

Partition of Unity Interpolation on Multivariate Convex Domains

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Abstract. In this paper we present a new algorithm for multivariate interpolation of scattered data sets lying in convex domains $\Omega \subseteq \mathbb{R}^N$, for any $N \geq 2$. To organize the points in a multidimensional space, we build a *kd-tree* space-partitioning data structure, which is used to efficiently apply a partition of unity interpolant. This global scheme is combined with local radial basis function approximants and compactly supported weight functions. A detailed description of the algorithm for convex domains and a complexity analysis of the computational procedures are also considered. Several numerical experiments show the performances of the interpolation algorithm on various sets of Halton data points contained in Ω , where Ω can be any convex domain like a 2D polygon or a 3D polyhedron.

Keywords: Meshfree Approximation, Multivariate Algorithms, Partition of Unity Methods, Scattered Data.

1 Introduction

In this paper we deal with the problem of interpolating a (usually) large number of multivariate scattered data points lying in convex domains or, more precisely, in convex hulls $\Omega \subseteq \mathbb{R}^N$, for any $N \geq 2$. In general, this problem is considered in literature supposing to interpolate data points which are situated in suitable or simple domains such as hypercubes or hyperrectangles (see e.g. [7,8,11]). Thus we construct a numerical algorithm which can efficiently be used for scattered data interpolation in Ω . To organize the points in a multivariate space, we make use of a space-partitioning data structure known as *kd-tree* (see [12]). This code is designed to numerically approximate data points by the partition of unity method, a global interpolation scheme which is combined with local radial basis function (RBF) approximants and compactly supported weight functions (see [9,13,14]). A detailed design of this algorithm as well as an analysis of its complexity is considered.

Moreover, we observe that the implemented code is completely automatic and any choice depending on the space dimension has suitably been studied so that this algorithm can work for any dimension. Numerical experiments show

the performances of the interpolation algorithm on various sets of Halton data points contained in $\Omega \subseteq \mathbb{R}^N$, for $N = 2, 3$. Here, Ω is any convex domain like a 2D polygon (e.g., a triangle or a hexagon) or a 3D polyhedron (e.g., a pyramid or a cylinder). Note that this algorithm for convex hulls extends our previous works on the topic [3,4,5,6].

The paper is organized as follows. In Section 2 we give a general presentation of the partition of unity interpolation combined with local radial basis functions, reporting some theoretical results. In Section 3, we describe the algorithm for convex hulls and analyze its complexity. In Section 4, in order to show accuracy and efficiency of the interpolation algorithm, we report numerical experiments considering various sets of scattered data points contained in 2D and 3D convex domains. Finally, Section 5 refers to conclusions and future work.

2 Partition of Unity Interpolation

Let $\mathcal{X}_n = \{\mathbf{x}_i, i = 1, 2, \dots, n\}$ be a set of distinct data points, arbitrarily distributed in a domain $\Omega \subseteq \mathbb{R}^N$, $N \geq 1$, with an associated set $\mathcal{F}_n = \{f_i, i = 1, 2, \dots, n\}$ of data values or function values, which are obtained by sampling some (unknown) function $f : \Omega \rightarrow \mathbb{R}$ at the data points, i.e., $f_i = f(\mathbf{x}_i)$, $i = 1, 2, \dots, n$.

The basic idea of the partition of unity method is to start with a partition of the open and bounded domain $\Omega \subseteq \mathbb{R}^N$ into d subdomains Ω_j such that $\Omega \subseteq \bigcup_{j=1}^d \Omega_j$ with some mild overlap among the subdomains. Associated with these subdomains we choose a partition of unity, i.e. a family of compactly supported, non-negative, continuous functions W_j with $\text{supp}(W_j) \subseteq \Omega_j$ such that

$$\sum_{j=1}^d W_j(\mathbf{x}) = 1, \quad \mathbf{x} \in \Omega. \quad (1)$$

The global approximant thus assumes the following form

$$\mathcal{I}(\mathbf{x}) = \sum_{j=1}^d R_j(\mathbf{x})W_j(\mathbf{x}), \quad \mathbf{x} \in \Omega. \quad (2)$$

