Numerical cubature over scattered data

Alvise Sommariva

NAMAS-24, Gaeta (I), September 16-20, 2024

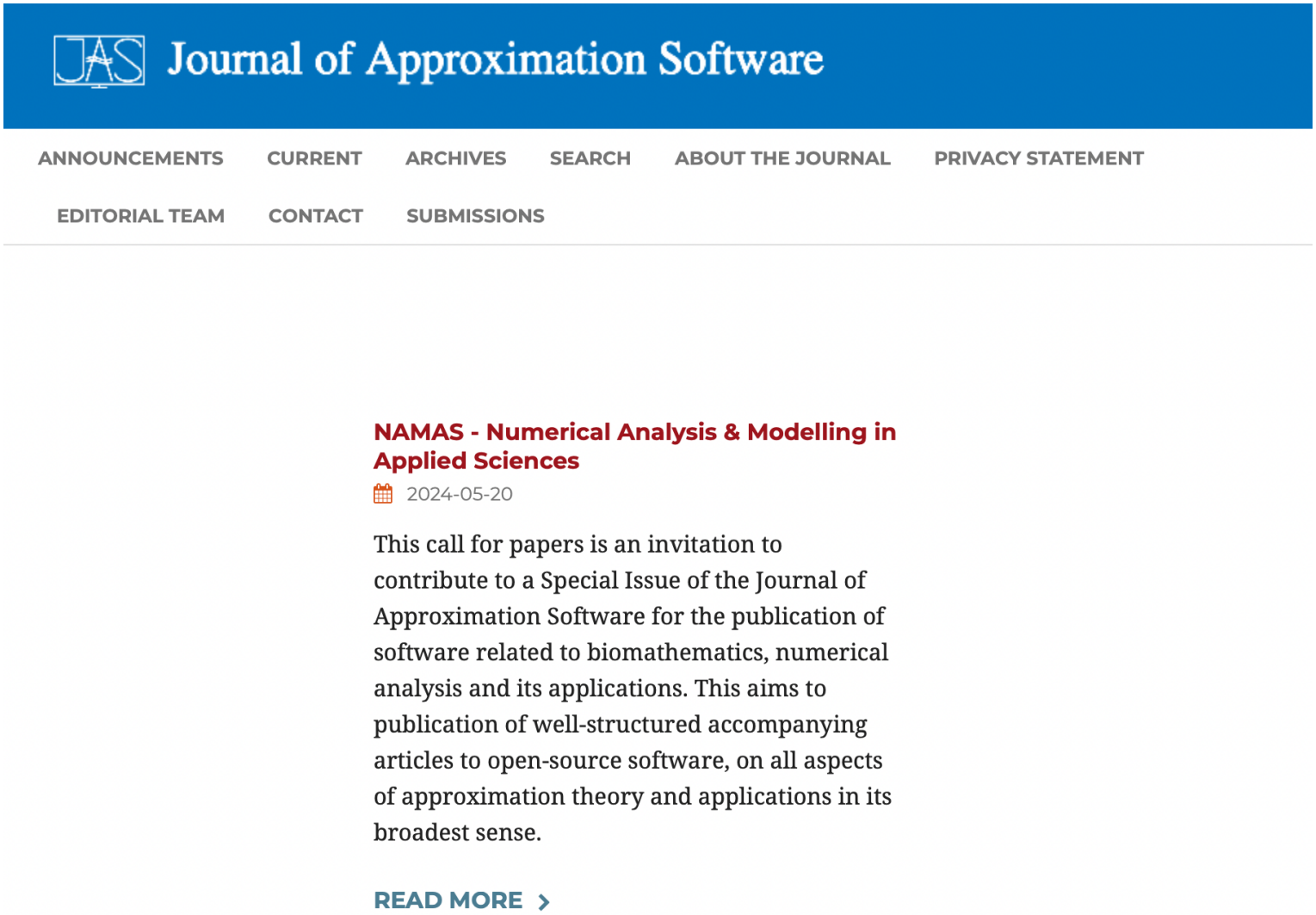
Numerical Analysis & Modelling in Applied Sciences congratulating Ezio Venturino on the occasion of his retirement

Dedication

This talk is dedicated to Ezio Venturino, for all the support that he gave to the development of Approximation Theory in Italy as well as the personal friendship that strongly bounds our group of researchers in Padua with that at the University of Turin.

Figure: From left to right: L. Bos, E. Venturino, A. De Rossi, A. Sommariva and R. Cavoretto (Matera 2022).

Announcement JAS/NAMAS



NAMAS and Journal of Approximation Software.

Announcement Workshop

The goal of SA2025 is to bring together researchers working in different fields of approximation and implementing algorithms using in particular the Matlab software, and other programming languages.

Purpose

In this talk we will briefly discuss

- numerical cubature over scattered data;
- introduce some basics on the topic;
- show the results that we have achieved on this topic since 2005.

Joint work with Marco Vianello (University of Padua), and RITA collaborators

- Roberto Cavoretto (University of Turin),
- Francesco Dell'Accio (University of Calabria),
- Alessandra De Rossi (University of Turin),
- Giacomo Elefante (University of Turin),
- Filomena Di Tommaso (University of Calabria),
- Nashua Siar (University Moulay Ismail, Morocco).

Work partially supported by

- the DOR funds of the University of Padova,
- INdAM-GNCS 2024 Project "Kernel and polynomial methods for approximation and integration: theory and application software".

Research accomplished within

- the RITA,
- the SIMAI Activity Group ANA&A,
- the UMI Group TAA.

Main problem

We intend to numerically approximate

$$\int_\Omega f(x)d\Omega \approx \sum_{i=1}^{N} w_i f(P_i).$$

where

- Ω is a domain of $\mathbb{R}^2$ or $\mathbb{R}^3$ (e.g. a sphere, a polygon, a polyhedron, etc.),
- $f \in C(\Omega)$,
- are available the samplings $f(P_i)$, $i = 1, \ldots, N$ at the scattered data $P_1, \ldots, P_N \in \Omega$.

In the case the set of nodes $\{P_i\}_{i=1,\dots,N}$ is a subset of sequence of points that is uniformly distributed in Ω, a classical approach is that of Monte Carlo-type methods

$$\int_\Omega f(x)d\Omega \approx \frac{\mu(\Omega)}{N}\sum_{i=1}^{N} f(P_i).$$

where $\mu(\Omega)$ is the measure of the domain Ω (or an approximation).

Notice that the weights are all equal to $\frac{\mu(\Omega)}{N}$.

Typically Ω is defined by set operations over

$$\Omega_1, \ldots, \Omega_M,$$

e.g. $\cap_{i=1}^{M}\Omega_i$ or $\cup_{i=1}^{M}\Omega_i$.

A basic approach is to

- determine a hyper-rectangle $\mathcal{R}$ containing Ω;
- define an uniformly distributed sequence $X^*_{\mathcal{R}}$ on $\mathcal{R}$;
- take the first N^* points $X_{\mathcal{R}}$ of $X^*_{\mathcal{R}}$ (usually N^* is very large);
- determine the sequence of points of $X^{(i)}_{\mathcal{R}} \subseteq X_{\mathcal{R}}$ belonging to Ω_i, $i = 1, \ldots, M$ (*in-domain* functions on each Ω_i must be available, it may not be a trivial task!);
- determine from these $X^{(i)}_{\mathcal{R}}$, $i = 1, \ldots, M$ the required sequence X_Ω on Ω as well as an approximation of $\mu(\Omega)$;
- choose N points $\{P_i\}_{i=1,\ldots,N}$ in X_Ω and from samplings of f compute $\int_\Omega f(x)d\Omega \approx \frac{\mu(\Omega)}{N}\sum_{i=1}^{N} f(P_i)$.

