RBFCUB: a numerical package for near-optimal meshless cubature on general polygons

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Abstract

In this paper we improve the cubature rules discussed in [12] for the computation of integrals by radial basis functions (RBFs). More precisely, we introduce in the context of meshless cubature a leave-one-out cross validation criterion for the optimization of the RBF shape parameter. This choice allows us to get highly reliable and accurate results for any kind of both infinity and finite regularity RBF. The efficacy of this approximation scheme is tested by numerical experiments on complicated polygonal regions. The related Matlab software is provided to the scientific community in [5].

Keywords: meshless cubature, radial basis functions, multivariate approximation, scattered data, polygonal regions
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1. Introduction

In [12] analytical formulas for computing integrals of the most popular *radial basis functions* (RBFs) are obtained. In particular, the previous work provides an efficient way to compute moments and cubature weights for a wide class of infinity and finite smooth RBFs, either globally or compactly supported. The resulting cubature rules can successfully be applied on general polygonal regions. However, due to severe ill-conditioning of the cubature matrix, the numerical method in [12] is able to provide good and predictable results for low-regularity (and shape parameter free) RBFs. On the contrary, when the basis functions need to be suitably scaled and/or high-regularity RBFs are considered, this direct method may result in deeply unpredictable and meaningless results, as observed in [12].

In this article we enhance the method [12] proposing in the context of RBF cubature the use of a technique that corresponds to a variant of cross validation, known as *leave-one-out cross validation* (LOOCV). By doing so, we are able to predict a "good" or a (near) optimal value of the RBF shape parameter. This procedure was originally introduced in RBF interpolation by Rippa [10], and more recently has widely been used in several fields of applied mathematics and scientific computing (see e.g. [3, 4, 6, 8]). As shown in our numerical experiments, the selection of optimal RBF shape parameters via LOOCV allows us to obtain precise and trustworthy results for any – even C^∞ smooth – type of RBF. The improved cubature process is tested by taking some 2D benchmark test functions and nonconvex or multiply disconnected polygonal regions, already considered in [12].

The paper is organized as follows. In Section 2 we give some preliminaries on RBF interpolation and cubature. In Section 3 we present the LOOCV method for selecting an optimal shape parameter. In Section 4 we show some numerical results in order to illustrate the performance of our cubature formulas for a wide range of RBFs. Section 5 contains conclusions.

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2. Problem statement

In this section we give a brief overview on RBF methods recalling some basic definitions and results, which are useful in the context of scattered data approximation. For further details on theoretical and computational issues, we refer the reader to [2, 8, 13].

2.1. RBF interpolation

Given a compact domain $\Omega \subset \mathbb{R}^d$, we denote by $X = \{(\boldsymbol{x}_i, f_i)\}_{i=1}^N$ a set of scattered data. The N distinct *data points* (or *nodes*) $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_N$ are assumed in Ω, while the corresponding *data* or *function values* $f_1, \ldots, f_N \in \mathbb{R}$ are obtained by possibly sampling any (unknown) function $f : \Omega \to \mathbb{R}$.

If we consider a RBF $\phi : \mathbb{R}_{\geq 0} \to \mathbb{R}$ that is *strictly conditionally positive definite* (SCPD) of order m, setting $\phi_i(\boldsymbol{x}) := \phi(||\boldsymbol{x} - \boldsymbol{x}_i||_2)$, we can determine a unique interpolating function $s : \Omega \to \mathbb{R}$ expressed as a linear combination of the basis functions ϕ_i, i.e.,

$$s(\boldsymbol{x}) = \sum_{i=1}^{N} c_i \phi_i(\boldsymbol{x}) + \sum_{i=N+1}^{N+M} c_i \pi_{i-N}(\boldsymbol{x}), \tag{1}$$

where $\{\pi_k\}_{k=1}^M$ form a basis for the $M = \binom{m-1+d}{m-1}$-dimensional linear space $\mathbb{P}_{m-1}^d$ of d-variate real valued polynomials of total degree less than or equal to $m-1$, and $||\cdot||_2$ denotes the Euclidean norm. The real (unknown) coefficients $c_1, \ldots, c_{N+M}$ are obtained by enforcing the interpolation conditions, that is, $s(\boldsymbol{x}_i) = f_i$, for $i = 1, \ldots, N$. Moreover, from RBF theory we know that a SCPD function of order 0 (i.e., $m = 0$) is called *strictly positive definite* (SPD), and so the polynomial in (1) vanishes [7].

