	6
5	6	7	7	7
6	10		10	10
7	10	12	12	12
8	15		15	15
9	15	17	17	19
10	21			22
11	24	24	24	27
12	28			33
13	28	31	33	36
14	36			42
15	36	40	44	48
16	45			52
17	45	49	57	61
18	55			66
19	55	60	68	73
20	66			78

Most cubature formulas mentioned above are obtained by solving the defining system of polynomial equations.

For □ that is true for $m \geq 15$.
For ◺ that is true for $m \geq 8$.

2.4 Direct approach

Solve the system of nonlinear equations

$$\sum_{i=1}^{N} w_i f_j(y^{(i)}) = I[f_j] \ , \quad j = 1, 2, \ldots, \dim \mathcal{P}_m^d.$$

directly.

Notation:
$\mathcal{G}$ = group of linear transformations.
$\mathcal{P}_m^d(\mathcal{G}) \subset \mathcal{P}^d(\mathcal{G})$, with only the polynomials of degree $\leq m$.

A $\mathcal{G}$-invariant cubature formula can be written as

$$Q[f] := \sum_{i=1}^{K} w_i Q_{\mathcal{G}}(y^{(i)})[f]$$

with $Q_{\mathcal{G}}(y)$ the average of the function values of f in the points of the $\mathcal{G}$-orbit of the point y.

Theorem: [Sobolev 1962]

Let Q be $\mathcal{G}$-invariant.
Q has degree m if

$$I[f] = Q[f], \forall f \in \mathcal{P}_m^d(\mathcal{G})$$

and

$$\exists g \in \mathcal{P}_{m+1}^d such \;\; that \;\; I[g] \neq Q[g].$$

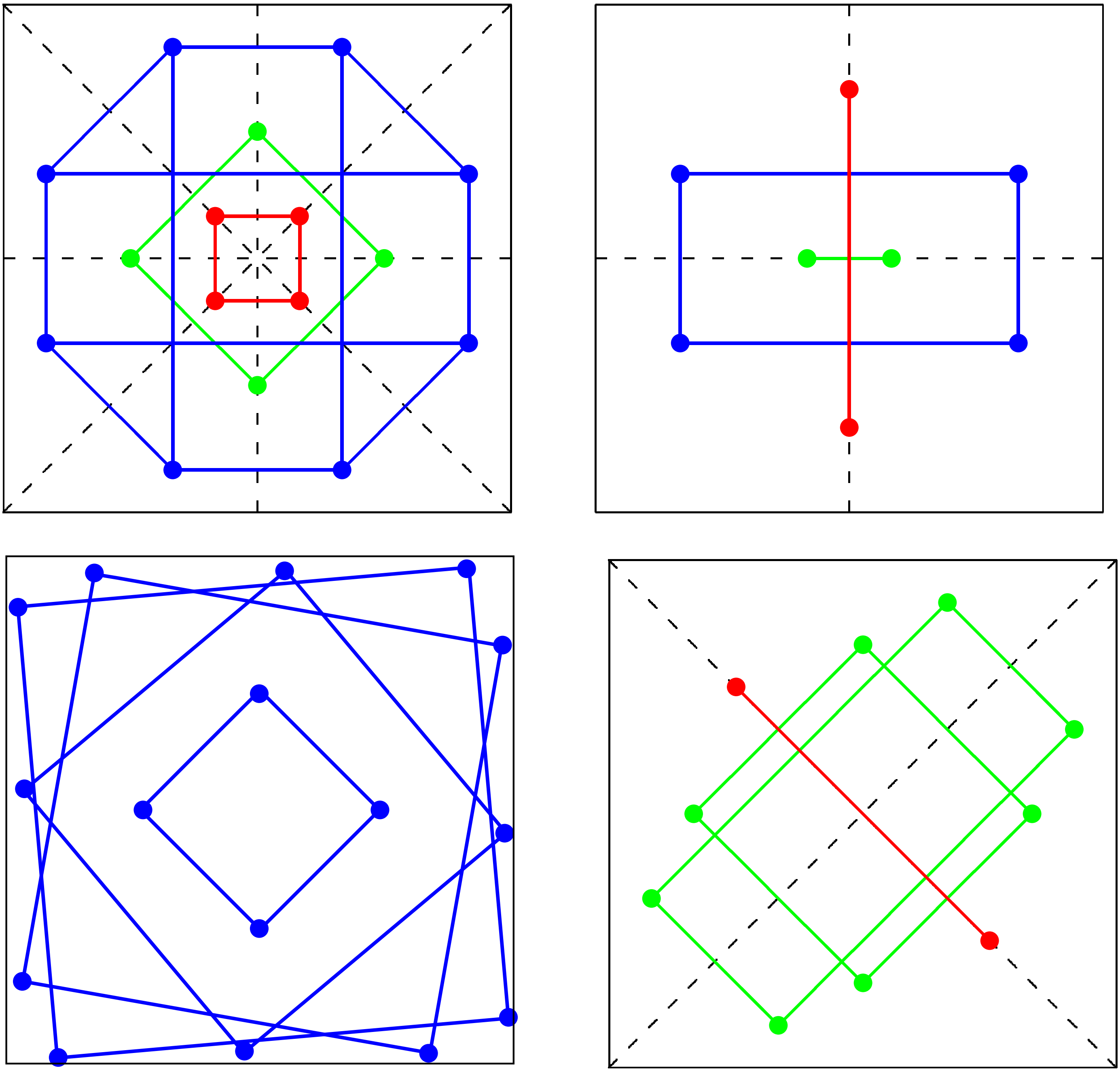
The $y^{(i)}$ and w_i are the solution of

