The approximation of multivariate integrals

Ronald Cools
Dept. of Computer Science, K.U.Leuven

Woudschoten 8 oktober 2008

Introduction

Given is an integral

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

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*.

Wishlist for a cubature rule

1. Rules must be efficient, i.e. use as few function evaluations as possible to obtain an approximation as good as requested.
2. The evaluation points and weights should be directly available, either hard coded or easy to generate.
3. We want to be able to obtain an error estimate.
4. If the estimated error is not sufficient, we would like to just add some more sample points.

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In this talk

1. OK for some settings
2. OK
3. completely ignored
4. maybe briefly

Quality criteria

One prefers cubature formulas where the points are inside Ω.

> *"... we meet with the curious result, that in certain cases the solution indicates that we are to employ values of the function some of which correspond to values of the variables outside the limits of integration. ... This, of course, renders the method useless in determining the integral from the measured values of the [integrand] as when we wish to determine the weight of a brick from the specific gravities of samples taken from 27 selected places in the brick, for we are directed by the method to take some of the samples from places outside the brick".* (Maxwell, 1877)

One prefers cubature formulas where all weights are positive.

- If relative error in computing $f(x)$ is bounded by ϵ then the error in computing $Q[f]$ is bounded by

$$\epsilon \sum_{j=1}^{N} |w_j|.$$

- Use a positive functional to approximate a positive functional.

A good quadrature or cubature formula has all points $y^{(j)}$ inside the region Ω and all weights w_j positive.

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

Will faster computers make everything trivial?

(Davis & Rabinowitz, 1984):

> *Given the present state of theory and hardware (1983), one can distinguish three dimensional ranges in addition to the two-dimensional case which deserves separate treatment:*
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> Range I: *integrals of dimension 3 to about 6 or 7,*
> Range II: *dimensions 7 or 8 to about 15,*
> Range III: *dimensions greater than 15.*

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Dimension 2: Situation satisfactory

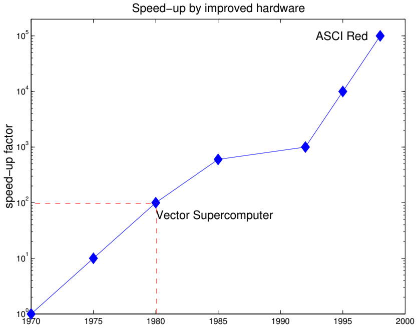
Range I: mainly polynomial-based methods

Range II: Monte Carlo and quasi-Monte Carlo become competitive

Range III: Monte Carlo and quasi-Monte Carlo are indicated.
One should not hope for more than 2 digits accuracy.

Is this much different today?

Improved hardware



TRIEX (De Doncker & Robinson, 1984) tested on
IBM 370/158 $\longrightarrow$ 1 MIPS
Now we have > 1000 MIPS′
1 CPU hour then $\longrightarrow$ 1 CPU second now.

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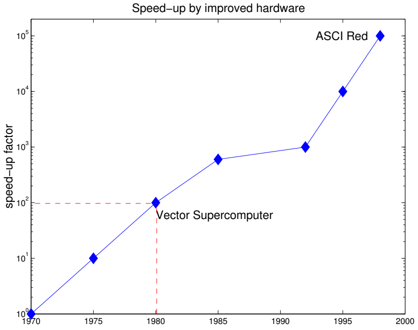
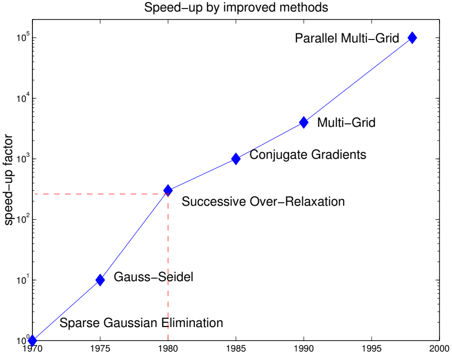


TRIEX (De Doncker & Robinson, 1984) tested on
IBM 370/158 → 1 MIPS
Now we have > 1000 MIPS′
1 CPU hour then → 1 CPU second now.
Original TRIEX tests limited to 23,000 function evaluations.
Who does 23,000,000 function evaluations nowadays?

Improved techniques

(Data from SIAM working group on CSE education long time go)



This is definitely not the picture for numerical integration techniques!

$\mathbb{P}^d$ = the vector space of all polynomials in d variables.
$\mathbb{P}^d_m$ = the subspace of $\mathbb{P}^d$ of polynomials with degree $\leq m$.
The cubature formula Q contains $2N+1$ parameters :

- the number N,
- the points $y^{(j)}$
- the weights w_j.