For each subdomain Ω_j we define a local RBF interpolant $R_j : \Omega \rightarrow \mathbb{R}$ of the form

$$R_j(\mathbf{x}) = \sum_{k=1}^{n_j} c_k \phi(d(\mathbf{x}, \mathbf{x}_k)), \quad (3)$$

where $d(\mathbf{x}, \mathbf{x}_k) = \|\mathbf{x} - \mathbf{x}_k\|_2$ is the Euclidean distance, $\phi : [0, \infty) \rightarrow \mathbb{R}$ is called *radial basis function*, and n_j indicates the number of data points in Ω_j . Moreover, R_j satisfies the interpolation conditions

$$R_j(\mathbf{x}_i) = f_i, \quad i = 1, 2, \dots, n_j. \quad (4)$$

In particular, we observe that if the local approximants satisfy the interpolation conditions (4), then the global approximant also interpolates at \mathbf{x}_i , i.e. $\mathcal{I}(\mathbf{x}_i) = f(\mathbf{x}_i)$, for $i = 1, 2, \dots, n_j$.

Solving the j -th interpolation problem (4) leads to a system of linear equations of the form

$$\Phi \mathbf{c} = \mathbf{f},$$

where entries of the interpolation matrix Φ are

$$\Phi_{ik} = \phi(d(\mathbf{x}_i, \mathbf{x}_k)), \quad i, k = 1, 2, \dots, n_j,$$

$$\mathbf{c} = [c_1, c_2, \dots, c_{n_j}]^T \text{ and } \mathbf{f} = [f_1, f_2, \dots, f_{n_j}]^T.$$

Now, we give the following definition (see [13]).

Definition 1. Let $\Omega \subseteq \mathbb{R}^N$ be a bounded set. Let $\{\Omega_j\}_{j=1}^d$ be an open and bounded covering of Ω . This means that all Ω_j are open and bounded and that Ω is contained in their union. A family of nonnegative functions $\{W_j\}_{j=1}^d$ with $W_j \in C^k(\mathbb{R}^N)$ is called a k -stable partition of unity with respect to the covering $\{\Omega_j\}_{j=1}^d$ if

- 1) $\text{supp}(W_j) \subseteq \Omega_j$;
- 2) $\sum_{j=1}^d W_j(\mathbf{x}) \equiv 1$ on Ω ;
- 3) for every $\beta \in \mathbb{N}_0^N$ with $|\beta| \leq k$ there exists a constant $C_\beta > 0$ such that

$$\|D^\beta W_j\|_{L^\infty(\Omega_j)} \leq C_\beta / \delta_j^{|\beta|}, \quad j = 1, 2, \dots, d,$$

where $\delta_j = \text{diam}(\Omega_j) = \sup_{\mathbf{x}, \mathbf{y} \in \Omega_j} \|\mathbf{x} - \mathbf{y}\|_2$.

In accordance with the statements in [13] we require some additional regularity assumptions on the covering $\{\Omega_j\}_{j=1}^d$.

Definition 2. Suppose that $\Omega \subseteq \mathbb{R}^N$ is bounded and $\mathcal{X}_n = \{\mathbf{x}_i, i = 1, 2, \dots, n\} \subseteq \Omega$ are given. An open and bounded covering $\{\Omega_j\}_{j=1}^d$ is called regular for (Ω, \mathcal{X}_n) if the following properties are satisfied:

- (a) for each $\mathbf{x} \in \Omega$, the number of subdomains Ω_j with $\mathbf{x} \in \Omega_j$ is bounded by a global constant K ;
- (b) each subdomain Ω_j satisfies an interior cone condition [14];
- (c) the local fill distances $h_{\mathcal{X}_{n_j}, \Omega_j}$, where $\mathcal{X}_{n_j} = \mathcal{X}_n \cap \Omega_j$, are uniformly bounded by the global fill distance $h_{\mathcal{X}_n, \Omega}$, i.e.

$$h_{\mathcal{X}_n, \Omega} = \sup_{\mathbf{x} \in \Omega} \min_{\mathbf{x}_k \in \mathcal{X}_n} d(\mathbf{x}, \mathbf{x}_k).$$

After defining the space $C_\nu^k(\mathbb{R}^N)$ of all functions $f \in C^k$ whose derivatives of order $|\beta| = k$ satisfy $D^\beta f(\mathbf{x}) = \mathcal{O}(\|\mathbf{x}\|_2^\nu)$ for $\|\mathbf{x}\|_2 \rightarrow 0$, we consider the following convergence result (see, e.g., [7, 14]).

