Constructing cubature formulas from scattered data by RBF

Alvise Sommariva and Marco Vianello

Dept. of Pure and Applied Mathematics, University of Padova (Italy)

Work supported by the "ex-60%" funds of the University of Padova, by the INdAM GNCS, and by the ARC MASCOS (research assistantship of A. Sommariva at the School of Mathematics, UNSW Sydney, Australia, 2004-2005).

Abstract

Survey of some recent results on the construction of numerical cubature formulas from scattered samples of small/moderate size, by using interpolation with Radial Basis Functions (RBF).

- **Unit square**: Error analysis and numerical tests with random points (Thin-Plate Splines and Wendland RBF).

- **Polygons**: Thin-Plate Splines over arbitary (convex as well as nonconvex and even multiply connected) polygons via Green's formula.

- **Sphere**: Construction of the formulas and tests some Franke functions.

The problem

Given a scattered sample of size n, say

$$X = \{P_i\} = \{(x_i, y_i)\} \subset \Omega; , \;\; i = 1, \ldots, n \; ,$$

and

$$\mathbf{f} = \{f(P_i)\}, \;\; i = 1, \ldots, n \; , \qquad (1)$$

of a given continuous function f on a multivariate compact set $\Omega \subset \mathbf{R}^N$ (the closure of an open and bounded set), and that we need to compute an approximate value of the integral

$$I(f) = \int_\Omega f(P)\, dP \; . \qquad (2)$$

Some basics: I

Fixed a suitable radial function $\phi : [0, +\infty) \to \mathbf{R}$, we can construct the RBF interpolant at the points $\{P_i\}$

$$s(P) := \sum_{j=1}^{n} c_j \, \phi_j(P) + p_m(P) \approx f(P) \; , \qquad (3)$$

with

$$P = (x, y) \in \Omega. \qquad (4)$$

In other words:

$$s(P_i) = f(P_i), \; i = 1, \ldots, n$$

where

- we use the notation

$$\phi_j(P) = \phi_j(P; \delta) := \phi(|P - P_j|/\delta) \; , \qquad (5)$$

- $p_m = \sum_{k=1}^{M} b_k \pi_k(P)$ polynomial of degree m ($\{\pi_k\}$ basis of the corresponding multivariate polynomial space),

- $|P - P_j|$ is a suitable distance (euclidean, geodesic, etc.),

- δ scaling parameter.

Some basics: II

The coefficients $\mathbf{c} = \{c_j\}$ are computed by solving (!) the augmented system of dimension $n + M$,

$$A\mathbf{c} + P\mathbf{b} = \mathbf{f},$$

$$P^T\mathbf{b} = \mathbf{0} \text{ where } P_{kj} = \pi_k(P_j)$$

is a symmetric matrix.

Key point: non-singularity of linear system, which depends on the choice of ϕ.

Some basics: III

Popular choices:

- Gaussians (G): $\phi(r) = \exp(-r^2)$

- Duchon's Thin-Plate Splines (TPS):
$$\phi(r) = r^2 \log(r)$$

- Hardy's MultiQuadrics (MQ):
$$\phi(r) = (1 + r^2)^{1/2}$$

- Inverse MultiQuadrics (IMQ):
$$\phi(r) = (1 + r^2)^{-1/2}$$

- Wendland's compactly supported (W2):
$$\phi(r) = (1 - r)_+^4 (4r + 1)$$

Cubature: I

Now, it is natural to approximate the integral $I(f)$ as

$$I(f) \approx I(s) = \sum_{j=1}^{n} c_j \, I(\phi_j) + I(p_m) \; ,$$

$$I(p_m) = \int_{\Omega} p_m(P) \, dP \; ,$$

$$I(\phi_j) = \int_{\Omega} \phi_j(P) \, dP \; , \quad j = 1, \ldots, n \; ,$$

where $p_m \equiv 0$ in positive definite instances.

