Effective numerical integration on complex shaped elements by discrete signed measures

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Dedicated to Ezio Venturino

Introduction

In this talk we will briefly discuss cheap numerical cubature on multivariate domains

- introduce some basics on the topic and theoretical results;
- show the numerical advantages of this approach.

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Let

- Ω be a domain of $\mathbb{R}^2$ or $\mathbb{R}^3$,
- $f \in C(\Omega)$.

We intend to numerically approximate the integration functional

$$\mathcal{L}(f) := \int_{\Omega} f(x) d\Omega$$

by a discrete one

$$\mathcal{L}_M(f) := \sum_{i=1}^{N_M} w_i f(P_i)$$

so that the degree of exactness ADE is M, i.e.

$$\mathcal{L}(p) = \mathcal{L}_M(p), \quad p \in \mathbb{P}_M,$$

being $\mathbb{P}_M$ the set of polynomials over Ω, of total degree M.

Concerning

$$\mathcal{L}_M(f) := \sum_{i=1}^{N_M} w_i f(P_i)$$

we suppose that

- the points P_i may be external to Ω;
- some weights w_i may be negative, but the index of stability named conditioning of the cubature formula

$$\text{cond}(\{w_i\}) := \frac{\sum_{i=1}^{N_M} |w_i|}{\sum_{i=1}^{N_M} w_i}$$

  tends to 1 when increasing the degree (of exactness) M;
- the determination of the nodes $\{P_i\}_{i=1,\ldots,N_M}$ and the weights $\{w_i\}_{i=1,\ldots,N_M}$ is fast;
- the latter does not require the solution of a linear system.

Suppose that

- $\Omega \subseteq B \subset \mathbb{R}^d$, where B is a hypercube (usually named *bounding box*),
- $f \in C(B)$;
- $\{\phi_k\}_{k=1,\dots,\nu_M}$ is an orthonormal basis of $\mathbb{P}_M$, w.r.t. some absolutely continuous measure μ on B.

One can approximate f in the bounding box B by the polynomial hyperinterpolant

$$\mathcal{H}_M(f) = \sum_{k=1}^{\nu_M} (f, \phi_k)\phi_k$$

where

$$(f, \phi_k) = \sum_{i=1}^{N_M} u_i f(P_i)\phi_k(P_i)$$

in which the r.h.s. is a cubature formula with positive weights u_i, $\{P_i\} \subset B$, with $ADE = 2M$.

Our approach to obtain such $\mathcal{L}_M$ is essentially the following:

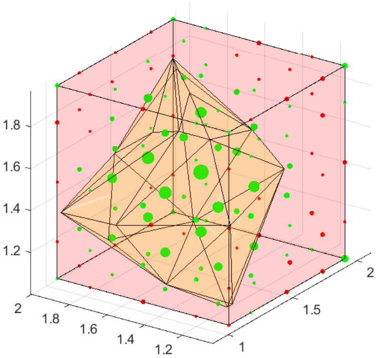
- *compute a polynomial hyperinterpolant $\mathcal{H}_M(f)$ of f on a hypercube B containing the domain Ω;*
- *apply the integration functional $\mathcal{L}$ to the hyperinterpolant $\mathcal{H}_M$.*

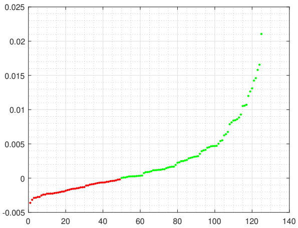
As in the similar case of classical interpolatory rules, these ideas can be converted in determining nodes and weights in the bounding box so that the rule has degree of exactness M on the integration domain Ω.