Monte Carlo type methods: example

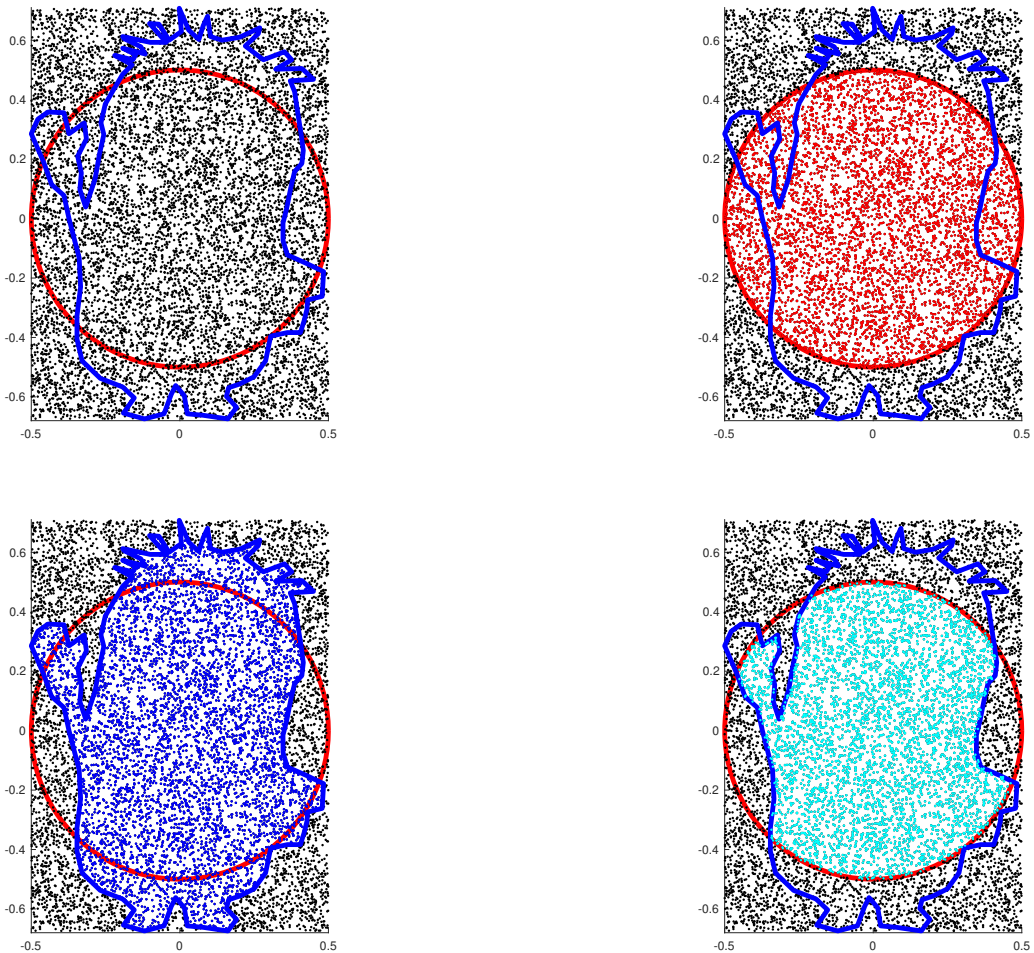


Figure: Intersection Ω of a polygonal minion with a disk. $N^* = 10000$ points in the bounding box $\mathcal{R} \approx [-0.5000, 0.5000] \times [-0.6741, 0.7077]$ of which $N = 4741$ are in Ω. Thus $\mu(\Omega) \approx \mu(\mathcal{R}) \cdot 4741/10000 \approx 0.6551$.

Pros:

- if indomains routines are available it may provide results even in complicated geometries without tracking the boundaries.
- many results in high dimensional spaces (curse of dimensionality!).

Cons:

- The basic version provides slow convergence to the integral. Some advantages using special sequences (Quasi-Monte Carlo methods). (see Koksma–Hlawka inequality).

If you are interested in this topic see

> J. Dick, F.Y. Kuo and I.H. Sloan,
> High-dimensional integration: The quasi-Monte Carlo way,

Numerical cubature by RBF: outline

Suppose that we have to approximate numerically

$$\int_\Omega f(P)d\Omega, \quad f \in C(\Omega)$$

being available the samplings of f at scattered data $P_k \in \Omega$, $k = 1, \ldots, N$.

In this part of the talk we

- give a short introduction of Radial Basis Functions (RBF),
- we show how to achieve specific cubature rules;
- introduce methods on certain domains as sphere and polygons;
- finish showing some new promising techniques.

For details about RBF see e.g. the monography

H. Wendland,
Scattered Data Approximation.

We will denote by $\mathbb{P}_m^d$ the vector space of $d-$variate real valued polynomials of total degree not exceeding m.

Definition (RBF Strictly positive definite)

A Radial Basis Function $\phi(r) : [0, +\infty) \to \mathbb{R}$, is *strictly positive definite* in $\mathbb{R}^d$ (sometimes referred as SPD), if for

- any N pairwise different points $P_1, \ldots, P_N \in \mathbb{R}^d$
- $c_1, \ldots, c_N \in \mathbb{R}$,

$$\sum_{j=1}^{N} \sum_{k=1}^{N} c_j c_k \phi(\|P_j - P_k\|_2) \geq 0 \tag{1}$$

being the quadratic form (1) null only when $c_1 = \ldots = c_N = 0$.

Some classical examples, just to mention some:

- Inverse Multiquadric: $\frac{1}{1+r^2}$,
- Wendland W2: $(1+4r) \cdot (\max(0, (1-r)))^4$, (compact support!),
- Gaussian: $\exp(-r^2)$.

One can prove the following important result.

Theorem (Uniqueness of the RBF interpolant)

Setting

$$\phi_i(P) := \phi(\|P - P_i\|_2)$$

for any choice of N distinct points $P_1, \ldots, P_N \in \mathbb{R}^d$, there is a unique interpolant

$$s(P) = \sum_{i=1}^{N} c_i \phi_i(P),$$

of the data $\{(P_i, f_i)\}_{i=1,\ldots,N}$, i.e. such that

$$s(P_i) = f_i \text{ for } i = 1, \ldots, N.$$

Definition (RBF strictly conditionally positive of order m)

The RBF function ϕ is *strictly conditionally positive of order m* (often shortened as SCPD), if

$$\sum_{j=1}^{N}\sum_{k=1}^{N} c_j c_k \phi(\|P_j - P_k\|_2) \geq 0 \tag{2}$$

holds

- for any N distinct points $P_1, \ldots, P_N \in \mathbb{R}^d$,
- $c_1, \ldots, c_N \in \mathbb{R}$ satisfying $\sum_{i=1}^{N} c_i p(P_i) = 0$ for any real valued polynomial $p \in \mathbb{P}^d_{m-1}$,

with the quadratic form (2) null only when $c_1 = \ldots = c_N = 0$.

Some classical examples:

- Multiquadric: $\sqrt{1+r^2}$ (order 1),
- Thin-Plate Spline: $r^2 \log(r)$ (order 2),
- Radial Powers: $r^\beta, \beta \notin 2\mathbb{N}$ (order $m = \lceil \beta/2 \rceil$).

Theorem (Uniqueness of the RBF interpolant)

If ϕ is a strictly conditionally positive RBF of order m then there exists a unique interpolant

$$s(P) = \sum_{i=1}^{N} c_i \phi_i(P) + \pi(P), \ \pi \in \mathbb{P}^d_{m-1}(\Omega) \tag{3}$$

of the data $X = \{(P_i, f_i)\}_{i=1,\dots,N}$.

Consequently, as in the case of algebraic rules of interpolatory type

$$\int_\Omega f(P)d\Omega \approx \int_\Omega s(P)d\Omega = \sum_{i=1,\dots,N} c_i \int_\Omega \phi_i(P)d\Omega + \int_\Omega \pi(P)d\Omega.$$

Thus is fundamental to approximate the moments

- $\int_\Omega \phi_i(P)d\Omega$, $i = 1, \dots, N$,
- $\int_\Omega \pi_k(P)d\Omega$, being $\{\pi_k(P)\}_k$ a basis of $\mathbb{P}^d_{m-1}(\Omega)$.

Numerical cubature by RBF: cubature weights

As in the case of algebraic interpolatory formula, one does not directly compute the interpolant, but the weights w_i, $i = 1, \ldots, N$ such that

$$\int_\Omega f(P) d\Omega \approx \sum_{i=1}^{N} w_i f(P_i).$$

To this purpose, one determines

1. the column vector of the moments, $\mathbf{I} = [\int_\Omega \phi_i(P) d\Omega; \int_\Omega \pi_k(P) d\Omega]^T$;
2. the generalized Vandermonde symmetric matrix

$$\mathcal{A} := \begin{bmatrix} A & B \\ B^T & 0_{M\times M} \end{bmatrix} \text{ where } A_{i,j} = \phi(\|P_i - P_j\|), B_{i,k} = \pi_k(P_i),$$

3. solve the square linear system

$$\mathcal{A}\,\mathbf{W} = \mathbf{I}\,, \quad \mathbf{W} = \begin{bmatrix} \mathbf{w} \\ \mathbf{z} \end{bmatrix} \quad \text{(moment matching system);} \qquad (4)$$

4. extract the first N components $\mathbf{w}$ of the solution $\mathbf{W}$.