Criterion to specify and classify cubature formulas:

Definition

A cubature formula Q for an integral I has degree m if

$$Q[f] = I[f], \forall f \in \mathbb{P}^d_m$$

and

$$\exists g \in \mathbb{P}^d_{m+1} \text{ such that } Q[g] \neq I[g].$$

Repeated quadrature

Not the topic of this talk...

Given a quadrature rule of degree m

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

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 m with $N = n^2$ points for

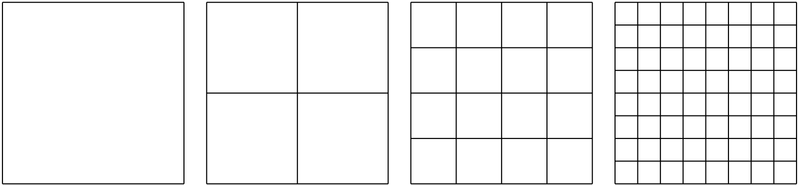
$$\int_0^1 \int_0^1 f(x, y)\mathrm{d}x\mathrm{d}y.$$

Copy rules and extrapolation

Not the topic of this talk...

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. ◺ :

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

Theorem

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 □ .

Let

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

Then

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

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

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

Polynomial-based methods

A cubature formula has **algebraic degree** m if it is exact for all polynomials of degree at most m.
The definition of degree is equivalent with

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

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

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

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

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

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Each point introduces $d+1$ unknowns.

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

Two aproaches

One can distinguish between 2 approaches to construct cubature formulas:

1. solve the system of nonlinear equations

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

   directly
   $\rightarrow$ **invariant theoretical approach**

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

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This 2nd approach has been very successful in quadrature.
In cubature, it has turned out to be difficult for $\square$,
significantly more difficult for $\triangle$ and
even more difficult for $d > 2$.

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

$\updownarrow$ $\updownarrow$ $\updownarrow$

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

The first century in a nutshell

1877: J.C. Maxwell constructed the first cubature formulas.
Fully symmetric, degree 7 for the square and cube.
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 d-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).

The quest for minimal formulas

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

Suppose a cubature formula has less than $\dim \mathbb{P}_k^d = \binom{d+k}{k}$ points.
$\Rightarrow$ there exists a $f \in \mathbb{P}_k^d$ that vanishes at the points
$\Rightarrow Q[f^2] = 0$.

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I is a positive functional $\Rightarrow I[f^2] > 0$.
$\Rightarrow Q$ does not have degree $2k$
or
a cubature formula of degree m has its number of points N bounded below by

$$N_{min} = \dim \mathbb{P}^d_{\lfloor \frac{m}{2} \rfloor} = \binom{d + \lfloor \frac{m}{2} \rfloor}{d}.$$

Used by Radon (1948).

Bounds for number of points

A very general upper and lower bound is given in

Theorem

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

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

For 'standard' space of algebraic polynomials this means

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

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

Radon's approach:
degree $m \to K = \dim \mathbb{P}^2_m = \frac{(m+1)(m+2)}{2}$ equations.
Each point introduces 3 unknowns.
If $m \neq$ multiple of 3, then K is a multiple of 3.
In that case, if the number of points in the cubature formula is

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then a system with the same number of equations as unknowns is obtained.
$m = 1 \to N = 1 = N_{min}$: trivial
$m = 2 \to N = 2 < N_{min}$
$m = 4 \to N = 5 < N_{min}$
$m = 5 \to N = 7 > N_{min}$: formulas for square, circle and triangle whose points are common zeros of 3 orthogonal polynomials.

Under what conditions is N_{min} sharp?
What is the highest lower bound for standard regions?

Construction of cubature formulas using ideal theory

Definition

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

Definition

$f \in \mathbb{P}^d$ is m-orthogonal for I if $I[fg] = 0$ for all g that satisfy $fg \in \mathbb{P}^d_m$.

There exist $(\dim \mathbb{P}^d_m - \dim \mathbb{P}^d_{m-1})$ unique orthogonal polynomials of degree m of the form

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

with $a_i \in \mathbb{N}, \sum_{i=1}^d a_i = m$ and $Q \in \mathbb{P}^d_{m-1}$.
$\longrightarrow$ *basic orthogonal polynomials*.