Theorem 1. *Let $\Omega \subseteq \mathbb{R}^N$ be open and bounded and suppose that $\mathcal{X}_n = \{\mathbf{x}_i, i = 1, 2, \dots, n\} \subseteq \Omega$. Let $\phi \in C_\nu^k(\mathbb{R}^N)$ be a strictly positive definite function. Let $\{\Omega_j\}_{j=1}^d$ be a regular covering for (Ω, \mathcal{X}_n) and let $\{W_j\}_{j=1}^d$ be k -stable for $\{\Omega_j\}_{j=1}^d$. Then the error between $f \in \mathcal{N}_\phi(\Omega)$, where \mathcal{N}_ϕ is the native space of ϕ , and its partition of unity interpolant (2) can be bounded by*

$$|D^\beta f(\mathbf{x}) - D^\beta \mathcal{I}(\mathbf{x})| \leq Ch_{\mathcal{X}_n, \Omega}^{(k+\nu)/2-|\beta|} |f|_{\mathcal{N}_\phi(\Omega)},$$

for all $\mathbf{x} \in \Omega$ and all $|\beta| \leq k/2$.

If we compare this result with the global error estimates (see e.g. [14]), we can see that the partition of unity preserves the local approximation order for the global fit. This means that we can efficiently compute large RBF interpolants by solving small RBF interpolation problems and then glue them together with the global partition of unity $\{W_j\}_{j=1}^d$. In other words, the partition of unity approach is a simple and effective technique to decompose a large problem into many small problems while at the same time ensuring that the accuracy obtained for the local fits is carried over to the global one.

3 Algorithm for Convex Hulls

In this section we present an algorithm for multivariate interpolation of scattered data sets lying in a convex domain (or convex hull) $\Omega \subseteq \mathbb{R}^N$, for any $N \geq 2$. This code is based on a global partition of unity interpolant using local RBF interpolants and compactly supported weight functions. To organize the points in a multivariate space, we build an efficient space-partitioning data structure as the *kd-trees*, because this enables us to efficiently answer a query, known as *range search* (see [1,2]). In fact, we need to solve the following computational issue:

Given a set X of points $\mathbf{x}_i \in X$ and a subdomain Ω_j , find all points situated in that subdomain, i.e. $\mathbf{x}_i \in X_j = X \cap \Omega_j$.

Note that the subdomain Ω_j denotes a generic region, so the index j is here fixed. For simplicity, all details of this algorithm concern a generic convex hull $\Omega \subseteq [0, 1]^N$, but its generalization is obviously possible and straightforward.

3.1 Description of the Algorithm

INPUT: N , space dimension; n , number of data; $\mathcal{X}_n = \{\mathbf{x}_i, i = 1, 2, \dots, n\}$, set of data points; $\mathcal{F}_n = \{f_i, i = 1, 2, \dots, n\}$, set of data values.

OUTPUT: $\mathcal{A}_s = \{\mathcal{I}(\tilde{\mathbf{x}}_i), i = 1, 2, \dots, s\}$, set of approximated values.

Stage 1. The set \mathcal{X}_n of data points and the set \mathcal{F}_n of data values are loaded.

Stage 2. After computing the number d of subdomain points, a set $\mathcal{C}_d = \{\tilde{\mathbf{x}}_j, j = 1, 2, \dots, d\} \subseteq \Omega$ of subdomain points is constructed¹. Note that the

¹ This set is obtained by generating a grid of equally spaced points on the hypercube $[0, 1]^N$. They are then automatically reduced taking only those in Ω by the `inhull` MATLAB function. Such points are the centres of partition of unity subdomains.

number d depends on both the data point number n and the space dimension N ; furthermore, it is suitably chosen assuming that the ratio $n/d \approx 2^{N+1}$.

Stage 3. The number s of evaluation points is computed and a set $\mathcal{E}_s = \{\tilde{\mathbf{x}}_i, i = 1, 2, \dots, s\} \subseteq \Omega$ of evaluation points is generated.

Stage 4. For each subdomain point $\tilde{\mathbf{x}}_j, j = 1, 2, \dots, d$, a local spherical subdomain is constructed, whose radius is

$$\delta_{\Omega_j} = \frac{\sqrt{2}}{D^{1/N}}, \quad (5)$$

where D is the number of subdomain points initially generated on $[0, 1]^N$.