Suppose that the integration domain Ω is a polyhedron. Determine:

1. a Cartesian bounding box for the polyhedron;
2. the nodes $\{P_i\}$ and weights $\mathbf{u} = \{u_i\}$, $1 \leq i \leq N_M$, of a cubature formula exact for $\mathbb{P}_{2M}$ for a given absolutely continuous measure $d\mu = \sigma(P)dP$ on the bounding box;
3. an orthonormal basis $\{\phi_1, \ldots, \phi_\nu\}$ of $\mathbb{P}_M$ with respect to $d\mu$,
4. the corresponding moments $\mathbf{m} = \{m_1, \ldots, m_N\}$ on Ω, $m_j = \int_\Omega \phi_j(P)\, dP$, e.g. by the divergence theorem;
5. the Vandermonde-like matrix
$$V = V_n(\{P_i\}) = [\phi_j(P_i)] \in \mathbb{R}^{N_M \times \nu}$$
6. compute the weights as
$$\mathbf{w} = diag(\mathbf{u})\, V\mathbf{m}\ ,$$
or in a Matlab-like notation $\mathbf{w} = \mathbf{u}.*\ V\mathbf{m}$.

Example





- On the left: quadrature nodes of the cheap rule on the nonconvex polyhedral element Ω_1 for degree 4, as red dots if the pertinent weight is negative, as green dots otherwise. The size of the dots is visually proportional to the weight magnitude.
- On the right, distribution of the weights in increasing order (in red: negative weights, in green: positive weights). We report that the smaller weight is $w_{\text{min}} \approx -3.6 \cdot 10^{-3}$, the larger is $w_{\text{max}} \approx 2.1 \cdot 10^{-2}$, and the smaller size is $|w|_{\text{min}} \approx 2.6 \cdot 10^{-5}$.

Pros:

- Application to polytopal FEM (fast and stable computation of the integrals of products of polynomials naturally arising on arbitrary polyhedral elements, avoiding sub-tessellation into tetrahedra);
- moment computation does not require polyhedral tesselation;
- many computations can be done just once and repeated on different integration domains;
- w.r.t. techniques based on approximate Fekete points
  - cubature stability is ensured;
  - no QR factorization or linear system solution is involved.

Cons:

- Though stability is ensured some weights may be negative;
- the integrands require in general evaluations outside the integration domain.

Using the previous notation and assumptions, let

- $(X, \mathbf{u}) = (\{P_i\}, \{u_i\})$, $1 \le i \le N_M$, be the nodes and positive weights of a quadrature formula for integration in $d\mu$, exact on $\mathbb{P}_{2M}$ (the polynomials with total degree not exceeding $2M$),
- $h \in L^2_\mu(K)$.
- $m_j = \int_\Omega \phi_j(P)\, h(P)\, d\mu$, $1 \le j \le \nu_M$.
- $w_i = u_i \sum_{j=1}^{\nu} \phi_j(P_i)\, m_j$, $1 \le i \le N_M$.

Then, the formula

$$\mathcal{L}(f) = \int_\Omega f(P)h(P)d\mu \approx \sum_{i=1}^{N_M} w_i\, f(P_i) = \mathcal{L}_M(f) \tag{1}$$

has degree of exactness M and is stable, since one can prove that

$$\lim_{M\to\infty} \sum_{i=1}^{N_M} |w_i| = \int_\Omega |h(P)|\, d\mu\,. \tag{2}$$

Recently we have extended this strategy to

- numerical cubature in multivariate domains as
  - bivariate domains whose boundary can be tracked by parametric splines,
  - multivariate domains with complicated gerometries in which moments are computed by Quasi-Montecarlo methods.
- general linear functionals $\mathcal{L}$, for example differentiation functionals as

$$\partial^{\alpha} f(P) \; , \quad P = (x_1, \ldots, x_d) \in B \; , \tag{3}$$

corresponding to (the pointwise evaluation of) a partial differential operator $\partial^{\alpha} = \partial_{x_1}^{\alpha_1} \ldots \partial_{x_d}^{\alpha_d}$.

Remark

All the Matlab and Python routines are available as open-source software.

In this last section, we give some hints on what has been done over polyhedra.

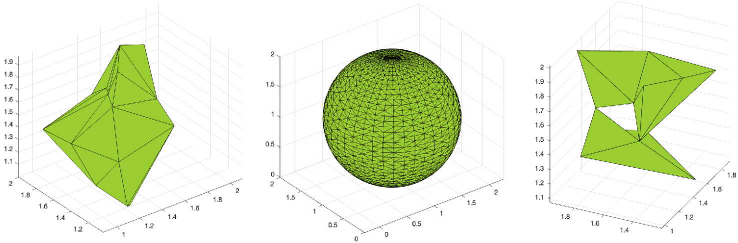


Figure: Examples of polyhedral domains. Left: Ω_1 (nonconvex, 20 facets); Center: Ω_2 (convex, 760 facets); Right: Ω_3 (multiply connected, 20 facets).