Cubature: II

Cubature formula

$$I(f) \approx I(s) = \sum_{j=1}^{n} c_j \, I(\phi_j) + I(p_m)$$

can be rewritten in the usual form of a weighted sum of the sample values.

The positive definite case: by symmetry of A

$$I(f) \approx I(s) \tag{6}$$

$$= \langle \mathbf{c}, \mathbf{I} \rangle = \langle A^{-1}\mathbf{f}, \mathbf{I} \rangle = \langle \mathbf{f}, \mathbf{w} \rangle = \sum_{j=1}^{n} w_j \, f_j \ , \tag{7}$$

$$A\mathbf{w} = \mathbf{I} \ , \ \text{ with } \mathbf{I} = \{I(\phi_j)\}_{1 \le j \le n} \tag{8}$$

where

- $\langle \cdot, \cdot \rangle$ is the scalar product in $\mathbf{R}^N$,
- $\mathbf{I}$ the vector of integrals on Ω of the radial basis functions.

Error Analysis

The error of the RBF cubature formula described above in the presence of approximate values of the basis functions integrals, can be estimated as

$$
\begin{aligned}
|I(f) - \langle \tilde{\mathbf{w}}, \mathbf{f} \rangle| &\leq \mathit{meas}(\Omega)\, \|f - s\|_\infty && (9)\\
&+ \|A^{-1}\|_2\, \|\mathbf{f}\|_2\, \|\mathbf{I} - \tilde{\mathbf{I}}\|_2 && (10)\\
&= \mathcal{O}(\alpha(h)) + \mathcal{O}(\beta(q))\, \|\mathbf{I} - \tilde{\mathbf{I}}\|_2\ ,
\end{aligned}
$$

where

$$\alpha(h) \to 0 \text{ as } h \to 0,$$

and

$$\beta(q) \to +\infty \text{ as } q \to 0,$$

h denoting the fill distance and q the separation distance

$$q = \min_{i \neq j} \{|P_i - P_j|\} \leq 2h\ . \tag{11}$$

Cubature on unit square: Gaussian basis

By separation of variables

$$\int_{[0,1]^2} e^{-|P-P_j|^2/\delta^2}\, dP =$$

$$\begin{aligned} &= \int_0^1 e^{-(x-x_j)^2/\delta^2}\, dx \int_0^1 e^{-(y-y_j)^2/\delta^2}\, dy \\ &= \frac{\pi\delta^2}{4} \left(\mathrm{erf}\left(\frac{1-x_j}{\delta}\right) - \mathrm{erf}\left(\frac{-x_j}{\delta}\right)\right) \qquad (12) \\ &\cdot \left(\mathrm{erf}\left(\frac{1-y_j}{\delta}\right) - \mathrm{erf}\left(\frac{-y_j}{\delta}\right)\right) , \end{aligned}$$

where

$$\mathrm{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x e^{-t^2}\, dt \, .$$