Stage 5. The kd -tree data structures are built for the set \mathcal{X}_n of data points and the set \mathcal{E}_n of evaluation points.

Stage 6. For each subdomain $\Omega_j, j = 1, 2, \dots, d$, the range query problem is considered, adopting the related searching procedure which consists of the following two steps:

- i) Find all data points (i.e. the set \mathcal{X}_{n_j}) belonging to the subdomain Ω_j and construct a local interpolation RBF matrix by \mathcal{X}_{n_j} , where n_j denotes the point number of \mathcal{X}_{n_j} .
- ii) Determine all evaluation points (i.e. the set \mathcal{E}_{s_j}) belonging to the subdomain Ω_j and build a local evaluation RBF matrix by \mathcal{E}_{s_j} , where s_j is the point number of \mathcal{E}_{s_j} .

Stage 7. A local RBF interpolant R_j and a weight function $W_j, j = 1, 2, \dots, d$, is computed for each evaluation point.

Stage 8. The global fit (2) is applied, accumulating all the R_j and W_j .

In this algorithm for convex domains the local interpolants are computed by using compactly supported RBFs as the Wendland functions. However, this approach is completely automatic and turns out to be very flexible, since different choices of local approximants, either globally or compactly supported, are allowed.

3.2 Complexity Analysis

The algorithm is based on the construction of kd -tree data structures. They enable us to efficiently determine all data points belonging to each subdomain $\Omega_j, j = 1, 2, \dots, d$, so that we can compute local RBF interpolants to be used in the partition of unity scheme. Then, assuming that the covering $\{\Omega_j\}_{j=1}^d$ is regular and local and the set \mathcal{X}_n of data points is quasi-uniform, we analyze the complexity of this interpolation algorithm.

In **Stages 1-4** we have a sort of preprocessing phase where we automatically load all data sets and define the parameters concerning data, subdomain and evaluation points. To construct an algorithm which efficiently works in a generic

space dimension N , we require that the subdomain number d is proportional to the data point number n , taking $n/d \approx 2^{N+1}$.

In **Stage 5** we build the kd -trees, which needs $\mathcal{O}(Nn \log n)$ time and $\mathcal{O}(Nn)$ space for n data points and $\mathcal{O}(Ns \log s)$ time and $\mathcal{O}(Ns)$ space for s evaluation points. Then, in **Stage 6** we make use of the range search procedure for each subdomain Ω_j , $j = 1, 2, \dots, d$, whose running times are $\mathcal{O}(\log n)$ and $\mathcal{O}(\log s)$, respectively (see [14]).

Since the number of centres in each subdomain Ω_j is bounded by a constant (see Definition 2), we need $\mathcal{O}(1)$ space and time for each subdomain to solve the local RBF interpolation problems. In fact, in order to obtain the local RBF interpolants, we have to solve d linear systems of (relatively) small sizes, i.e. $n_j \times n_j$, with $n_j \ll n$, thus requiring a constant running time $\mathcal{O}(n_j^3)$, $j = 1, 2, \dots, d$, for each subdomain. Besides reporting the points in each subdomain in $\mathcal{O}(1)$, as the number d of subdomains Ω_j is bounded by $\mathcal{O}(n)$, this leads to $\mathcal{O}(n)$ space and time for solving all of them.

Thus, in **Stage 7** and **8** we have to add up a constant number of local RBF interpolants to get the value of the global fit (2). This can be computed in $\mathcal{O}(1)$ time.

4 Numerical Experiments

In this section we present some numerical experiments we made to test our procedures implemented in MATLAB environment. All the tests have been carried out on a Intel Core i7-4500U 1.8 GHz processor. In our results we report errors and CPU times obtained by running the algorithm on a few scattered data sets, which are located in a convex hull $\Omega \subseteq [0, 1]^N$, for $N = 2, 3$. As interpolation points, we take uniformly random Halton data points. They are generated by using the program `haltonseq.m`, available at [10], and then suitably reduced to Ω . We observe that this code for convex domains is completely automatic and, though we here focus only on bivariate and trivariate interpolation, it might also be used in higher dimensions.