Illustration

A generalisation of a property of Gauss quadrature formulas:

Theorem

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

Illustration

A generalisation of a property of Gauss quadrature formulas:

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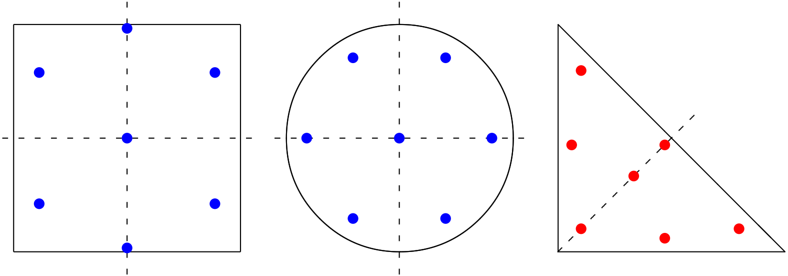
The condition of this theorem does not hold for regions Ω such as a □ or ◺ with $w(x) = 1$.

Degree 5 cubature formulas of Radon (1948)



Classical lower bound: $N \geq 6$
appears to be unreachable for standard regions!

Introduction to ideal theory

Definition

A polynomial ideal $\mathfrak{A}$ is a subset of $\mathbb{P}^d$ such that if $f_1, f_2 \in \mathfrak{A}$ and $g_1, g_2 \in \mathbb{P}^d$, then $f_1 g_1 + f_2 g_2 \in \mathfrak{A}$.

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

Definition

The zero set of an ideal $\mathfrak{A}$ is

$$NG(\mathfrak{A}) := \{y \in \mathbb{C}^d \mid \forall f \in \mathfrak{A} : f(y) = 0\}.$$

Definition

An ideal $\mathfrak{A} \subset \mathbb{P}^d$ is a real ideal if

$$f \in \mathfrak{A} \Leftrightarrow f(y) = 0 \ , \ \forall y \in NG(\mathfrak{A}) \cap \mathbb{R}^d.$$

Several types of bases for $\mathfrak{A}$:
H-basis (= Macaulay basis = canonical basis)
$\longrightarrow$ theoretical importance
G-basis (= Gröbner basis) $\longrightarrow$ practical importance
Under mild restrictions, a G-basis is an H-basis.

Definition

Let $\mathfrak{A}$ be a polynomial ideal. $\{f_1, f_2, \ldots, f_s\} \subset \mathfrak{A}$ is an H-basis for $\mathfrak{A}$ if for all $f \in \mathfrak{A}$ polynomials $g_1, g_2, \ldots, g_s$ exist such that

$$f = \sum_{i=1}^{s} f_i g_i \quad \text{and} \quad \deg(f_i g_i) \leq \deg(f), i = 1, 2, \ldots, s.$$

Theorem (Möller 1973)

For any polynomial ideal an H-basis exists.

Definition

The Hilbert function $\mathcal{H}$ is defined as

$$\begin{aligned}\mathcal{H}(k;\mathfrak{A}) &:= \dim \mathbb{P}_k^d - \dim(\mathfrak{A} \cap \mathbb{P}_k^d), k \in \mathbb{N} \\ &:= 0, -k \in \mathbb{N}_0\end{aligned}$$

$$\mathcal{H}(K;\mathfrak{A}) = \#NG(\mathfrak{A})$$

The relation between polynomial ideals, Hilbert function and cubature formulas is given by...

Relation between ideal theory and cubature formulas

Theorem (Möller 1973)

Let I be an integral over an d-dimensional region and $m \in \mathbb{N}$. Let $\{y^{(1)}, y^{(2)}, \dots, y^{(N)}\} \subset \mathbb{C}^d$ and

$$\mathfrak{A} := \{f \in \mathbb{P}^d | f(y^{(i)}) = 0, i = 1, 2, \dots, N\}.$$

Then the following statements are equivalent.

1. $f \in \mathfrak{A} \cap \mathbb{P}^d_m \Rightarrow I[f] = 0.$
2. *There exists a cubature formula*

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

such that $I[f] = Q[f], \forall f \in \mathbb{P}^d_m$, with at most $\mathcal{H}(d; \mathfrak{A})$ weights different from zero.

Points can have weight equal to zero !

H-bases are important because

Theorem (Möller 1973)

If $\{f_1, f_2, \ldots, f_s\}$ is an H-basis of $\mathfrak{A}$ and if the set of common zeros of $f_1, f_2, \ldots, f_s$ is finite and nonempty, then the following statements are equivalent :

1. *There is a cubature formula of degree m for the integral I which has as points the common zeros of $f_1, f_2, \ldots, f_s$. These zeros may be multiple, leading to the use of function derivatives in the cubature formula.*
2. *f_i is m-orthogonal for $I, i = 1, 2, \ldots, s$.*

Improved lower bound

For degree $m = 2k - 1$

$$\tilde{N}_{min} = \frac{k(k+1)}{2} + \left\lfloor \frac{k}{2} \right\rfloor = \dim \mathbb{P}^2_{k-1} + \left\lfloor \frac{k}{2} \right\rfloor$$

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

Cubature formulas with $\tilde{N}_{min}$ points do *not* always exist.
But $\tilde{N}_{min}$ is the best possible
if one only takes into account the central symmetry.