Theorem

Denote by

- $\tilde{\mathbf{I}} \approx \mathbf{I}$ *the approximate RBF moments,*
- $\tilde{\mathbf{W}}$ *and* $\tilde{\mathbf{w}}$ *the corresponding perturbed weights,*
- *by* $\tilde{\mathbf{f}} \approx \mathbf{f}$ *the noisy functional data at* $\{P_i\}_{i=1,\dots,N}$*,*
- $h = \max_{P\in\Omega} \min_{1\le i\le n} |P - P_i|$ *is the* fill distance*;*
- $q = \min_{j\neq i} \{|P_j - P_i|\} \le 2h$ *is the* separation distance*,*
- $\alpha(h) \downarrow 0$ *as* $h \to 0$*,*
- $\lambda(q) \downarrow 0$ *as* $q \to 0$*.*

Then the cubature error $E(f) = |\int_\Omega f(P)d\Omega - \sum_{i=1}^N \tilde{w}_i \tilde{f}_i|$ *is such that*

$$E(f) \le \mathcal{O}\left(\alpha(h)\right) + \mathcal{O}\left(\frac{1}{\lambda(q)}\right) \|\mathbf{I} - \tilde{\mathbf{I}}\|_2 + \|\mathbf{f} - \tilde{\mathbf{f}}\|_\infty \sum_{i=1}^N |\tilde{w}_i|.$$

Numerical cubature by RBF: error estimate

From

$$E(f) \leq \mathcal{O}\left(\alpha(h)\right) + \mathcal{O}\left(\frac{1}{\lambda(q)}\right) \|\mathbf{l} - \tilde{\mathbf{l}}\|_2 + \|\mathbf{f} - \tilde{\mathbf{f}}\|_\infty \sum_{i=1}^{N} |\tilde{w}_i|.$$

and

- $\alpha(h) \downarrow 0$ as $h \to 0$,
- $\lambda(q) \downarrow 0$ as $q \to 0$.

we understand that

1. small fill distance h may help;
2. small separation distance q may harm when small and a not too precise computation of moments;
3. negative weights harms in case of noisy function evaluations.

More details can be found in the seminal paper

A. Sommariva, M. Vianello

Numerical cubature on scattered data by Radial Basis Functions

Numerical cubature by RBF: numerical considerations

Though everything seems straightforward theoretically, things are more complicated on the numerical side.

- the linear system may be severely ill-conditioned, depending on the choosen RBF, on its scaling factor and on the nodes;
- the computation of the moments must be *accurate* and fast.

Remark

The last item is particularly difficult, depending on the RBF and on the shape of the domain since we need to compute numerically

- $\int_\Omega \phi_i(P)d\Omega := \int_\Omega \phi(\|P - P_i\|_2)d\Omega$, $i = 1, \dots, N$,
- $\int_\Omega \pi_k(P)d\Omega$, *being* $\{\pi_k(P)\}_k$ *a basis of* $\mathbb{P}^d_{m-1}(\Omega)$ *(mandatory only on conditionally positive RBFs).*

As example, think about the case of $N \approx 1000$ *and* Ω *a polygon with complicate geometry: one has to quickly compute all those integrals close to machine precision.*

Numerical cubature by RBF: numerical considerations

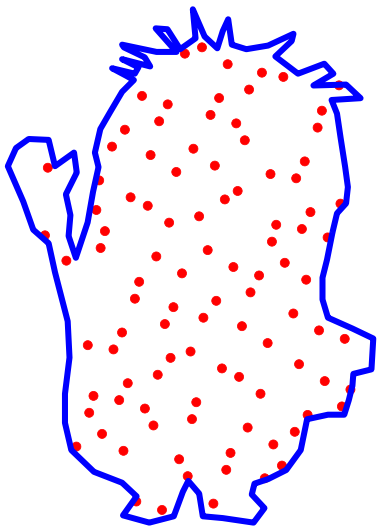


Figure: A domain Ω given by a polygonal minion and 100 centers (red dots).

From the figure above, one understands how complicated is to compute in the TPS case, on many RBF centers P_i, integrals of the form

$$\int_\Omega \|P - P_i\|_2^2 \log(\|P - P_i\|_2) d\Omega.$$

1. It becomes more challenging to compute them quickly and with high precision.
2. Issues for RBF with compact support $\mathrm{supp}(\phi)$ (role of $\Omega \cap \mathrm{supp}(\phi)$).

Unit-sphere and moments computation

Let $\Omega = \mathbb{S}^2$ be the unit-sphere and suppose we have to compute the moments

1. $\int_{\mathbb{S}^2} \phi_i(P) d\mathbb{S}^2$, $i = 1, \ldots, N$,
2. $\int_{\mathbb{S}^2} \pi_k(P) d\mathbb{S}^2$, being $\{\pi_k(P)\}_k$ a basis of $\mathbb{P}^d_{m-1}(\mathbb{S}^2)$ (mandatory only on conditionally positive RBFs).

The second problem above is easily solvable by means of one of the many algebraic rules available on the sphere (see, e.g. those suggested by R.S. Womersley).

Consequently, we focus our attention on the computation of RBF moments, varying the centers P_i, $i = 1, \ldots, N$.

Using the spherical coordinates

$$x = \cos(\psi)\sin(\theta), \quad y = \sin(\psi)\sin(\theta), \quad z = \cos(\theta),$$

with $0 \leq \psi < 2\pi, 0 \leq \theta \leq \pi$ and taking into account the jacobian determinant,

$$\begin{aligned} \int_{\mathbb{S}^2} \phi_i(P) d\mathbb{S}^2 &= \int_{\mathbb{S}^2} \phi(\|P - P_i\|_2) d\mathbb{S}^2 \\ &= \int_0^{2\pi} \int_0^{\pi} \phi(\sqrt{2(1-\cos(\theta))}) \sin(\theta) d\theta d\psi \\ &= \pi \int_0^4 \phi(\sqrt{s}) ds \end{aligned} \tag{5}$$

Remark

The last integral is available explictly for a large class of RBFs on the sphere and independent of the center, thus the computation of the RBF moments is particularly simple.

Remark

In the previous example, we have considered the distance of two points on the sphere as in $\mathbb{R}^3$.

One can do similar computations based on the geodesic distance, for those that are known as SRBF (acronym of spherical RBFs).

For additional details and considerations see

A. Sommariva and R.S. Womersley
Integration by RBF over the Sphere.

Let $\Omega \subset \mathbb{R}^2$ be a polygonal region and suppose we have to compute the moments

- $\int_\Omega \phi_i(P)d\Omega$, $i = 1, \ldots, N$,
- $\int_\Omega \pi_k(P)d\Omega$, being $\{\pi_k(P)\}_k$ a basis of $\mathbb{P}^d_{m-1}(\Omega)$ (mandatory only on conditionally positive RBFs).

Again, we focus our attention on the computation of the integrals

$$\int_\Omega \phi_i(P)d\Omega = \int_\Omega \phi(\|P - P_i\|_2)d\Omega, \quad i = 1, \ldots, N.$$

since there exist formulas with low cardinality that compute the polynomial moments.

Polygonal regions: first approach

As first approach one can

- subdivide the polygonal region in a minimal number of triangles $\{\mathcal{T}_k\}_{k=1,\dots,L}$ (use e.g. Matlab environment `polyshape`);
- compute all the moments over the triangles, i.e.

$$\int_{\mathcal{T}_k} \phi(\|P - P_i\|_2) d\mathcal{T}_k \text{ for } i = 1\dots, N, k = 1, \dots, L;$$

- sum up the contributions to get the moments

$$\int_{\Omega} \phi(\|P - P_i\|_2) d\Omega, \text{ for } i = 1\dots, N.$$

The key point is that we have reduced the problem to the moment computation over triangles.

Notice that, using the notation above, une has to compute NL integrals.

Polygonal regions: first approach

In the paper

A. Sommariva, M. Vianello,
RBF moment computation and meshless cubature on general polygonal regions,

we have provided an algorithm (not trivial!) to compute explicitly these integrals for a large class of RBF including

- Thin-Plate Splines,
- Multiquadrics,
- Inverse Multiquadrics,
- Wendland W0, W2, W4, W6,
- Radial Powers,
- Gaussians.

The corresponding mathematical formulas are too long to be included in this talk but can be found in the Matlab codes available at the author's homepage.

Polygonal regions: first approach

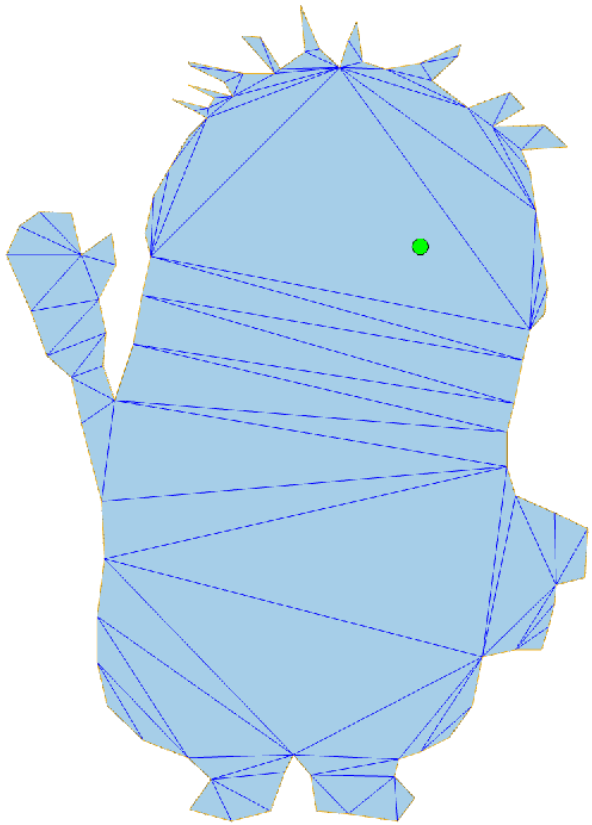


Figure: A polygonal minion with 99 vertices, a center (in green) and a minimal triangulation of the domain (97 triangles).