In order to point out accuracy of this algorithm, we compute on a reduced grid of s evaluation points² Maximum Absolute Error (MAE) and Root Mean Square Error (RMSE), whose formulas are

$$MAE = \max_{1 \leq i \leq s} |f(\tilde{\mathbf{x}}_i) - \mathcal{I}(\tilde{\mathbf{x}}_i)|, \quad (6)$$

and

$$RMSE = \sqrt{\frac{1}{s} \sum_{i=1}^s |f(\tilde{\mathbf{x}}_i) - \mathcal{I}(\tilde{\mathbf{x}}_i)|^2}. \quad (7)$$

² The number s depends on the convex domain Ω ; at first, we construct a uniform grid of 40^N points, and then we automatically reduce them taking only those in Ω through the `inhull` MATLAB function.

Moreover, we report results obtained by using as basis the Wendland C^2 function, i.e.,

$$\phi(r) = (1 - \delta r)_+^4 (4\delta r + 1),$$

where $\delta \in \mathbb{R}^+$ is a *shape parameter*, $r = \|\cdot\|_2$ is the Euclidean distance, and $(\cdot)_+$ denotes the truncated power function. We remark that this RBF is compactly supported (i.e., its support is $[0, 1/\delta]$) and strictly positive definite in \mathbb{R}^N for $N \leq 3$ (see [14]). Note that here it is used as both a basis function and a localizing function of Shepard's weight W_j in the global fit (2).

4.1 Results for 2D Convex Hulls

In this subsection we focus on bivariate interpolation, analyzing performances of our algorithm for convex hulls and showing the numerical results obtained by considering five sets of Halton data points. These tests are carried out considering different convex domains, i.e., a triangle, a disk and a hexagon (see Figure 1).

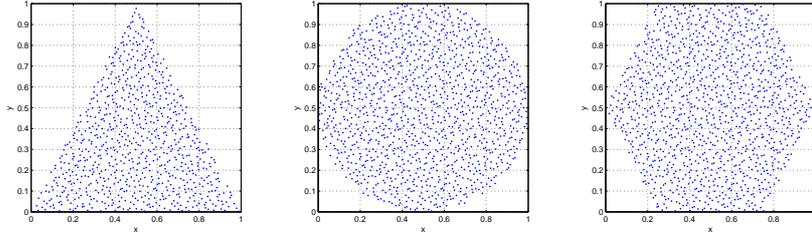


Fig. 1: Examples of points in 2D convex hulls. Left: triangle, 805 nodes; center: disk, 1257 nodes; right: hexagon, 1204 nodes.

In the various experiments we investigate accuracy of the interpolation algorithm taking the data values by the well-known 2D Franke's test function

$$f_2(x_1, x_2) = \frac{3}{4}e^{-\frac{(9x_1-2)^2+(9x_2-2)^2}{4}} + \frac{3}{4}e^{-\frac{(9x_1+1)^2}{49} - \frac{9x_2+1}{10}} + \frac{1}{2}e^{-\frac{(9x_1-7)^2+(9x_2-3)^2}{4}} - \frac{1}{5}e^{-(9x_1-4)^2 - (9x_2-7)^2}.$$

After showing in Figure 2 the stable behavior of RMSEs by varying the value of $\delta \in [0.1, 3]$, for each of convex domains we report MAEs and RMSEs taking $\delta = 0.1$ as shape parameter of the Wendland C^2 function. Then, since we are also concerned to point out the efficiency of the algorithm, in Tables 1–3 we show CPU times computed in seconds.

Finally, in Figure 3 we represent the 2D Franke's function (left) and the absolute errors (right) computed on convex domains. This study shows that the

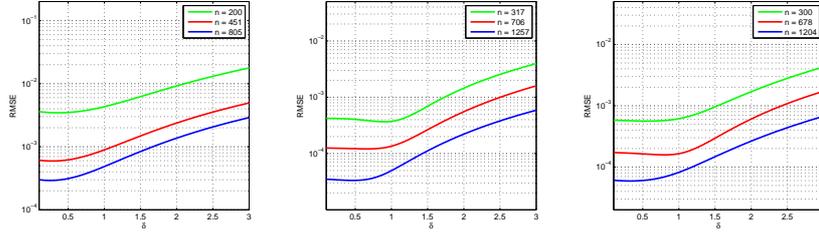


Fig. 2: RMSEs by varying the value of δ . Left: triangle; center: disk; right: hexagon.