Overview of known bounds and formulas

degree	N_{min}	$\tilde{N}_{min}$	$\square$	$\triangle$
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	21	24	24	27

Overview of known bounds and formulas

degree	N_{min}	$\tilde{N}_{min}$	$\square$	$\triangle$
9	15	17	17	19
10	21			22
11	21	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 $\square$ that is true for $m \geq 15$.

For $\triangle$ that is true for $m \geq 8$.

Direct approach

Solve the system of nonlinear equations

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

directly.

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Note: Special methods for systems of polynomial equations
(special homotopies, Gröbner bases)
are not useful.

Introduction to invariant theory

$\mathcal{G}$ = group of linear transformations.

Definition

The $\mathcal{G}$-orbit or $\mathcal{G}$-corona of a point $y \in \mathbb{R}^d$ is $\{g(y) | \forall g \in \mathcal{G}\}$.

Definition

$\Omega \subset \mathbb{R}^d$ is said to be invariant with respect to $\mathcal{G}$ if $g(\Omega) = \Omega$ for all $g \in \mathcal{G}$. An invariant polynomial of $\mathcal{G}$ is a polynomial ϕ which is left unchanged by every transformation in $\mathcal{G}$.

$$\begin{aligned}
\mathbb{P}^d(\mathcal{G}) &= \text{the vector space of all invariant polynomials of } \mathcal{G} \\
\mathbb{P}^d_m(\mathcal{G}) &= \text{the subspace of } \mathbb{P}^d(\mathcal{G}) \text{ with only} \\
&\quad\ \text{the polynomials of degree} \leq m.
\end{aligned}$$

Definition

Let $\phi_1, \phi_2, \ldots, \phi_l$ be invariant polynomials of $\mathcal{G}$.
$\phi_1, \phi_2, \ldots, \phi_l$ form an integrity basis for the invariant polynomials of $\mathcal{G}$ $\Leftrightarrow$ any invariant polynomial of $\mathcal{G}$ is a polynomial in $\phi_1, \phi_2, \ldots, \phi_l$.
Each polynomial ϕ_i is called a basic invariant polynomial of $\mathcal{G}$.

Note that $l \geq d$.
For reflection groups $l = d$.
For rotation groups $l = d + 1$.

Relation between invariant theory and cubature formulas

Definition

A cubature formula is $\mathcal{G}$-invariant if Ω and $w(x)$ are $\mathcal{G}$-invariant, and if the set of points is a union of $\mathcal{G}$-orbits. The points of one and the same orbit have the same weight.

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

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

and

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

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

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

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

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

Historic perspective for $\triangle$

a. No structure imposed $\Rightarrow$ the monomials

$$x^i y^j \ , \ 0 \leq i + j \leq m \ ,$$

form a basis of $\mathcal{P}_m^2$.
The number of moment equations is then

$$\frac{1}{2}(m^2 + 3m + 2).$$

Historic perspective for △

b. In the 1960s, it appeared that for ◺ a significant reduction was available if one structured the rule to be invariant under coordinate interchange, and fitted only monomials

$$x^\alpha y^\beta \text{ with } \alpha \geq \beta \geq 0.$$

The number of independent moment equations is then

$$\left\lfloor \frac{1}{4}(m^2 + 4m + 4) \right\rfloor .$$

$\Rightarrow$ minimal formulas of degrees 2, 3, 4, 5, and 6.

Historic perspective for $\triangle$

c. The full symmetry of $\triangleleft$ was systematically exploited for the first time in 1975 (Lyness & Jespersen). A basis for the $\mathcal{D}_3$-invariant polynomials of degree m and less is

$$(r^2)^i (r^3 \cos 3\theta)^j \ , \ 0 \le 2i + 3j \le m,$$

and the number of independent moment equations is

$$\left\lfloor \frac{1}{12}(m^2 + 6m + 12) \right\rfloor .$$

Historic perspective for $\triangle$

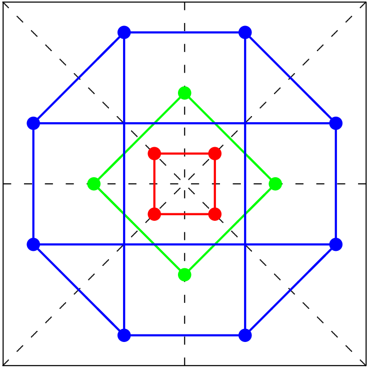
d. In the late 1980s, search for minimal formulas for degrees > 5, using the subgroup of $\mathcal{D}_3$ generated by the rotations.
$\Rightarrow$ minimal formulas of degree 7 and 8.
(Gatermann 1988, C & Haegemans 1987)
For this symmetry, a basis using $\triangleleft$ is