In the example above, since the polygonal minion can be obtained as union of 97 triangles (with non overlapping interior), if there are 1000 centers, then one has to compute 97000 integrals to determine the RBF moments over the centers.

Polygonal regions: second approach

As second approach one may compute the RBF moments over Ω by means of Gauss-Green formula (no need of subvidiving the domain in triangles!).

$$\int_{\Omega} \phi(\|P - P_i\|_2) dP = \oint_{\partial\Omega} \left(\int \phi(\|P - P_i\|_2) dx \right) dy, \; P = (x, y). \quad (6)$$

We suppose that the polygon Ω

- is simple, i.e. without self-intersections,
- has vertices V_j, $j = 1, \ldots, n+1$ (ordered counterclockwise), with $V_{n+1} = V_1$, denoting by
- $\overline{V_j V_{j+1}}$ the segment connecting V_j with V_{j+1}.

We sketch our procedure:

- compute an explicit primitive

$$\Phi_i(P) = \int \phi(\|P - P_i\|_2) dx;$$

- since

$$\begin{aligned} \int_\Omega \phi(\|P - P_i\|_2) dP &= \oint_{\partial\Omega} \left(\int \phi(\|P - P_i\|_2) dx \right) dy \\ &= \oint_{\partial\Omega} \Phi_i(P) dy = \sum_{j=1}^{n} \int_{\overline{V_j V_{j+1}}} \Phi_i(P) dy, \end{aligned}$$

we focus on the computation of each $\int_{\overline{V_j V_{j+1}}} \Phi_i(P) dy$, for $j = 1, \ldots, n$ and $i = 1, \ldots N$.

Polygonal regions: second approach

The key point is that, also in this case, each integral

$$\int_{\overline{V_j V_{j+1}}} \Phi_k(P) dy, j = 1, \ldots, n, k = 1, \ldots N$$

can be explictly determined for a wide class of RBF including

- Multiquadrics,
- Inverse Multiquadrics,
- Thin-Plate Splines,
- Radial Powers of the form $\phi(r) = r^k$ with $k = 3, 5, 7$,
- RBFs with compact support as $W0$, $W2$, $W4$, $W6$.

For

- Gaussian,
- the Matérn,

we were only able to determine Φ_k and compute the required integrals by high order shifted Gauss-Legendre rules.

On the RBF scaling (technical!)

Sometimes, for achieving a better approximation quality, for some RBF one may use its scaled version

$$\phi_\epsilon(r) := \phi(\epsilon\, r)$$

with $\epsilon > 0$ choosen in view of the centers and function evaluations.

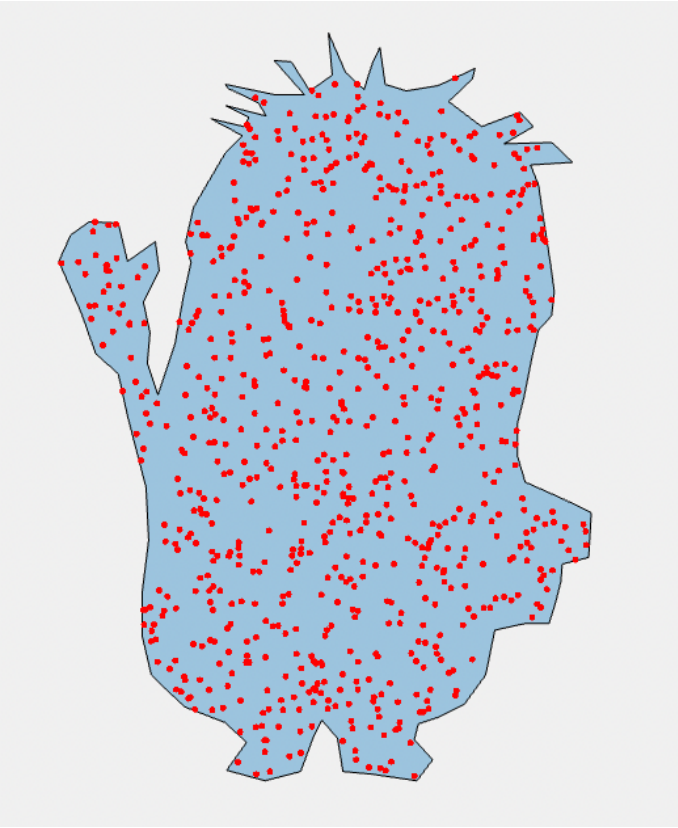
All the previous techniques can be adopted. By means of a specific algorithm, known in literature as LOOCV, one can compute a certain scale ϵ so to

- get highly reliable and precise results for any kind of RBF, even infinity smooth;
- reduce the cubature error for those finite regularity RBFs, such as W2, for which an optimal choice of ϵ is noteworthy.

For the interested reader, we have explored this subject in

R. Cavoretto, A. De Rossi, A. Sommariva, M. Vianello,
RBFCUB: a numerical package for near-optimal meshless cubature on general polygons.

Numerical example



```
***  TPS: r^2*log(r))

RBF SCALE    : OPTIMAL, 1.0e+00

FUNCTION TYPE:  1
*** f=@(x,y) franke(x,y);

POLYGON TYPE:    9
NODES CARDIN.:  800

* CUBATURE RES.: 6.499997962359514e-01
* EXACT VALUE  : 6.500164167333661e-01
** ABSOLUTE ERR.: 1.662e-05
** RELATIVE ERR.: 2.557e-05
* norm(w,1) : 9.297e-01
* COND. VAND.MATRIX  : 5.071e+07
NOTE: FORMULA WITH NEGATIVE WEIGHTS

CPU: CUBATURE MATRIX 0.0e+00
CPU: MOMENTS         1.4e-01
CPU: POLYNO. MOMENTS 3.4e-03
CPU: WEIGHTS COMPUT. 1.2e-02
CPU: TOTAL TIME      1.6e-01
```

Figure: Minion: 800 random points. Approach via Gauss-Green and TPS.

Numerical example

```
***  INVERSE MULTIQUADRIC: (1+r^2)^(-1/2)

RBF SCALE    : OPTIMAL, 2.4e-01

FUNCTION TYPE:  1
*** f=@(x,y) franke(x,y);

POLYGON TYPE:    9
NODES CARDIN.:  800

* CUBATURE RES.: 6.500161482921571e-01
* EXACT VALUE  : 6.500164167333661e-01
** ABSOLUTE ERR.: 2.684e-07
** RELATIVE ERR.: 4.130e-07
* norm(w,1) : 9.661e+01
* COND. VAND.MATRIX  : 2.278e+17
NOTE: FORMULA WITH NEGATIVE WEIGHTS

CPU: CUBATURE MATRIX 0.0e+00
CPU: MOMENTS         5.5e+00
CPU: POLYNO. MOMENTS 3.5e-05
CPU: WEIGHTS COMPUT. 6.2e-03
CPU: TOTAL TIME      5.5e+00
```

```
***  INVERSE MULTIQUADRIC: (1+r^2)^(-1/2)

RBF SCALE    : OPTIMAL, 2.4e-01

FUNCTION TYPE:  1
*** f=@(x,y) franke(x,y);

POLYGON TYPE:    9
NODES CARDIN.:  800

* CUBATURE RES.: 6.500161482921571e-01
* EXACT VALUE  : 6.500164167333661e-01
** ABSOLUTE ERR.: 2.684e-07
** RELATIVE ERR.: 4.130e-07
* norm(w,1) : 9.661e+01
* COND. VAND.MATRIX  : 2.278e+17
NOTE: FORMULA WITH NEGATIVE WEIGHTS

CPU: CUBATURE MATRIX 0.0e+00
CPU: MOMENTS         5.4e+00
CPU: POLYNO. MOMENTS 3.5e-05
CPU: WEIGHTS COMPUT. 6.9e-03
CPU: TOTAL TIME      5.4e+00
```

Figure: Minion: 800 random points. Approach via triangulation and Gauss-Green on IMQ.

In the recent paper

R.Cavoretto, A. De Rossi, F. Dell'Accio, F. Di Tommaso, N. Siar, A. Sommariva, M Vianello,
Numerical cubature on scattered data by adaptive interpolation,

we have used an alternative approach.