Solving the interpolation problem in the general case of a SCPD function ϕ of order m results in a linear system of the form

$$\mathcal{A}\mathbf{c} = \mathbf{b}, \tag{2}$$

where

$$\mathcal{A} := \begin{bmatrix} A & P \\ P^T & O \end{bmatrix}, \qquad \mathbf{b} := \begin{bmatrix} \mathbf{f} \\ \mathbf{0} \end{bmatrix}.$$

The entries of the (symmetric) *interpolation matrix* $\mathcal{A}$ in (2) are $A_{i,j} := \phi(||\boldsymbol{x}_i - \boldsymbol{x}_j||_2)$, $P_{ik} := \pi_k(\boldsymbol{x}_i)$, with $i, j = 1, \ldots, N$, $k = 1, \ldots, M$, and O is a $M \times M$ zero matrix. Furthermore, $\mathbf{c} := [c_1, \ldots, c_{N+M}]^T$, $\mathbf{f} := [f_1, \ldots, f_N]^T$ and $\mathbf{0}$ is a zero vector of length M. It is also important to note that in the particular case of a SPD RBF the matrix reduces simply to $\mathcal{A} = A$, and the polynomial part disappears.

Usually, in literature, several RBFs are scaled in terms of a *shape parameter* $\varepsilon > 0$ such that

$$\phi_\varepsilon(r) = \phi(\varepsilon r).$$

In the following, for the sake of simplicity, we refer to $\phi_i(\boldsymbol{x})$ as $\phi_\varepsilon(||\boldsymbol{x} - \boldsymbol{x}_i||)$, keeping always implicit (unless necessary) the dependence on ε. For these RBFs the selection of a suitable value of ε is a crucial task, but also a big issue (cf. [4]). Though there are also families of RBFs that do not need a scaling of their argument (i.e., they are shape parameter free), in this work we only take into account RBFs depending on ε. In Table 1 we list some of the most popular SCPD RBFs together with their orders, see e.g. [7]. Note that Gaussian, Inverse MultiQuadric and MultiQuadric functions are globally supported, while the Wendland functions are compactly supported and their support is given by $[0, 1/\varepsilon]$, see [13].

2.2. RBF cubature by moment computation

In the numerical cubature we consider the problem of computing an approximate value of the integral

$$I(f) := \int_\Omega f(\boldsymbol{x}) \, d\boldsymbol{x},$$

RBF	$\phi_\varepsilon(r)$	SCPD order
Gaussian C^∞ (GA)	$\exp(-\varepsilon^2 r^2)$	0
Inverse MultiQuadric C^∞ (IMQ)	$(1+\varepsilon^2 r^2)^{-1/2}$	0
MultiQuadric C^∞ (MQ)	$(1+\varepsilon^2 r^2)^{1/2}$	1
Wendland C^4 (W4)	$\max(1-\varepsilon r, 0)^6 \, (35\varepsilon^2 r^2 + 18\varepsilon r + 3)$	0
Wendland C^2 (W2)	$\max(1-\varepsilon r, 0)^4 \, (4\varepsilon r + 1)$	0
Matérn C^2 (M2)	$\exp(-\varepsilon r)(\varepsilon r + 1)$	0
Matérn C^0 (M0)	$\exp(-\varepsilon r)$	0

Table 1: Some of the most popular RBFs.