Numerical results: cubature

deg	4	6	8	10	12	14	16	18	20
Ω_1	1.2e-03	1.4e-03	1.7e-03	2.3e-03	3.4e-03	5.1e-03	7.7e-03	1.9e-02	3.4e-02
Ω_2	3.0e-02	3.4e-02	4.3e-02	5.9e-02	8.2e-02	1.2e-01	1.8e-01	4.4e-01	9.7e-01
Ω_3	8.1e-04	9.0e-04	1.1e-03	1.7e-03	2.3e-03	3.5e-03	5.4e-03	1.3e-02	2.6e-02

Table: Average cputimes (in seconds) of *CheapQ* on the domains above, varying the algebraic degree of exactness.

deg n	4	6	8	10	12	14	16	18	20
Ω_1	1.55	1.40	1.30	1.25	1.23	1.21	1.19	1.17	1.17
Ω_2	1.30	1.14	1.21	1.12	1.13	1.12	1.10	1.10	1.09
Ω_3	1.63	1.81	1.89	1.86	1.82	1.79	1.74	1.67	1.63

Table: Ratios $\sum_{j=1}^{\nu} |w_j| / vol(\Omega_i)$ for *CheapQ* on the domains above, varying the algebraic degree of exactness.

Numerical results: differentiation

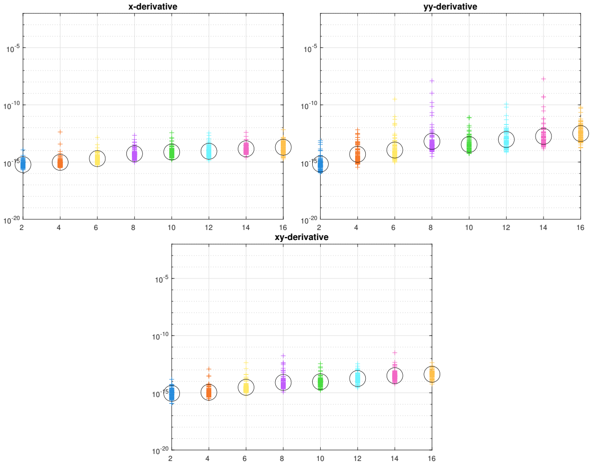


Figure: Small crosses: relative differentiation errors in the 2-norm on the first 100 Halton points in $[-1,1]^2$, for 100 trials of random polynomials $p_n(x,y) = (c_0 + c_1 x + c_2 y)^n$, $n = 2, 4, \ldots, 16$. Circles: geometric mean of the relative errors.

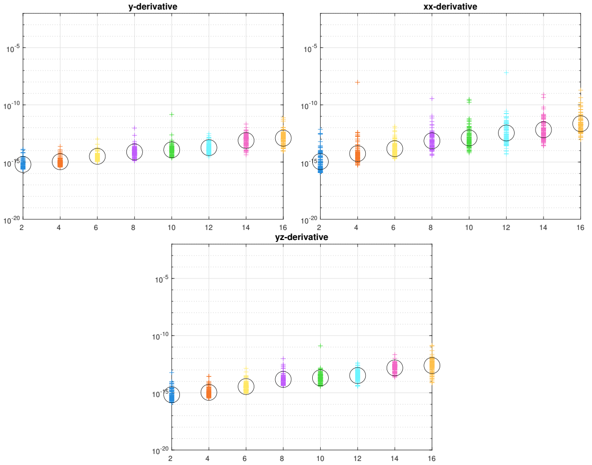


Figure: Small crosses: relative differentiation errors in the 2-norm on the first 100 Halton points in $[-1,1]^3$, for 100 trials of random polynomials $p_n(x,y,z) = (c_0 + c_1 x + c_2 y + c_3 z)^n$ in $[-1,1]^3$, $n = 2, 4, \ldots, 16$. Circles: geometric mean of the relative errors.

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