We observed that for many complex domains

- the RBF moments computation can be difficult,
- yet, an algebraic rule with degree of exactness $ADE = \delta$ is available.

We will take advantage of this to compute integrals on complicated regions, where the RBF techniques previously shown are not directly applicable.

Basic idea: one can

- determine an approximant ψ of the integrand f, based on the scattered data $\{P_i\}_{i=1,\ldots,N}$;
- evaluate ψ on the nodes $\{Q_k\}_{k=1,\ldots,L}$ of the algebraic formula,
- evaluate the algebraic formula with degree of exactness $ADE = \delta$,

$$\int_\Omega f(P)d\Omega \approx \sum_{i=1}^{N_\delta} w_i f(Q_i) \approx \sum_{i=1}^{N_\delta} w_i \psi(Q_i),$$

providing the required approximation of the integral.

We easily have the following error estimate

$$\left| \int_\Omega f(P)d\Omega - \sum_{i=1}^{N_\delta} w_i \psi(Q_i) \right| \leq \mu(\Omega) \left(2E_\delta(f) + \max_{i=1,\ldots,N_\delta} (|f(Q_i) - \psi(Q_i)|) \right)$$

where $E_\delta(f)$ is the best approximation error in ∞ norm of f in $\mathbb{P}_\delta$.

Problem: we said

> *determine an approximant* $\psi \approx f$, *based on the scattered data* $\{P_i\}_{i=1,\dots,N}$ *and evaluate* ψ *on the nodes* $\{Q_k\}_{k=1,\dots,L}$ *of the algebraic formula*

In literature there are many approximants on scattered data, as

- Matlab basic routine `Scattered Interpolation` (SCATTINT),
- adaptive moving interpolation `Disc`,
- RBF with LOOCV (choice of a good shape parameter ϵ), e.g. via Multiquadrics,
- methods in the family of Partition of unity known as `adaptive RBF-PUM`,
- methods in the family of Shepard methods known as `multinode Shepard methods`,

just to mention some.

Cubature on scattered data via algebraic formulas: numerical examples, I

As illustration, we consider the numerical integration over certain squares Ω of the functions

1. Franke's test function

$$\begin{aligned} f_1(x,y) &= \frac{3}{4}\exp\left(-\frac{(9x-2)^2+(9y-2)^2}{4}\right)+\frac{3}{4}\exp\left(-\left(\frac{(9x+1)^2}{49}+\frac{9y+1}{10}\right)\right) \\ &+ \frac{1}{2}\exp\left(-\frac{(9x-7)^2+(9y-3)^2}{4}\right)-\frac{1}{5}\exp(-((9x-4)^2+(9y-7)^2)), \end{aligned}$$

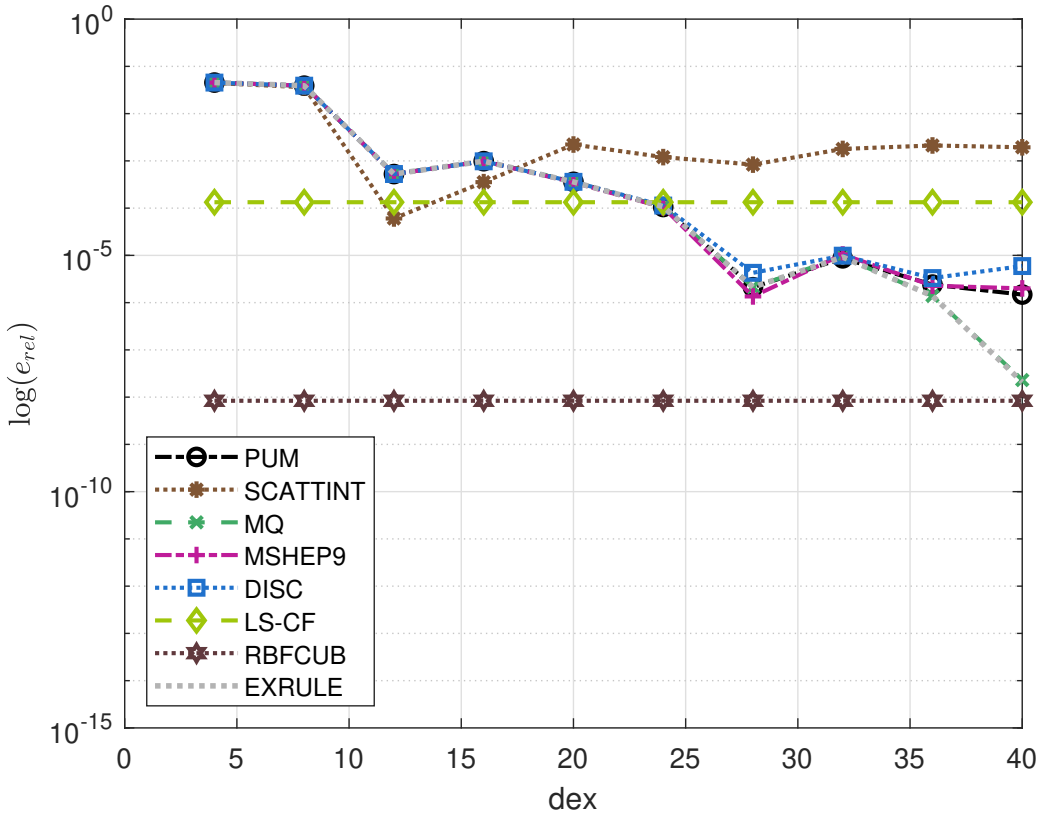
2. $f_2(x,y)=\frac{1}{(1+x^2)(1+y^2)}$;
3. $f_3(x,y)=((x-0,5)^2+(y-0.5)^2)^{3/2}$,
4. $f_4(x,y)=((x-0.5)^2+(y-0.5)^2)^{7/2}$.

As for the domains Ω we considered

- the square $[0,1]\times[0,1]$ for f_1, f_3, f_4,
- the square $[-1,1]\times[1,1]$ for f_2.

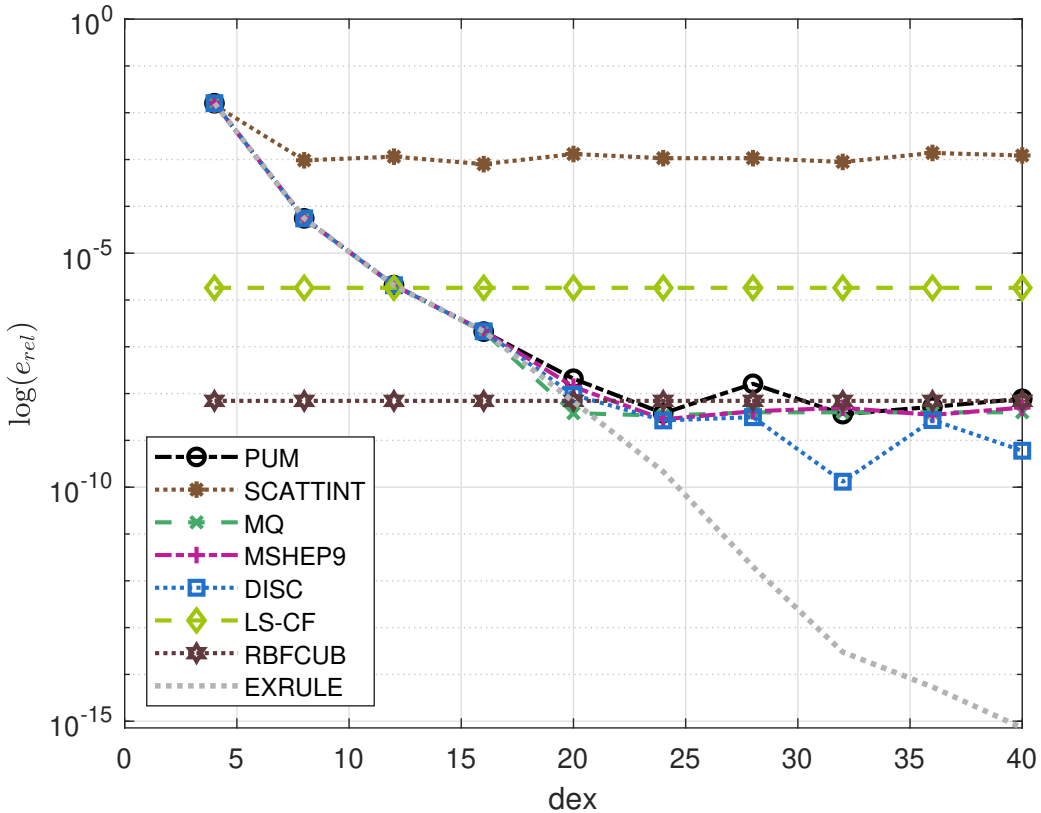
Algebraic rules are taken from those of almost minimal cardinality .