Cubature on unit square: other popular basis, reduction to a right triangle, I

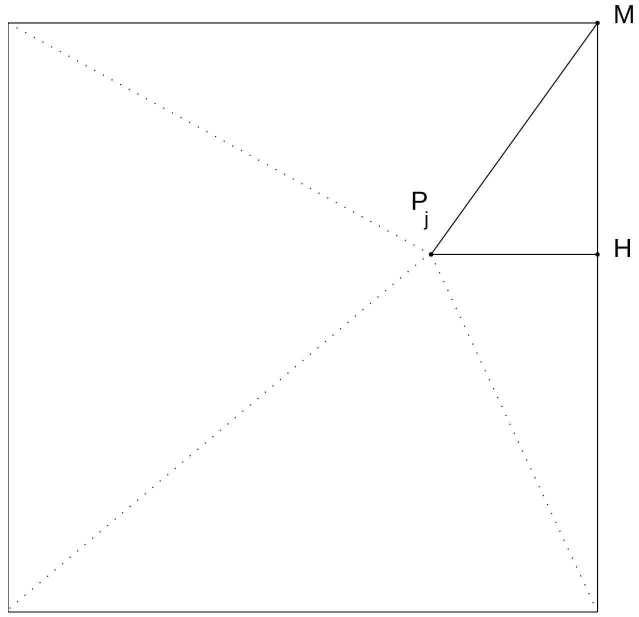
Fixing the interpolation point P_j, we

1. split the unit square with vertices $A = (0,0)$, $B = (1,0)$, $C = (1,1)$, $D = (0,1)$, into four triangles $\mathcal{T}_1 = P_jAB$, $\mathcal{T}_2 = P_jBC$, $\mathcal{T}_3 = P_jCD$, $\mathcal{T}_4 = P_jDA$;

2. split further for convenience each $\mathcal{T}_k$ into two right triangles $\mathcal{T}_k^{(1)}$, $\mathcal{T}_k^{(2)}$, each one with a vertex in P_j.

Cubature on unit square: other popular basis, reduction to a right triangle, II

Geometric explanation of the previous slide



Cubature on unit square: other popular basis, reduction to a right triangle, III

At this point, we have only to compute integrals of the form $\int_{\mathcal{T}} \phi_j(P)\, dP$ where $\mathcal{T}$ is a certain right triangle, say $\mathcal{T} = P_j H M$, with the right angle at H.

Cubature on unit square: other popular basis, reduction to a right triangle, IV

Set

- $r_0 = |P_j - H|$, $r_1 = |P_j - M|$.

- θ^* the angle $H\widehat{P_j}M$.

Integrating in polar coordinates,

$$\int_{\mathcal{T}} \phi_j(P)\, dP =$$

$$\begin{aligned}
&= \int_0^{\theta^*} \int_0^{r_0/\cos\theta} \phi_j(r\cos\theta, r\sin\theta) r\, dr\, d\theta \\
&= \int_0^{\theta^*} \int_0^{r_0/\cos\theta} \phi(r/\delta) r\, dr\, d\theta \\
&= \delta^2 \int_0^{\theta^*} \Psi\left(\frac{r_0}{\delta\cos\theta}\right) d\theta \quad ,
\end{aligned}$$

where $\theta^* = \arccos(r_0/r_1)$ and Ψ is the following primitive

$$\Psi(\rho) = \int_0^\rho \phi(r) r \, dr \; , \tag{13}$$

and

$$r_0/\delta \leq r_0/(\delta \cos\theta) \leq r_0/(\delta \cos\theta^*) = r_1/\delta \leq \sqrt{2}/\delta.$$

Cubature on unit square: other popular basis, reduction to a right triangle, V

The primitive Ψ is immediately derived analytically

- Duchon's Thin-Plate Splines (TPS):

$$\Psi(\rho) = \frac{\rho^4}{4}\left(\log \rho - \frac{1}{4}\right)$$

- Hardy's MultiQuadrics (MQ):

$$\Psi(\rho) = \frac{1}{3}\left((1+\rho^2)^{3/2} - 1\right)$$

- Inverse MultiQuadrics (IMQ):

$$\Psi(\rho) = (1+\rho^2)^{-1/2} - 1$$

- Wendland's compactly supported (W2):

$$\Psi(\rho) = -\frac{1}{7}(1-\rho)_+^5(4\rho^2 + \frac{5}{2}\rho + \frac{1}{2}) + \frac{1}{14}$$

Cubature on unit square: a summary, step I

1. The cubature problem on the unit square of some popular RBF, is reduced to the cubature of the same RBF on 8 right triangles.

2. The cubature of any RBF in one of those triangles is obtained by a *double integral*.

3. The first double integral is known explicitly.

Cubature on unit square: a summary, step II

For Thin-Plate splines and Wendland functions, also the second double integral can be computed explicitly!

See details in

A. Sommariva and M. Vianello, *Numerical cubature on scattered data by radial basis functions*, Computing **76** (2005), 295–310.

Cubature on unit square: numerical results

RBF cubature with sets of $n = 50$ and $n = 100$ random points generated with a uniform probability distribution in $[0,1]^2$: Spectral norm of the inverses of the collocation matrices and 1-norm of the computed weights vectors (average values on 50 independent trials).