where $f(\boldsymbol{x})$ is an integrable function, which is generally known only on a scattered data set X. A direct approach to solve this problem consists in integrating the RBF interpolant s in (1), i.e.,

$$I(f) \approx I(s) = \int_\Omega s(\boldsymbol{x})\; d\boldsymbol{x} = \sum_{i=1}^{N} c_i \int_\Omega \phi_i(\boldsymbol{x})\; d\boldsymbol{x} + \sum_{i=N+1}^{N+M} c_i \int_\Omega \pi_{i-N}(\boldsymbol{x})\; d\boldsymbol{x}.$$

Defining the moment vectors $\mathbf{I}_\phi = \{I(\phi_i)\}_{i=1}^N$, $\mathbf{I}_\pi = \{I(\pi_k)\}_{k=1}^M$ and denoting by $\langle \cdot, \cdot \rangle$ the scalar product in $\mathbb{R}^d$, we obtain that

$$I(s) = \langle \mathbf{c}, \mathbf{I} \rangle, \quad \text{with } \mathbf{I} := \begin{bmatrix} \mathbf{I}_\phi \\ \mathbf{I}_\pi \end{bmatrix}. \tag{3}$$

For a more comprehensive study and a detailed error analysis, the reader can refer to [12].

2.3. RBF moment computation

In [12] the authors introduced a triangulation-free algorithm for moment computation of the most common RBFs on polygonal regions that we briefly describe in this section.

Let Ω be a simple polygon, i.e. without self intersections, described counterclockwise by the sequence of vertices $\{\boldsymbol{v}_j\}_{j=1,\dots,n+1}$, where $\boldsymbol{v}_{n+1} = \boldsymbol{v}_1$. In view of Gauss-Green theorem in polar coordinates, we have that the moment $I_\Omega(\phi_k) = \int_\Omega \phi(\varepsilon\|\boldsymbol{x} - \boldsymbol{x}_k\|_2)\, d\boldsymbol{x}$ of the scaled RBF ϕ centered in $\boldsymbol{x}_k$ with shape parameter ε, is such that

$$I_\Omega(\phi_k) = \oint_{\partial\Omega} \left(\int r\phi(\varepsilon\, r) dr \right) d\theta = \sum_{j=1}^{n} \int_{\overline{\boldsymbol{v}_j \boldsymbol{v}_{j+1}}} \int r\phi(\varepsilon\, r) dr\; d\theta.$$

where $r = \|\boldsymbol{x} - \boldsymbol{x}_k\|_2$ and $\overline{\boldsymbol{v}_j \boldsymbol{v}_{j+1}}$ is the segment joining the vertex $\boldsymbol{v}_j$ with $\boldsymbol{v}_{j+1}$.

Now set $\mu_0 = 1$ if the non-degenerate triangle with vertices $\boldsymbol{x}_k, \boldsymbol{v}_j, \boldsymbol{v}_{j+1}$ is ordered counterclockwise and $\mu_0 = -1$ otherwise. Next, let r_0 be the length of the segment $\overline{\boldsymbol{x}_k \boldsymbol{v}_j}$, θ_0 and θ^* respectively the absolute values of the angles $\boldsymbol{x}_k \widehat{\boldsymbol{v}_j \boldsymbol{v}}_{j+1}$ and $\boldsymbol{v}_j \widehat{\boldsymbol{x}_k \boldsymbol{v}}_{j+1}$, $\Psi(\rho) := \int_0^\rho t\phi(t)dt$, $c_{\theta_0,\varepsilon} := \varepsilon\, r_0 \sin(\theta_0)$. In [12] it is proven that

$$\int_{\overline{\boldsymbol{v}_j \boldsymbol{v}_{j+1}}} \int r\phi(\varepsilon\, r) dr\; d\theta = \mu_0\, \varepsilon^{-2} \int_{\theta_0}^{\theta^*+\theta_0} \Psi(c_{\theta_0,\varepsilon} / \sin(s))\, ds. \tag{4}$$