Cubature on scattered data via algebraic formulas: numerical examples, I



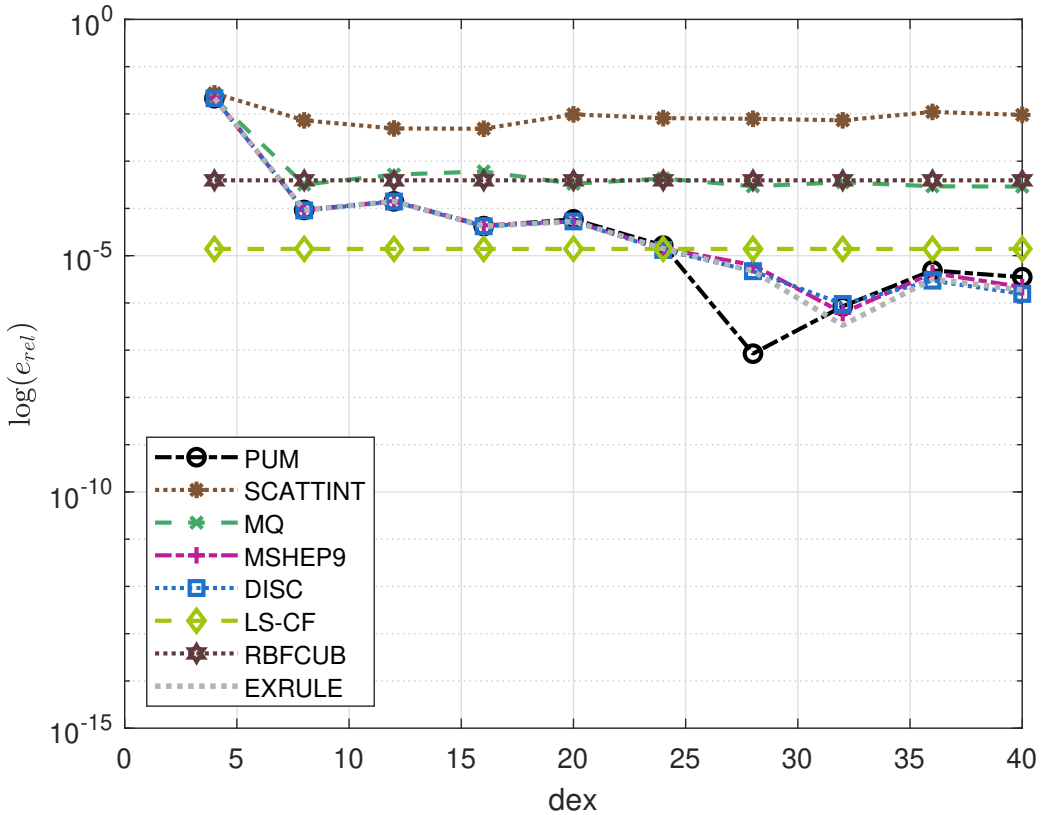
- Comparison of scattered cubature methods on 800 Halton points for f_1 ;
- horizontal lines: RBFCUB with MultiQuadrics and LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, I



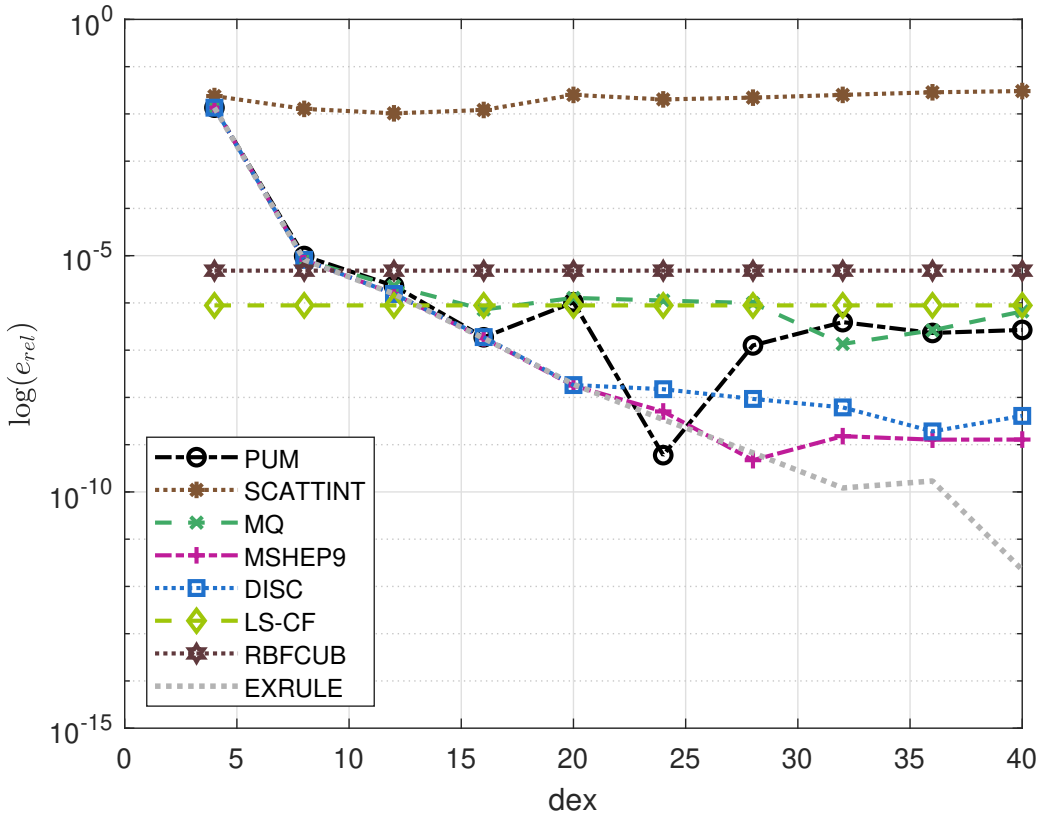
- Comparison of scattered cubature methods on 800 Halton points for f_2;
- horizontal lines: RBFCUB with MultiQuadrics and LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, I



- Comparison of scattered cubature methods on 800 Halton points for f_3;
- horizontal lines: RBFCUB with MultiQuadrics and LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, I



- Comparison of scattered cubature methods on 800 Halton points for f_4
- horizontal lines: RBFCUB with MultiQuadrics and LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, II

As second battery of tests, we consider the numerical integration over two nonstandard domains with curved boundaries,

- a circular lune (non-convex domain),
- an asymmetric circular annulus (multiply connected domain).