50	δ	MQ	IMQ	G	$W2$	TPS
	0.1	4E+03	1E+03	1E+03	2E+01	9E+02
$\|A^{-1}\|_2$	1	2E+12	3E+11	5E+15	5E+03	6E+03
	10	>E+17	>E+17	>E+17	7E+06	6E+05
	0.1	2E+00	1E+00	1E+00	2E-01	2E+00
$\|\tilde{\mathbf{w}}\|_1$	1	7E+01	9E+01	3E+02	2E+00	1E+00
	10	6E+05	6E+04	3E+02	2E+00	1E+00

100	scaling	MQ	IMQ	G	$W2$	TPS
	0.1	1E+04	5E+03	1E+04	2E+02	9E+02
$\|A^{-1}\|_2$	1	2E+16	6E+15	>E+17	5E+04	8E+03
	10	>E+17	>E+17	>E+17	3E+07	1E+06
	0.1	2E+00	2E+00	2E+00	3E-01	1E+00
$\|\tilde{\mathbf{w}}\|_1$	1	8E+02	5E+02	1E+03	2E+00	1E+00
	10	4E+06	1E+05	6E+02	2E+00	1E+00

Cubature on unit square: numerical results II

Errors of RBF interpolation (I_n) and cubature (C_n) for the test function $f(x,y) = e^{x-y}$, with $n = 50$ and $n = 100$ random points generated with a uniform probability distribution in $[0,1]^2$ (average values on 50 samples of size n).

	δ	MQ	IMQ	G	$W2$	TPS
	0.1	8E-02	3E-01	8E-01	9E-01	5E-02
I_{50}	1	4E-03	8E-03	3E-04	2E-01	6E-02
	10	1E-03	5E-04	1E-03	3E-02	7E-02
	0.1	2E-03	3E-02	3E-01	8E-01	9E-04
C_{50}	1	6E-05	1E-04	6E-06	1E-02	2E-03
	10	7E-01	3E-02	7E-04	4E-04	2E-03
	0.1	6E-02	3E-01	5E-01	9E-01	4E-02
I_{100}	1	3E-04	8E-04	8E-04	1E-01	2E-02
	10	2E-03	7E-04	2E-03	2E-02	3E-02
	0.1	6E-04	1E-02	8E-02	7E-01	5E-04
C_{100}	1	2E-06	5E-06	1E-05	4E-03	2E-04
	10	4E+00	6E-02	1E-03	1E-04	5E-04

Cubature on polygons: Green's formula approach and TPS, I

The core of the Green's formula approach is given by computing

$$\int_{\Omega} \phi(|P-Q|)\, dQ = \int_{\partial\Omega} \left(\int \phi(|P-Q|)\, dx \right) dy \tag{14}$$

(with $P=(x,y)$. $Q=(u,v)$), as a function of the point Q.

We have put the scaling parameter $\delta = 1$ for notation simplicity, but with TPS this is not really restrictive.

Cubature on polygons: Green's formula approach and TPS, II

In the case of TPS the x-primitive above is (since $\phi(r) = r^2 \log r$)

$$\begin{aligned}
\Phi_Q(P) &:= \int \phi(|P-Q|)\,dx \\
&= \frac{1}{9}(u-x)^3 + \frac{2}{3}(u-x)(v-y)^2 \\
&- \frac{2}{3}(v-y)^3 \text{ arctan}\left(\frac{u-x}{v-y}\right) \\
&- \frac{1}{6}(u-x)((u-x)^2 + 3(v-y)^2) \\
&\cdot \log\Big((u-x)^2 + (v-y)^2\Big).
\end{aligned}$$