with $0 \le \theta_0 < \theta^* + \theta_0 < \pi$, $c_{\theta_0,\varepsilon} > 0$. Since

$$\int_{\theta_0}^{\theta^*+\theta_0} \Psi(c_{\theta_0,\varepsilon} / \sin(s))\, ds = \int_{\pi/2}^{\theta^*+\theta_0} \Psi(c_{\theta_0,\varepsilon} / \sin(s))\, ds - \int_{\pi/2}^{\theta_0} \Psi(c_{\theta_0,\varepsilon} / \sin(s))\, ds$$

the required moment is at hand as soon as one is able to evaluate

$$I_{c,\pi/2,t^*}(\Psi) = \int_{\pi/2}^{t^*} \Psi(c/\sin(s))\, ds,\ c > 0,\ t^* \in (0, \pi).$$

In the appendix of [12] there is an explicit formulation of $I_{c,\pi/2,t^*}(\Psi)$ for Multiquadrics, Inverse Multiquadrics, Thin-Plate Splines, Radial Powers of the form $\phi(r) = r^k$ with $k = 3, 5, 7$, RBFs with compact support such as the Wendland RBFs $W0$, $W2$, $W4$, $W6$, while for the Gaussian and the Matérn RBFs $\phi(r) = \exp(-r)$ and $\phi(r) = (1 + r) \exp(-r)$, the authors were only able to determine Ψ in closed form and next compute the required integrals by suitable shifted Gauss-Legendre rules.

We finally point out that some care should be taken with RBFs that are compactly supported (see [12] for additional details). We conclude observing that if Ω consists of a simple polygon Ω_0 with some non overlapping simple polygonal *holes* $\Omega_1, \ldots, \Omega_M$, then $I_\Omega(\phi_k) = I_{\Omega_0}(\phi_k) - \sum_{j=1}^{M} I_{\Omega_j}(\phi_k)$ where all the values $I_{\Omega_0}(\phi_k), \ldots, I_{\Omega_M}(\phi_k)$ can be computed by the technique described above.

3. Selecting an optimal shape parameter via LOOCV

As it is well-known, from the *uncertainty* or *trade-off principle* [11] we know that using a RBF one cannot have high accuracy and stability at the same time. In fact, when the best accuracy is typically achieved, i.e., in the *flat limit* $\varepsilon \to 0$, the interpolation matrix might suffer from severe ill-conditioning. In order to get trustworthy solutions, it is therefore essential to find an optimal value of the shape parameter ε.

3.1. Error computation

A popular strategy for estimating the RBF shape parameter ε based on the given data set $X = \{(\boldsymbol{x}_i, f_i)\}_{i=1}^N$ is the LOOCV method [10]. In this technique an optimal value of ε is selected by minimizing a cost function that collects the errors for a sequence of partial fits to the data. To estimate the unknown true error, we split the data into two parts: a *training* data set consisting of $N-1$ data to obtain a "partial interpolation", and a *validation* data set that contains a single (remaining) data used to compute the error. After repeating in turn this procedure for each of the N given data, the result is a vector of error estimates and the cost function is used to determine the optimal value of ε, see [9].

For this discussion we define by

$$\boldsymbol{x}^{[k]} := [\boldsymbol{x}_1, \ldots, \boldsymbol{x}_{k-1}, \boldsymbol{x}_{k+1}, \ldots, \boldsymbol{x}_N]^T, \qquad \mathbf{f}^{[k]} := [f_1, \ldots, f_{k-1}, f_{k+1}, \ldots, f_N]^T,$$

the vectors of data points and corresponding values with the removed data $(\boldsymbol{x}_k, f_k)$, denoted by the superscript $[k]$. In the sequel, all other qualities are represented similarly.