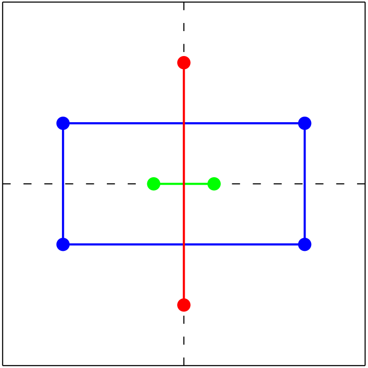
$$(r^2)^i (r^3 \cos 3\theta)^j (r^3 \sin 3\theta)^l \ , \ 0 \leq 2i + 3(j+l) \leq m \ , \ l = 0 \text{ or } 1,$$

and the number of independent moment equations is

$$\left\lfloor \frac{1}{6}(m^2 + 3m + 6) \right\rfloor .$$

Which structures should one use for $\square$?





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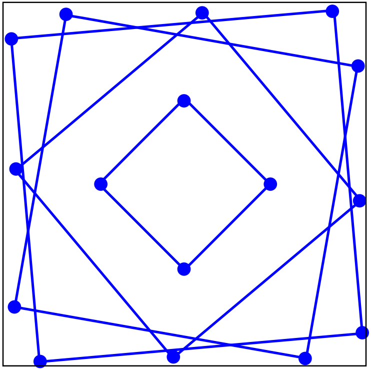
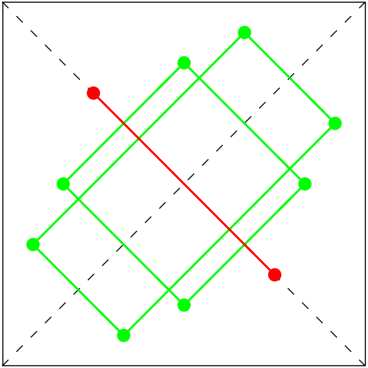
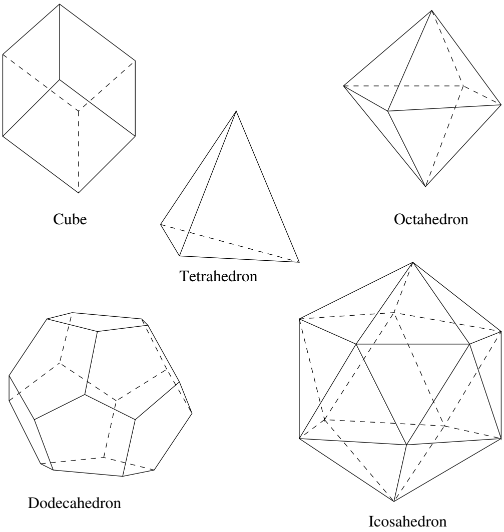




Higher dimensions = less groups to play with



$B_{3,0}$

$A_{3,0}$

$I_{3,0}$

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.

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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.

1-dimensional fully symmetric

The basic invariant polynomial is $\phi := x^2$.
The different types of Z_2-orbits:

type	generator	number of unknowns	number of points in an orbit	unknowns
0	(0)	1	1	weight
1	(a)	2	2	a, weight

Theorem

The consistency conditions for one-dimensional symmetric quadrature formulas of degree $2k-1$ are :

$$\begin{aligned} K_0 \;+\; 2K_1 &\geq k \\ 2K_1 &\geq k-1 \\ K_0 &\leq 1 \end{aligned}$$

A symmetric quadrature formula has $N = K_0 + 2K_1$ points.