of the functions f_1, f_2, f_3, f_4

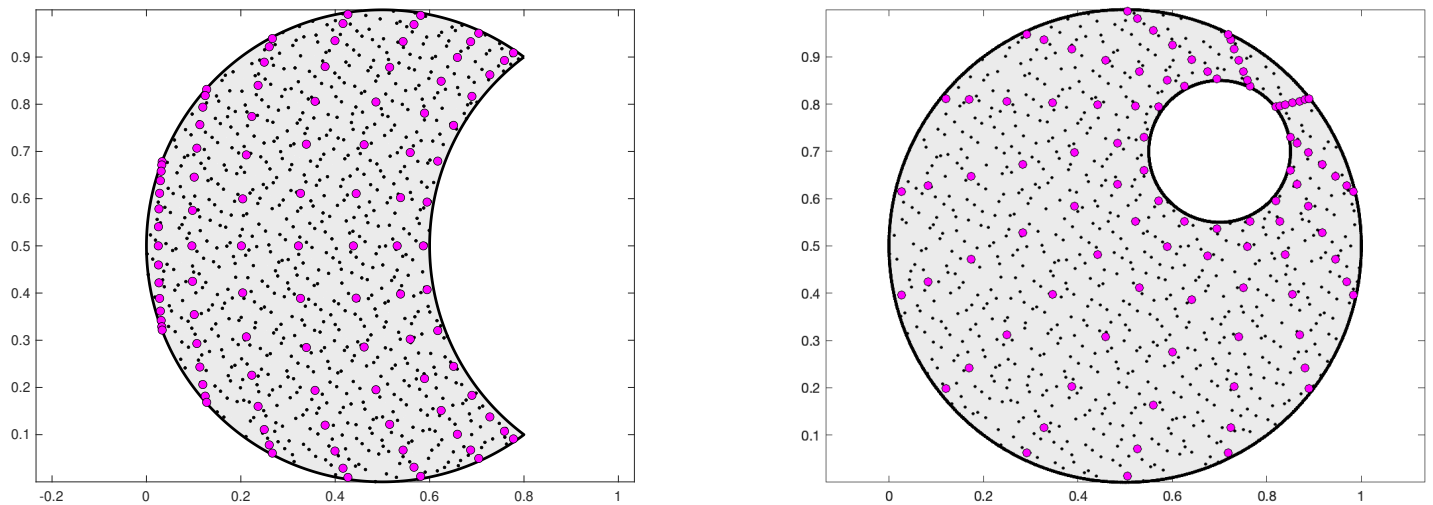


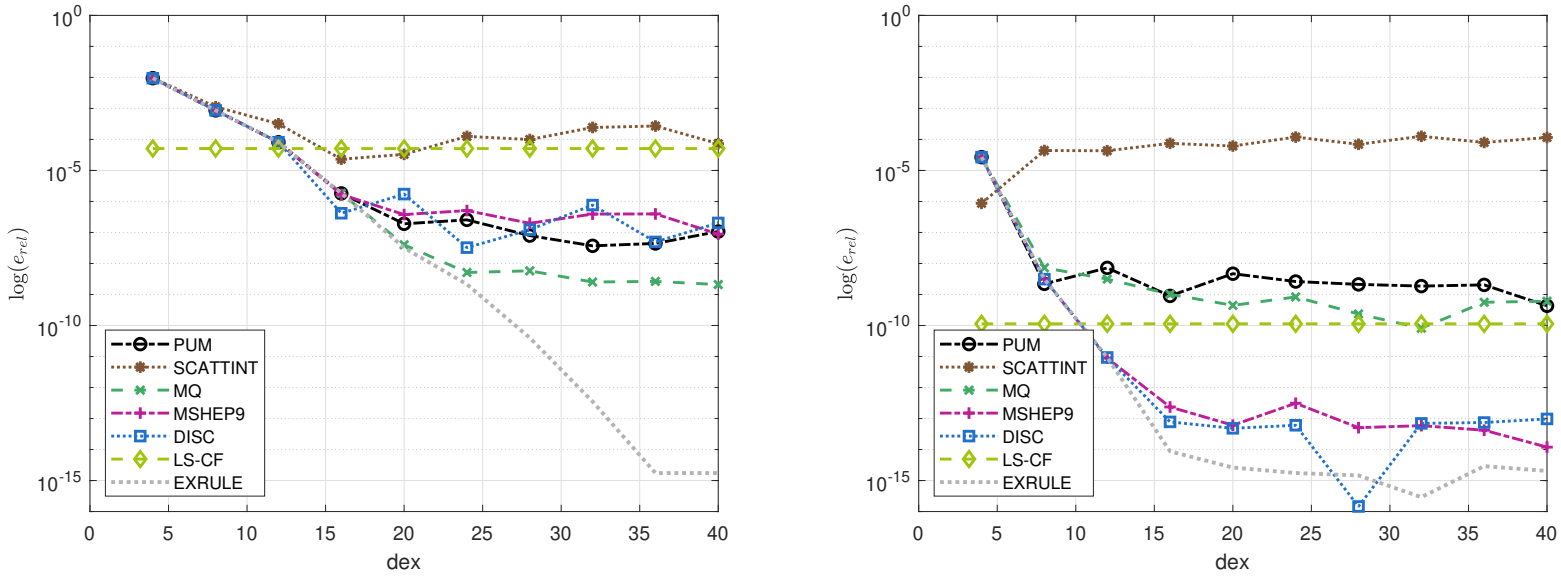
Figure: Halton points on a circular lune and an asymmetric circular annulus (black dots), and cubature nodes of an algebraic rule of degree 12 (in magenta).

Cubature on scattered data via algebraic formulas: numerical examples, II

Some observations:

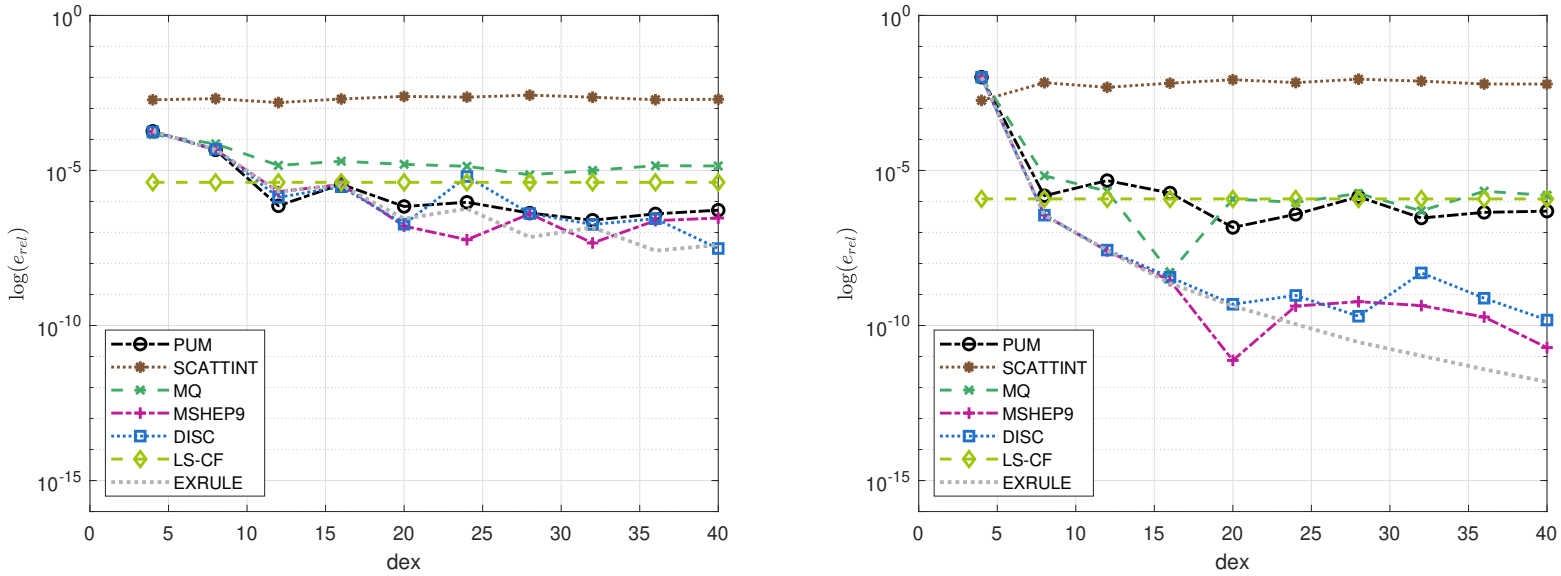
- Algebraic cubature rules are available (via subperiodic trigonometric Gaussian quadrature);
- our routine RBFCUB with LOOCV is not applicable, being for the moment restricted to linear polygons;
- we have modified the codes LS-CF, based on a work by Glaubitz, to work with the appropriate polynomial moments on such curved domains (this option is not present in the original package of the author);
- in the presence of a very high number of scattered points, PUM and LS-CF are faster and could be methods of choice in order to control the computing time.

Cubature on scattered data via algebraic formulas: numerical examples, II



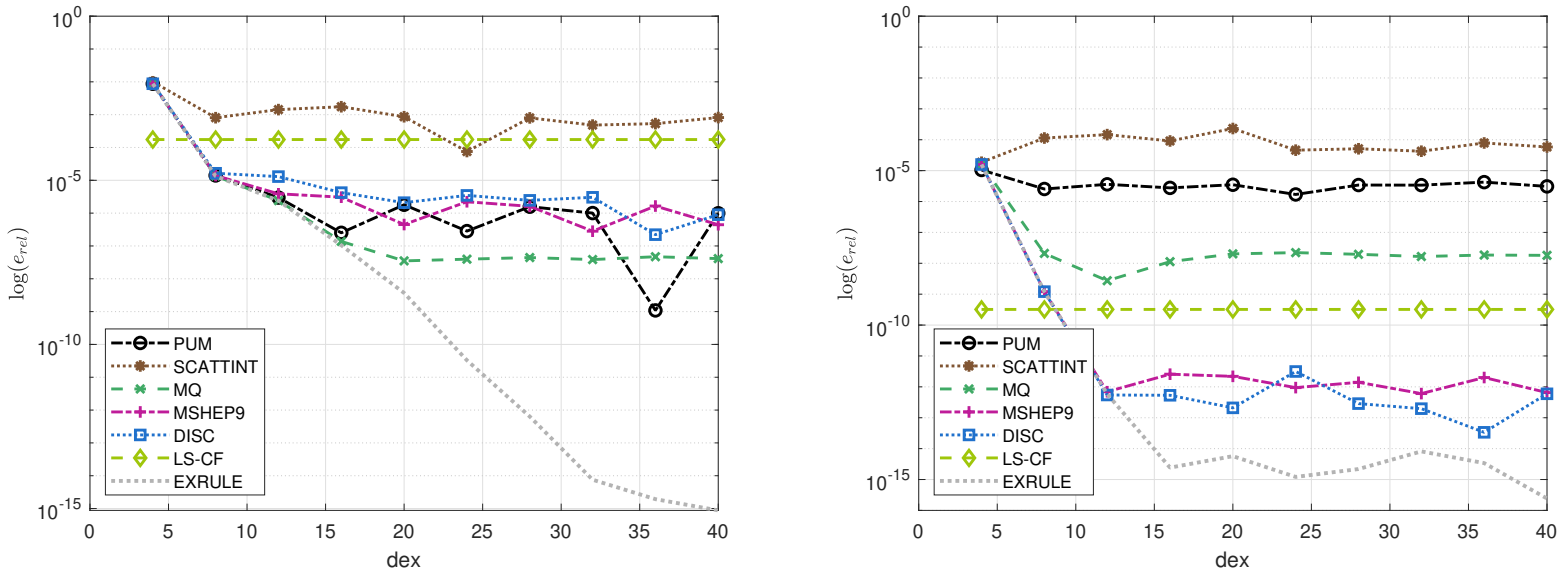
- Comparison of scattered cubature methods on 800 Halton points for f_1 (left) and f_2 (right) with Ω being a circular lune;
- the horizontal line correspond to LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, II