Table 1: Errors and CPU times (in seconds) for triangle using $\delta = 0.1$.

n	MAE	RMSE	time
51	1.04E - 01	1.06E - 02	0.1
200	6.57E - 02	3.60E - 03	0.2
451	1.26E - 02	6.11E - 04	0.3
805	7.39E - 03	3.00E - 04	0.4
1256	3.72E - 03	1.65E - 04	0.6

Table 2: Errors and CPU times (in seconds) for disk using $\delta = 0.1$.

n	MAE	RMSE	time
80	2.64E - 02	4.94E - 03	0.1
317	5.12E - 03	4.22E - 04	0.2
706	1.99E - 03	1.25E - 04	0.4
1257	3.29E - 04	3.51E - 05	0.6
1960	3.23E - 04	2.39E - 05	0.9

Table 3: Errors and CPU times (in seconds) for hexagon using $\delta = 0.1$.

n	MAE	RMSE	time
76	4.43E - 02	6.35E - 03	0.1
300	5.56E - 03	5.82E - 04	0.2
678	2.38E - 03	1.72E - 04	0.4
1204	6.40E - 04	6.07E - 05	0.6
1877	6.32E - 04	3.98E - 05	0.8

maximum errors mainly concentrate on or close to the boundary of the convex hull. Note that, for shortness, in this paper we report numerical results obtained on a single example (or data set), but similar situations appear in all considered cases.

4.2 Results for 3D Convex Hulls

In this subsection we instead report numerical results concerning trivariate interpolation. As earlier, we analyze accuracy and efficiency of the partition of unity algorithm for convex hulls, taking also in this case some sets of Halton scattered data points. Such points are located in three different convex domains: a pyramid, a cylinder and a hexagonal prism (see Figure 4).

In the various tests we analyze the performances of the proposed algorithm taking the data values by 3D Franke's function, whose analytic expression is

$$f_3(x_1, x_2, x_3) = \frac{3}{4}e^{-\frac{(9x_1-2)^2+(9x_2-2)^2+(9x_3-2)^2}{4}} + \frac{3}{4}e^{-\frac{(9x_1+1)^2}{49} - \frac{9x_2+1}{10} - \frac{9x_3+1}{10}} + \frac{1}{2}e^{-\frac{(9x_1-7)^2+(9x_2-3)^2+(9x_3-5)^2}{4}} - \frac{1}{5}e^{-(9x_1-4)^2-(9x_2-7)^2-(9x_3-5)^2}.$$

As in the bivariate case, for each of convex hulls in Tables 4–6 we show MAEs, RMSEs and CPU times obtained by running our interpolation algorithm. These results are obtained taking $\delta = 0.1$. Here, we omit the graphs of RMSEs by varying δ because this study revealed a behavior similar to that outlined in Figure 2. Moreover, in dimension three we observed a even more relevant concentration of maximum errors on (or close to) the boundary of convex hulls.

Table 4: Errors and CPU times (in seconds) for pyramid using $\delta = 0.1$.

n	MAE	RMSE	time
335	1.15E-01	5.03E-03	4.8
2670	3.42E-02	5.88E-04	17.4
8995	1.21E-02	1.60E-04	30.1
21337	1.66E-02	1.59E-04	49.5
41665	5.96E-03	5.95E-05	83.7

5 Conclusions and Future Work

In this paper we presented a new algorithm for multivariate interpolation of scattered data sets lying in convex domains (or hulls) $\Omega \subseteq \mathbb{R}^N$, for any $N \geq 2$. It is based on the partition of unity interpolation using local RBF interpolants