Cubature on polygons: Green's formula approach and TPS, III

Suppose that the domain Ω is a *polygon* (convex or nonconvex, but simply connected), whose boundary is described *counterclockwise* by a sequence of vertices $V_j = (\xi_j, \nu_j)$, $j = 1, \ldots, p$ with $p \geq 3$,

$$\partial\Omega = [V_1, V_2] \cup [V_2, V_3] \cup \cdots \cup [V_p, V_{p+1}] \;, \quad V_{p+1} = V_1 \;. \tag{15}$$

Then

$$\int_\Omega \phi(|P - Q|)\, dQ =$$

$$\begin{aligned} &= \sum_{j=1}^{p} \int_{[V_j, V_{j+1}]} \Phi_Q(P)\, dy \\ &= \sum_{\xi_j \neq \xi_{j+1}} \frac{\Delta\nu_j}{\Delta\xi_j} \int_{\xi_j}^{\xi_{j+1}} \Phi_Q\left(x, \frac{\Delta\nu_j}{\Delta\xi_j} x + \nu_j\right) dx \\ &+ \sum_{\xi_j = \xi_{j+1}} \int_{\nu_j}^{\nu_{j+1}} \Phi_Q(\xi_j, y)\, dy \end{aligned}$$

where Δ denotes the forward difference operator.

Cubature on polygons: Green's formula approach and TPS, IV

Assume that the side $[V_j, V_{j+1}]$ is not parallel to the y-axis. By putting $u - x = t$, so that $v - y = at + b$ along the side for $a = -\Delta\nu_j/\Delta\xi_j$ and $b = \nu_j - v + (u - \xi_j)\Delta\nu_j/\Delta\xi_j$, the problem is eventually reduced to computing explicitly a *second level primitive* like

$$\int \Phi_Q(u - t, v - at - b)\, dt = A(t) + B(t) + C(t) \ , \tag{16}$$

The functions A, B, C are known explicitly. See details in

A. Sommariva and M. Vianello, *Meshless cubature by Green's formula*, 2006, submitted (preprint UNSW AMR06/10, available online at http://www.maths.unsw.edu.au/applied/apphome.html).

Cubature on polygons: Some numerical results, I

We have considered the following test functions

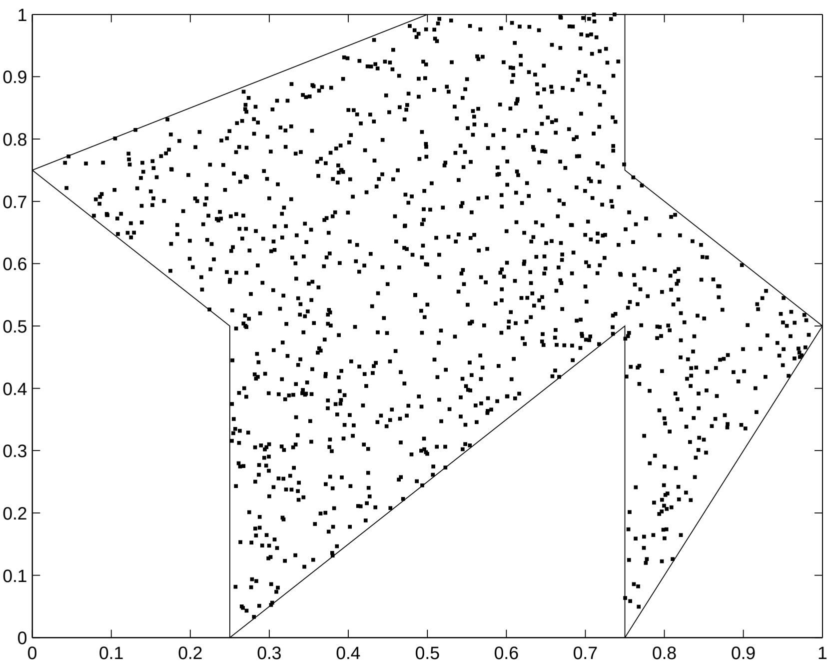
$$f_1(x,y) = \exp(x-y)\ ,\ \ f_2(x,y) = \exp(5(x-y))\ ,$$