$$Q[\phi_i] = I[\phi_i], i = 1, 2, \ldots, \dim \mathcal{P}_m^d(\mathcal{G}),$$

where the ϕ_i form a basis for $\mathcal{P}_m^d(\mathcal{G})$.

Reduce to smaller system by imposing symmetry:
more symmetry $\Rightarrow$ smaller system

Which structures should one use for □ ?



Consistency conditions

Each orbit $\Rightarrow$

- a number of unknowns in the nonlinear equations
- a number of points in the formula.

$K_i :=$ the number of orbits of type i in Q.

A **consistency condition** is an inequality for the K_is that must be satisfied in order to obtain a system of nonlinear equations where the number of unknowns $\geq$ the number of equations in each subsystem.

Cubature formulas which do not satisfy the consistency conditions are called "fortuitous".

Strictly speaking, consistency conditions are not sufficient and not necessary conditions.
And they don't distinguish between real and complex solutions, and solutions with all points inside or some outside.

Why imposing structure ?

1. reduction of the number of nonlinear equations and unknowns.

   The larger the symmetry group $\mathcal{G}$, the lower is $\dim \mathcal{P}_d^n(\mathcal{G})$ and, consequently, the lower is the number of nonlinear equations that determine a $\mathcal{G}$-invariant cubature formula.

   $\longrightarrow$ In general, the system is still too large to be solved completely.

   E.g. cubature formula of degree 7 for a 2D-region
   is a solution of $\dim \mathcal{P}_7^2 = 36$ equations.
   A $\square$ -invariant formula of degree 7 is a solution of 6 equations.

2. possibility of finding a basis, such that the original system splits into subsystems.

3. possibility that subsystems are easy to solve (e.g. quadrature)

Critical notes

Regularly articles attacking the system of polynomial equations appear in application journals.
Ofter their authors are unaware of ‘invariant theory’, ‘consistency conditions’ and results published after Stroud (1971)...

⇒ many reconstructions, or constructions of rules that are inferior to rules that where obtained earlier.

New results are often a matter of ‘luck’.
New higher degree results are obtained simply because computers can deal with bigger problems now than 10 years ago,
not as a consequence of fundamental progress in this area.

The condition of the system of nonlinear equations is often ignored.