Example: symmetric formula of degree 11

$$I[f] = \int_{-1}^{1} f(x)\mathrm{d}x$$

$\mathcal{G} = \{x \to x, x \to -x\}$, $\mathcal{G}$-orbit of $a = \{a, -a\}$ and the basic invariant polynomial is x^2.

$$Q[f] = \sum_{i=1}^{k} w_i(f(x_i) + f(-x_i))$$

quadrature formula has degree 10 iff it is exact for

$$1\ ,\ x^2\ ,\ x^4\quad x^6\ ,\ x^8\ ,\ x^{10}$$

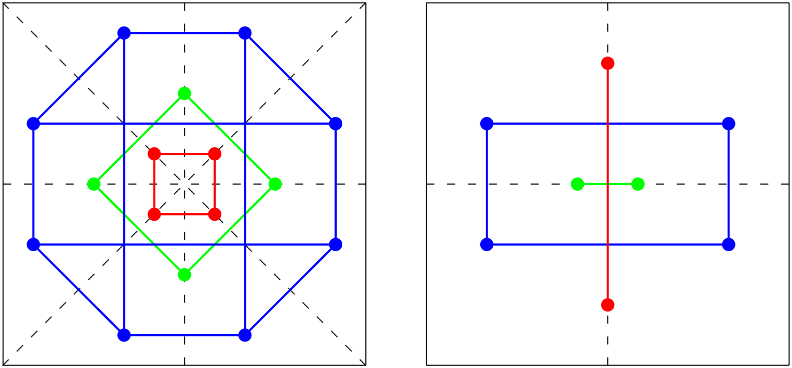
($\Rightarrow$ degree 11)
6 equations: $Q[x^j] = I[x^j]\ ,\ j = 0, 2, \ldots, 10$
6 unknowns: $w_1\ ,\ x_1\ ,\ w_2\ ,\ x_2\ ,\ w_3\ ,\ x_3$

$$Q[x^j] = \sum_{i=1}^{3} w_i(x_i^j + (-x_i)^j)\ ,\ j = 0, 2, \ldots, 10$$

2-dimensional fully symmetric

As basic invariant polynomials one can choose
$\phi_1 := x^2 + y^2$ and $\phi_2 = x^2 y^2$.
The different types of $\mathcal{D}_4$-orbits:

type	generator	number of unknowns	number of points in an orbit	unknowns
0	(0,0)	1	1	weight
1	(a,0)	2	4	a, weight
2	(a,a)	2	4	a, weight
3	(a,b)	3	8	a, b, weight



Theorem (Mantel & Rabinowitz 1977)

The consistency conditions for two-dimensional fully symmetric cubature formulas of degree $2k-1$ are :

$$\begin{array}{rcl} 3K_3 & \geq & A_1(k)-k \\ 2K_2+3K_3 & \geq & A_1(k) \\ 2K_1+3K_3 & \geq & A_1(k) \\ K_0+2K_1+2K_2+3K_3 & \geq & A_1(k)+k \\ K_0 & \leq & 1 \end{array}$$

$$A_1(k)=\begin{cases} \frac{(k-1)^2}{4} & if\ k\ is\ odd \\ \frac{k}{2}(\frac{k}{2}-1) & if\ k\ is\ even \end{cases}$$

A fully symmetric cubature formula has $N=K_0+4K_1+4K_2+8K_3$ *points.*

The construction of a cubature formula with the lowest possible number of points, requires two steps :

1. Solve the integer programming problem:

$$\text{minimize} \;\; N(K_i, i = 0, 1, \ldots)$$

   where the K_is satisfy the consistency conditions.
2. Solve the system of nonlinear (polynomial) equations.

Example: fully symmetric formula of degree 7

The consistency conditions are

$$\begin{aligned} 3K_3 &\geq -2 \\ 2K_2 + 3K_3 &\geq 2 \\ 2K_1 + 3K_3 &\geq 2 \\ K_0 + 2K_1 + 2K_2 + 3K_3 &\geq 6 \\ K_0 &\leq 1 \end{aligned}$$

An optimal solution is $[K_0, K_1, K_2, K_3] = [0, 1, 2, 0]$.

$$\begin{aligned} \to Q[f] \quad = \quad & w_1(f(x_1,0) + f(-x_1,0) + f(0,x_1) + f(0,-x_1)) \\ + \quad & w_2(f(x_2,0) + f(-x_2,0) + f(0,x_2) + f(0,-x_2)) \\ + \quad & w_3(f(x_3,x_3) + f(-x_3,x_3) + f(x_3,-x_3) + f(-x_3,-x_3)) \end{aligned}$$

Example

Use $\phi_1 = x^2 + y^2$ and $\phi_2 = x^2 y^2$.

$$\begin{cases} 4w_3\phi_2(x_3,x_3) & = 4w_3x_3^4 & = I[\phi_2] \\ 4w_3\phi_1(x_3,x_3)\phi_2(x_3,x_3) & = 8w_3x_3^6 & = I[\phi_1\phi_2] \end{cases}$$

$$\begin{cases} 4w_1 + 4w_2 & = I[0] - 4w_3 \\ 4w_1\phi_1(x_1,0) + 4w_2\phi_1(x_2,0) & = I[\phi_1] - 4w_3\phi_1(x_3,x_3) \\ 4w_1\phi_1^2(x_1,0) + 4w_2\phi_1^2(x_2,0) & = I[\phi_1^2] - 4w_3\phi_1^2(x_3,x_3) \\ 4w_1\phi_1^3(x_1,0) + 4w_2\phi_1^3(x_2,0) & = I[\phi_1^3] - 4w_3\phi_1^3(x_3,x_3) \end{cases}$$

Why imposing structure?