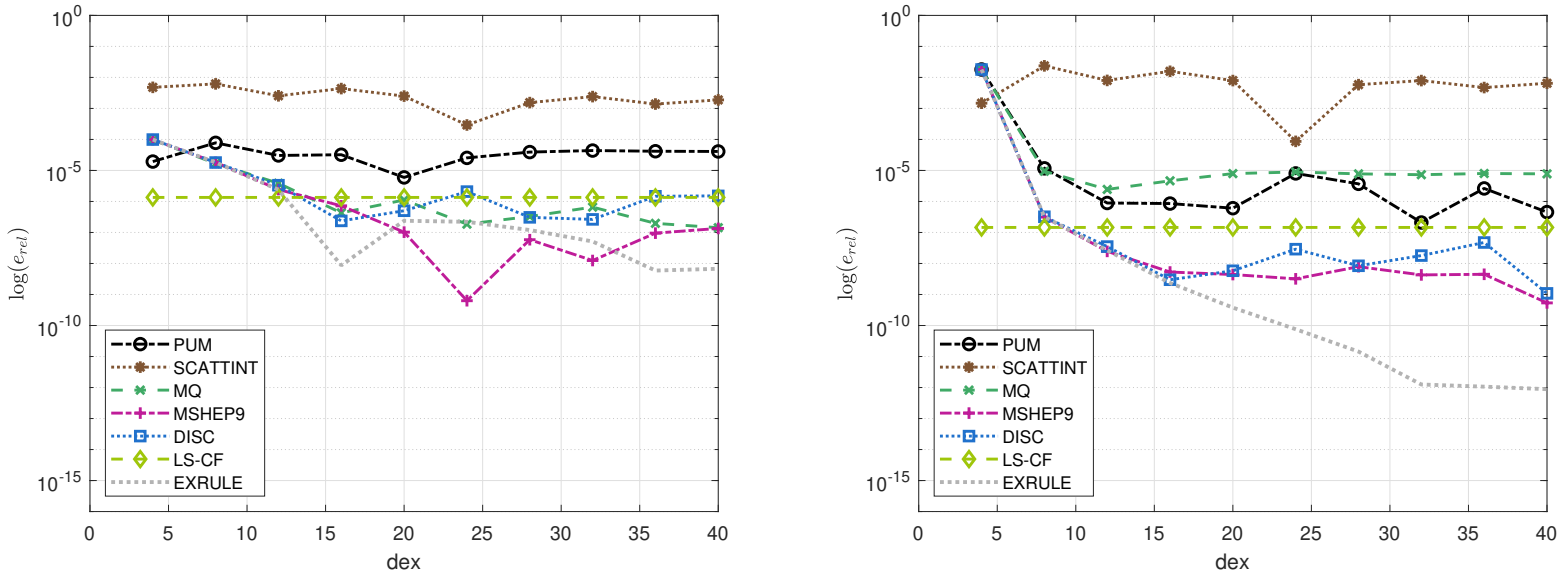
- Comparison of scattered cubature methods on 800 Halton points for f_3 (left) and f_4 (right) with Ω being a circular lune;
- the horizontal line correspond to LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, II



- Comparison of scattered cubature methods on 800 Halton points for f_1 (left) and f_2 (right) with Ω being a circular annulus;
- the horizontal line correspond to LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, II



- Comparison of scattered cubature methods on 800 Halton points for f_3 (left) and f_4 (right) with Ω being a circular annulus;
- the horizontal line correspond to LS-CF method;
- grey dotted line: algebraic rule with exact function values;
- x-axis: degree of exactness `dex` of the underlying (almost-)minimal algebraic rule;
- y-axis: relative cubature errors in the logarithmic scale ($\log(e_{rel})$).

Cubature on scattered data via algebraic formulas: numerical examples, II

1. A hidden difficulty, not to be disregarded, is that it is not trivial to set all the parameters of the approximants over scattered data as PUMs or RBFs interpolants or Shepard-type methods;
2. complicated domains can be treated, e.g. those whose boundary can be tracked by bivariate NURBS;
3. all the codes are available open-source at the author's homepage.

Present research

The research of our group, at present focuses on

- implementing these methods for domains in $\mathbb{R}^3$ as polyhedra and spherical polygons;
- improving the approximation quality and speed of PUMs or methods of Shepard-type;
- determining numerically estimates of cubature errors.

In this direction we are preparing

R. Cavoretto, A. De Rossi, G. Elefante, A. Sommariva and M. Vianello

Adaptive RBF cubature by scattered data on spherical polygons

- using TPS and radial powers,
- a LOOCV-like algorithm to compute the approximation via an optimal RBF (search for the best power of $\phi(r) = r^{2k+1}$);
- estimate of the integration error via LOOCV error estimates.

Bibliography

- J. Dick, F.Y. Kuo and I.H. Sloan, High-dimensional integration: The quasi-Monte Carlo way, Acta Numerica, April 2013.
  → Survey on quasi-Monte Carlo methods.
- H. Wendland, *Scattered Data Approximation*, Cambridge University Press, 2010.
  → Introduction to RBF.
- A. Sommariva, M. Vianello, Numerical cubature on scattered data by Radial Basis Functions, Computing, Volume 76, 2005, 295-310.
  → One of the first papers on RBF cubature.
- A. Sommariva and R.S. Womersley, *Integration by RBF over the Sphere*, report of UNSW.
  → RBF cubature on the sphere.
- A. Punzi, A. Sommariva, M. Vianello, Meshless cubature over the disk by Thin-Plates Splines, Journal of Computational and Applied Mathematics, Volume 221, 2008, 430-436.
  → RBF cubature on unit-disk.
- A. Sommariva, M. Vianello, RBF moment computation and meshless cubature on general polygonal regions, Applied Mathematics and Computation, Volume 409, 15 November 2021, 126375.
  → RBF cubature on polygonal regions.

Bibliography

- R. Cavoretto, A. De Rossi, A. Sommariva, M. Vianello, RBFCUB: a numerical package for near-optimal meshless cubature on general polygons, Applied Mathematics Letters, Volume 125, March 2022, 107704.
  → RBF cubature on polygonal regions with LOOCV.
- R.Cavoretto, A. De Rossi, F. Dell'Accio, F. Di Tommaso, N. Siar, A. Sommariva, M Vianello, Numerical cubature on scattered data by adaptive interpolation, Journal of Computational and Applied Mathematics, Volume 444, July 2024, 115793.
  → RBF cubature via interpolation.
- J. Glaubitz, J. Reeger, Towards stability of radial basis function based cubature formulas, BIT Numer. Math., Volume 63, 2023.
  → Cubature via scattered data (extraction of algebraic rule).
- J. Reeger, Adaptivity in Local Kernel Based Methods for Approximating the Action of Linear Operators, SIAM Journal on Scientific Computing, Vol. 46-4, 2024.
  → Recent research on this topic.
- A. Sommariva, Matlab software for cubature over scattered data
  → Software for cubature over scattered data.

Q: Are adaptive codes available for polynomial interpolation? Have you used them for comparisons?

A: Yes, there are many, from the interval (see `integral`) as well as in bivariate/trivariate hyper-rectangles (see `integral2`, `integral3`). These routines may help to compute specific integrals on many other domains (e.g. disks or sphere).

Also `Chebfun` environment allows that for the same domains (see, e.g., `sumdisk`, `sum2`).

In our homepage `Alvise Sommariva, software`, you may find these routines for polygons and spherical polygons. They are used for reference results over polygonal regions.

A: Is it important the property triangulation of the polygons (like for PDEs)?

No, it is important to be minimal so to have low cardinality rules based on formula on a reference triangle then applying barycentric coordinates. In order to decrease the cardinality of the rule, one can use compression of the rule (see `Alvise Sommariva, software`, for already implemented routines).