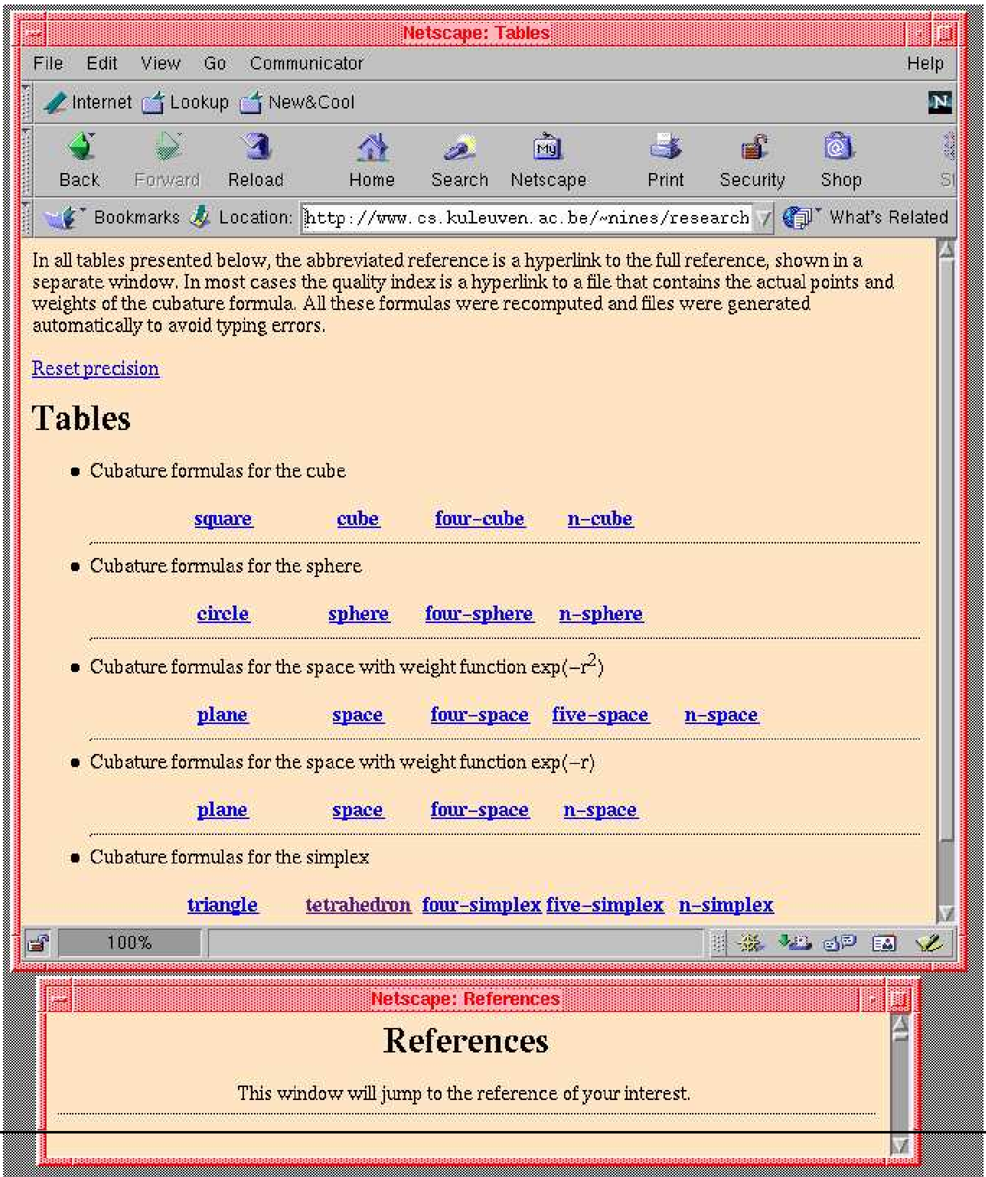
Warning: iterative zero finders often minimize a residue,
so not always a zero is obtained.

Watch out for... a couple of new approaches (for higher dimensions) appeared recently based on results from e.g. coding theory.
Names to look for: N. Victoir, G. Kuperberg, M. Taylor.

2.5 Encyclopaedia of Cubature Formulas

Origin: joint work with Philip Rabinowitz (1993); sequel (1999)

`www.cs.kuleuven.be/~nines/research/ecf/ecf.html`



3 Quasi-Monte Carlo methods

Monte Carlo

(S. Ulam, N. Metropolis & J. von Neumann, 1945)

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

Random points (according to pdf $w(x)$) $y^{(j)} \in \Omega$.