The key idea is to predict the parameter ε considering the partial RBF interpolant to the data $(\boldsymbol{x}^{[k]}, \mathbf{f}^{[k]})$, i.e.,

$$s^{[k]}(\boldsymbol{x}) = \sum_{i=1,\ i\neq k}^{N} c_i \phi_i(\boldsymbol{x}) + \sum_{i=N+1}^{N+M} c_i \pi_{i-N}(\boldsymbol{x}).$$

If e_k is the error estimator

$$e_k(\varepsilon) = f_k - s^{[k]}(\boldsymbol{x}_k), \tag{5}$$

the norm of the vector of errors $\mathbf{e} = [e_1, \ldots, e_N]^T$ as a function of ε can be used to minimize the cost function and find the optimal value of ε. Thus, this vector is computed by removing in turn each node of X, then comparing the resulting fit with the known value at the removed point.

Since this LOOCV implementation is quite expensive, the error computation can be simplified by using the rule

$$e_k(\varepsilon) = \frac{c_k}{\mathcal{A}^{-1}_{kk}}, \tag{6}$$

where c_k is the kth coefficient of the solution vector $\mathbf{c} = \mathcal{A}^{-1}\mathbf{b}$ in (2), and $\mathcal{A}^{-1}_{kk}$ is the kth diagonal element of the inverse of the *full* RBF matrix $\mathcal{A}^{-1}$. Notice that this formulation needs to only solve a single linear system, considering the entire data set X.

In summary, the problem is solved by minimizing the cost function

$$\mathrm{LOOCV}(\varepsilon) = ||\mathbf{e}(\varepsilon)||_\infty = \max_{k=1,\ldots,N} \left| \frac{c_k}{\mathcal{A}^{-1}_{kk}} \right|. \tag{7}$$

where $||\cdot||_\infty$ denotes the ∞-norm, even if in principle any norm is enabled.

Remark 3.1. One may wonder whether it is convenient writing the cubature formula (3) in a more standard form, as a linear combination of function values with cubature weights. This is clearly possible, following the lines of [12], by solving the relevant moment matching system with the transposed interpolation matrix. In the present context, however, there is no computational advantage, since the optimal shape parameter is function dependent and so are consequently the weights, preventing from using them for different functions.

3.2. Computational complexity and implementation details

While the naive implementation of LOOCV algorithm by the estimator (5) is rather costly (i.e., of the order $\mathcal{O}(N^4)$), the use of the single formula (6) reduces the computational complexity to $\mathcal{O}(N^3)$. Furthermore, all entries of the error vector $\mathbf{e}$ can be computed simply by a single statement in Matlab, provided that the component rule (6) is vectorized. Finally, in order to quickly find an optimal shape parameter, the minimum of the cost function (7) can be determined by the Matlab function `fminbnd`. For further implementation details, see the Matlab codes available in [5].

4. Numerical results

In this section we report some results of extensive experiments carried out to test our numerical cubature technique. Since we want to verify accuracy and effectiveness of our integration formulas for ε-dependent RBFs w.r.t. the ones studied in [12], we consider the same 2D complex polygonal domains Ω_s, $s = 1, 2$, see Figure 1. In particular, we analyze the precision/behavior of infinity smooth RBFs such as GA, IMQ and MQ, and finite regularity RBFs like W4, W2, M2 and M0 (cf. Table 1). As test functions, we take

$$f_1(x, y) = \exp(x - y), \qquad f_2(x, y) = \sqrt{(x - 0.3)^2 + (y - 0.3)^2}.$$

In order to measure the quality of our results, we compute the *maximum relative errors* (MREs) assuming as *reference* (or *exact*) values the ones obtained by the algebraic cubature algorithm in [1], with algebraic degree of exactness equal to 1000.