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

   > The larger the symmetry group $\mathcal{G}$, the lower is $\dim \mathbb{P}_m^d(\mathcal{G})$ 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 $\dim \mathbb{P}_7^2 = 36$ 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)...
$\Rightarrow$ many reconstructions, or constructions of rules that are inferior to rules that where obtained earlier.

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New higher degree results are obtained simply because computers can deal with bigger problems now than 10 years ago,
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There are a few new insights however (N. Victoir, G. Kuperberg, M. Taylor).

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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.

Is there a need for higher degree formulas?

Yes!

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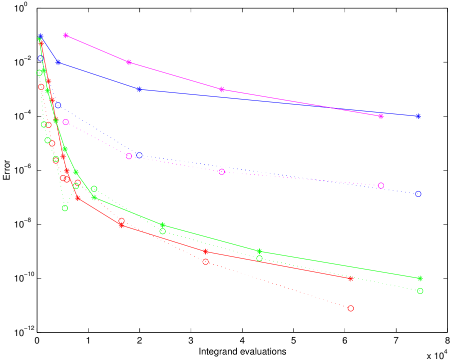
Yes!

$$\int_0^1\int_0^1\int_0^1 r^{-0.5}\log r \exp(xy+z)\mathrm{d}x\mathrm{d}y\mathrm{d}z \quad \text{with} \quad r := \sqrt{x^2+y^2+z^2}.$$

Using DCUHRE (Berntsen, Espelid & Genz, 1991)
and CUBPACK (C. & Haegemans, 2001)



2-division with degree 7 ($N = 39$)
2-division with degree 9 ($N = 77$)
2-division with degree 13 ($N = 89$)
2/4/8-division with degree 13

Results are scattered around

(C. & Rabinowitz, 1993):

> "This paper is concerned with continuing the work of Stroud in one specific area, namely the compilation of all so-called monomial cubature rules which have appeared since the publication of (Stroud, 1971) plus some cubature rules which appeared earlier but were not included..."

Main problem: different representations of the same cubature rule.

- $\sum w_j = 1$ or $\sum w_j = \mathrm{vol}(\Omega)$
- Different cubes, $[0,1]^d$ and $[-1,1]^d$
  different triangles, ◿ , ◁, ◺
  ...
- Geometric equivalent cubature rules.

$\Rightarrow$ The surface of the ball was excluded.

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This implies a validation (recomputation) of published results!
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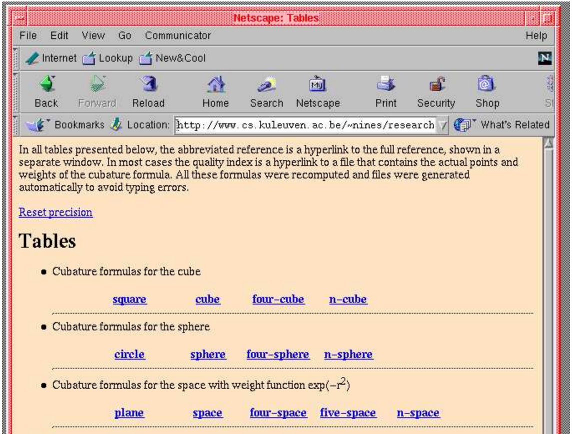
Some published rules contain errors. Types of errors:

- Even (Stroud, 1971) contains misprints. E.g.:
  - misplaced power in C_n:3-1
  - missing $\sqrt{\ }$ in C_2: 3-1
  - wrong weight $\frac{31}{649}$ instead of $\frac{31}{648}$ in C_2:7-3
- Misprints and/or inaccurate results:
  not all published digits are correct
- False formula
  $\rightarrow$ These are included in web-tables but with label Error.
  - Easy to recognise (by an expert)
    E.g.: Formula for S_2 of degree 11 with 25 points and negative weights. Theory learns us that this is impossible!
  - Difficult to recognise (even by an expert) (e.g., error in system)

Encyclopaedia of Cubature Formulas

Origin: joint work with Philip Rabinowitz (1993); sequel (1999)
www.cs.kuleuven.be/∼nines/research/ecf/

Google helps
if you know the magic word (=cubature).



This concluses the introduction to
the construction of cubature formulas of algebraic degree.