$$f_3(x,y) = \sqrt{(x-0.5)^2 + (y-0.5)^2}\ , \qquad (17)$$

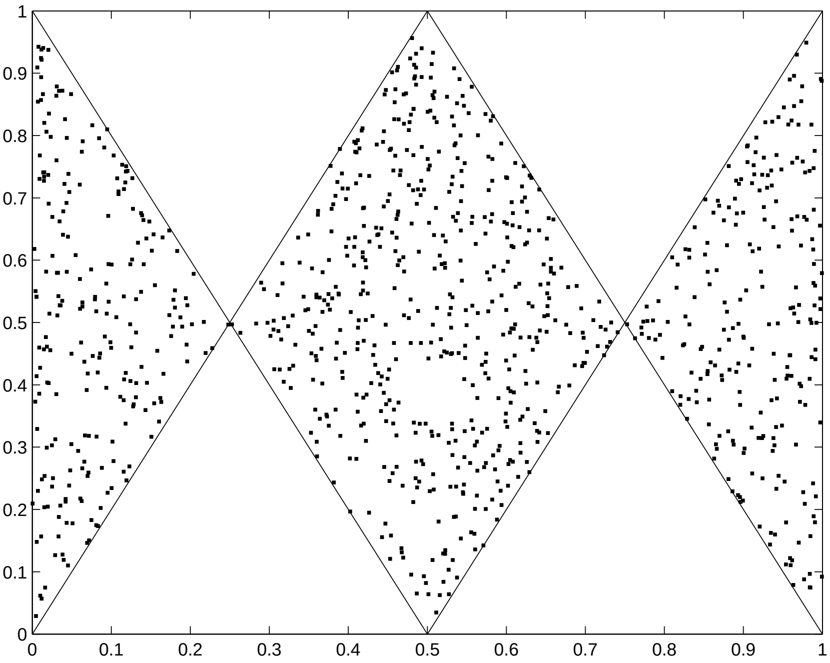
and the two nonconvex polygons. Observe that f_1 and f_2 are C^∞, whereas f_3 has a singularity of the gradient in $(0.5, 0.5)$.

Cubature on polygons: Some numerical results, II

First non-convex polygon and scattered data



Second non-convex polygon and scattered data



Cubature on polygons: Some numerical results, III

Errors of TPS interpolation and TPS-Green compared to Monte Carlo cubature with $n =$ 100, 800 *uniform random points on the 1st nonconvex polygon (average values on* 50 *independent trials, rounded to the 1st significant digit).*

function	formula	100 pts	800 pts
f_1	TPS_intp	5E-02	1E-02
	TPS_Green	1E-04	8E-06
	MC	1E-02	5E-03
f_2	TPS_intp	8E+00	1E+00
	TPS_Green	2E-02	9E-04
	MC	2E-01	7E-02
f_3	TPS_intp	4E-02	8E-03
	TPS_Green	2E-04	6E-06
	MC	4E-03	2E-03

Cubature on polygons: Some numerical results, IV

Examples on the 2nd nonconvex polygon.

function	formula	100 pts	800 pts
f_1	TPS_intp	1E-01	2E-02
	TPS_Green	3E-04	1E-05
	MC	2E-02	6E-03
f_2	TPS_intp	2E+01	2E+01
	TPS_Green	2E-02	8E-04
	MC	4E-01	2E-01
f_3	TPS_intp	5E-02	9E-03
	TPS_Green	2E-04	9E-06
	MC	6E-03	2E-03

Cubature on the sphere: a note, I

As we have previously seen, the key-point is the integration of the RBF functions, i.e.

$$\int_{\Omega} \phi(\|P - P_i\|)\, d\Omega$$

where P_i is the center of the RBF. In the case of the sphere, the symmetry makes the integral independent of the point P_i. Again, the integrals of the more popular RBF

$$\int_{\Omega} \phi(\|P - P_i\|)\, d\Omega$$

are known explicitly. For their representation and some numerical examples, consider

A. Sommariva, R. Womersley, *Integration by RBF over the Sphere*.

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