In Tables 2 and 3 we show the cubature MREs obtained by selecting optimal values of the shape parameter ε. As discussed in Section 3, the ε-detection via LOOCV is determined by the use of Matlab `fminbnd` minimization routine. The optimal shape parameters are searched for $\varepsilon \in [0.5, 15]$, while all other routine parameters were set by their default values. Although the cubature matrix $\mathcal{A}$ may be extremely ill-conditioned (in particular, with C^∞ RBFs and small values of ε), the LOOCV approach still enables to make good predictions of ε, thus permitting to get reliable results, a feature not available in the previous work [12].

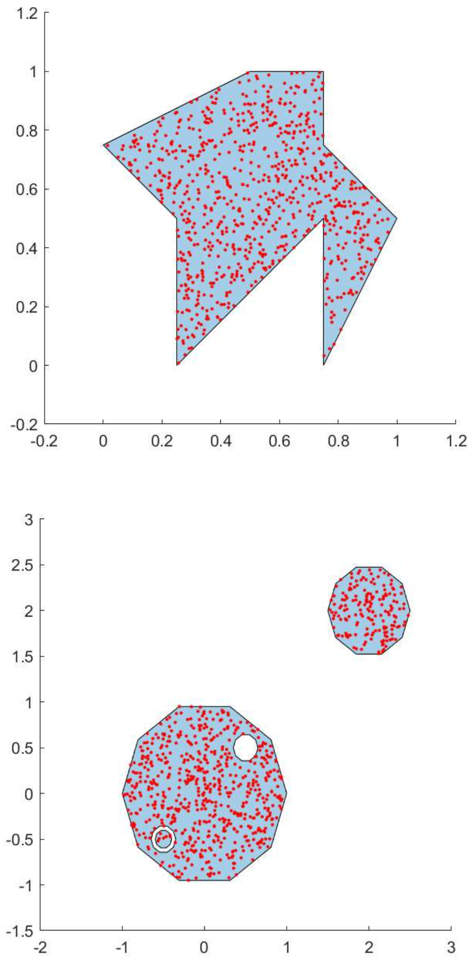

Figure 1: Polygonal regions Ω_1 (top) and Ω_2 (bottom) with scattered data points.

Test	N	GA	IMQ	MQ	W4	W2	M2	M0
f_1	200	2e−7	5e−7	4e−7	2e−4	6e−4	2e−4	2e−3
	400	1e−7	1e−5	3e−7	1e−5	4e−5	9e−6	3e−4
	800	7e−8	6e−7	2e−7	1e−6	2e−5	8e−6	6e−5
f_2	200	4e−3	1e−3	7e−4	9e−4	5e−4	1e−4	2e−3
	400	4e−3	8e−4	3e−4	2e−4	1e−4	1e−4	6e−4
	800	2e−3	3e−5	2e−5	1e−5	4e−6	5e−6	3e−5

Table 2: MREs computed by RBF cubature on Ω_1.

5. Conclusions

In this paper we solved the main open problem in [12]. While the original method provided reasonably accurate and numerically stable cubature rules for finite regularity RBFs, such as thin plate splines, radial powers and W2 (for $\varepsilon = 1$ fixed), this new approach based on the LOOCV criterion for the ε-prediction

Test	N	GA	IMQ	MQ	W4	W2	M2	M0
f_1	200	6e−6	2e−4	3e−6	8e−4	2e−3	4e−4	4e−3
	400	2e−7	3e−6	7e−6	7e−5	3e−4	3e−5	7e−4
	800	6e−8	7e−7	9e−8	2e−5	9e−5	9e−6	4e−4
f_2	200	7e−4	5e−5	1e−4	5e−4	1e−3	1e−4	7e−4
	400	6e−4	1e−4	1e−4	5e−5	6e−4	1e−4	2e−4
	800	5e−4	3e−5	2e−5	2e−5	7e−5	4e−6	1e−4

Table 3: MREs computed by RBF cubature on Ω_2.

leads to a two-fold benefit: (i) obtaining highly reliable and precise results for any kind of RBF, even infinity smooth; (ii) reducing the cubature error for those finite regularity RBFs, such as W2, for which an optimal choice of ε is noteworthy.

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