It should be clear now that
cubature is significantly different from quadrature.

It should be clear that these methods apply only in low dimensions.
Remember the 'Range 1' of Davis & Rabinowitz!

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Let’s have a quick look at Monte Carlo and quasi-Monte Carlo methods.

The Monte Carlo principle

Aim: compute a number I that arises in a mathematical problem.
Suppose I is also the *expected value* of a certain *stochastic process*.

The expected value of the process is estimated by sampling,
and the estimate is used as an approximation to I.

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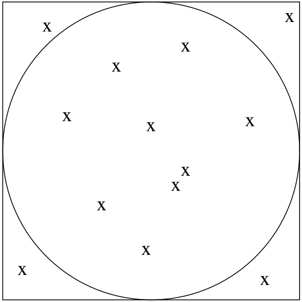
What is π again?



$$\frac{\pi}{4} \approx \frac{9}{13}$$

Monte Carlo methods

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

$$Q[f] := \frac{1}{N}\sum_{j=1}^{N} f(y^{(j)}) \text{ with } \mathrm{Vol}(\Omega) = 1$$

Random points (according to pdf $w(x)$) $y^{(j)} \in \Omega$.
For any given $\varepsilon > 0$

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

Central limit theorem $\rightarrow$

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

For a fixed level of confidence (i.e., for $\lambda =$ constant), the error bound

$$\frac{\lambda\sigma}{\sqrt{N}}$$

varies directly as σ and inversely by $N^{1/2}$.
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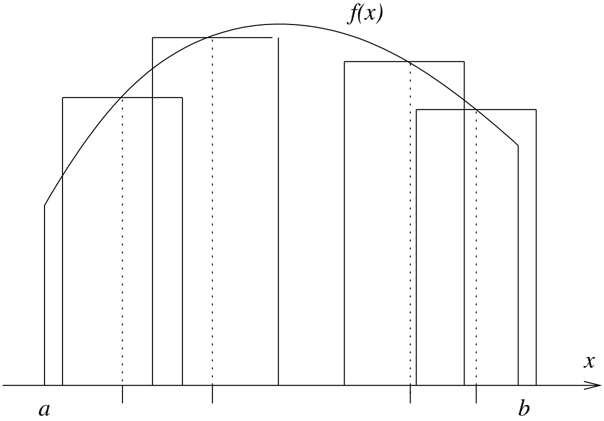
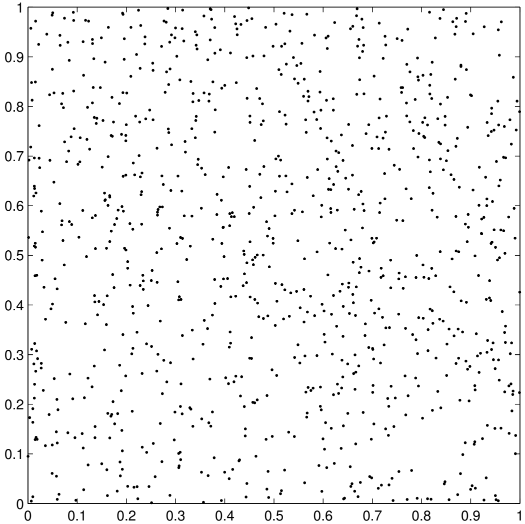
Note also that the variance is defined only for integrands which are square-integrable even though this is not required for the convergence (in probability) of the Monte Carlo method.

Observe that the approximation does not look like a usual approximation of an integral.

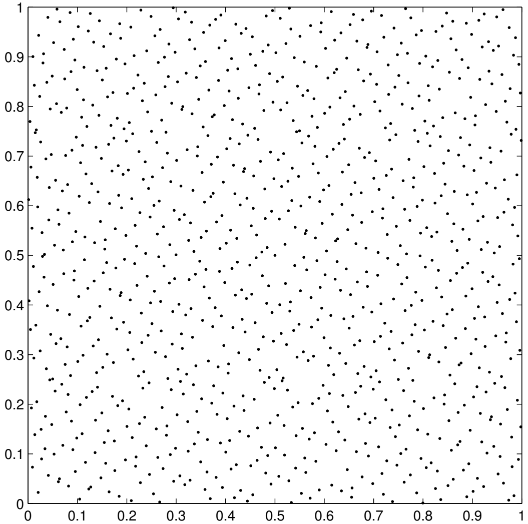
$$\int_a^b f(x)dx = \frac{1}{N}\sum_{i=1}^{N} f(x_i)$$



Random points appear in clusters with blind spots in between



The same number of points, more pleasingly distributed



To be continued.