For any given $\varepsilon > 0$

$$\lim_{N\to\infty} \text{prob}\left(I[f] - \varepsilon \leq Q[f] := \frac{1}{N} \sum_{j=1}^{N} f(y^{(j)}) \leq I[f] + \varepsilon \right) = 1.$$

Central limit theorem →

$$\lim_{N\to\infty} \text{prob}\left(\left| \frac{1}{N} \sum_{j=1}^{N} f(y^{(j)}) - I[f] \right| \leq \frac{\lambda\sigma}{\sqrt{N}} \right) = \frac{1}{\sqrt{2\pi}} \int_{-\lambda}^{\lambda} e^{-t^2/2} \mathrm{d}t.$$

Quasi-Monte Carlo

(R.D. Richtmyer, 1952)
Points $y^{(j)}$ are chosen "**better than random**"

→ based on **low-discrepancy sequences**
(Richtmyer, Sobol, Halton, Niederreiter, Faure,... generalisations)

Theorem:

If f has bounded variation $V(f)$ on $[0,1]^d$ in the sense of Hardy and Krause, then, for any $y^{(1)}, \ldots, y^{(N)} \in [0,1]^d$, we have

$$\left| \frac{1}{N} \sum_{j=1}^{N} f(y^{(j)}) - \int_{[0,1]^d} f(x) \mathrm{d}x \right| \leq V[f] D_N^\star (y^{(1)}, \ldots, y^{(N)}).$$

$$D_N^\star \asymp \frac{(\log N)^d}{N}$$

→ **lattice rules**
so-called "good lattice points" (Korobov, 1959)
more general (Frolov, 1977), (Sloan & Kachoyan, 1987)

Integral over cube

$$I[f] = \int_0^1 \cdots \int_0^1 f(x_1, \ldots, x_d) \mathrm{d}x_1 \ldots \mathrm{d}x_d = \int_{[0,1)^d} f(\mathbf{x}) \, \mathrm{d}\mathbf{x}$$

Definition:

An d-dimensional rank-t lattice rule is given by

$$Q[f] = \frac{1}{n_1 n_2 \ldots n_t} \sum_{k_1=1}^{n_1} \sum_{k_2=1}^{n_2} \cdots \sum_{k_t=1}^{n_t} f\left(\left\{ \frac{k_1 \mathbf{z}_1}{n_1} + \frac{k_2 \mathbf{z}_2}{n_2} + \ldots + \frac{k_t \mathbf{z}_t}{n_t} \right\}\right),$$

where $n_i \in \mathbb{N}_0$ and $\mathbf{z}_i \in \mathbb{Z}^d$ for all i.

Further restriction: an extremely simple form...

Definition: [Rank-1 lattice rule]

Given an d-dimensional **generating vector** $\mathbf{z}$ we get a **rank-1** lattice rule

$$Q[f] = \frac{1}{N} \sum_{k=1}^{N} f\left(\left\{ \frac{k\mathbf{z}}{N} \right\}\right).$$

Common *misconceptions* about lattice rules

- **"Lattice rules are for integrating periodic functions."**
  $\rightarrow$ therefore the use of periodising transformations

  However:
  Lattice rules can just as well be used for non-periodic functions.

- **"For every N one needs another rule."**

  Surprise: one can create point sets of which you can take points in a particular order and it works out all right.

  This is a sequence from an extensible/embedded lattice rule.

Lattice rules can be used as just a set of low discrepancy points.

Good introductions to Quasi-Monte Carlo methods are in books by Niederreiter (1992), Tezuka (1995), Drmota & Tichy (1997) and survey articles by Spanier & Maize (1994) and Caflisch (1998)

Research activities on qMC: see proceedings of International Conferences on Monte Carlo & quasi-Monte Carlo methods (Springer).s
Next one in August 2006 in Ulm, Germany!

A good introduction to lattice rules is Sloan & Joe (1994).
Additional names to look for: F. Kuo, D. Nuyens, M. Hill.

4 Final remarks

The survey books by Stroud (1971) and Davis & Rabinowitz (1984) are out of date.

There are no quadrature/cubature specific journals.

Relevant results are scattered around in many journal publications. Different research communities don't look enough at each others journals, which is not good for progress.

During the past few years several new ideas where introduced to this area of research. Some look promising, but they need time to mature.