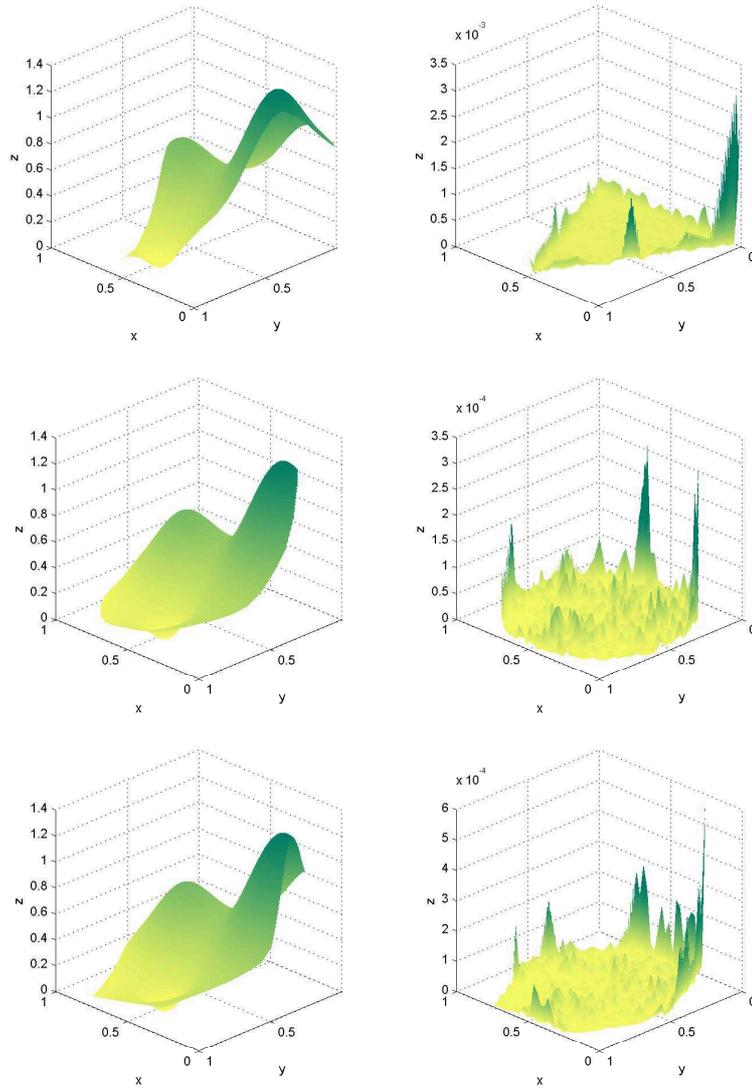


Fig. 3: 2D Franke's function (left) and absolute errors (right) defined on convex domains. Top: triangle, 1256 nodes; middle: disk, 1960 nodes; bottom: hexagon, 1877 nodes.

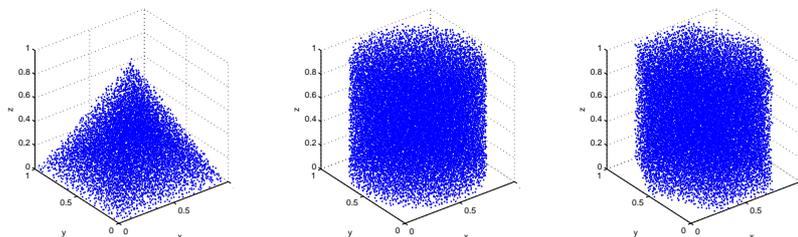


Fig. 4: Examples of points in 3D convex hulls. Left: pyramid, 8995 nodes; center: cylinder, 21177 nodes; right: hexagonal prism, 20249 nodes.

Table 5: Errors and CPU times (in seconds) for cylinder using $\delta = 0.1$.

n	MAE	RMSE	time
787	$3.47\text{E} - 01$	$7.93\text{E} - 03$	15.2
6271	$9.91\text{E} - 03$	$1.65\text{E} - 04$	44.6
21177	$2.00\text{E} - 03$	$3.35\text{E} - 05$	77.6
50184	$1.48\text{E} - 03$	$1.86\text{E} - 05$	130.7
97997	$8.58\text{E} - 04$	$1.08\text{E} - 05$	209.0

Table 6: Errors and CPU times (in seconds) for hexagonal prism using $\delta = 0.1$.

n	MAE	RMSE	time
754	$1.65\text{E} - 01$	$4.49\text{E} - 03$	15.1
6002	$7.25\text{E} - 03$	$1.33\text{E} - 04$	44.5
20249	$3.02\text{E} - 03$	$3.78\text{E} - 05$	77.3
47997	$1.78\text{E} - 03$	$2.00\text{E} - 05$	127.0
93754	$1.15\text{E} - 03$	$1.27\text{E} - 05$	202.9

and compactly supported weight functions. To partition the points in Ω , we used a kd-tree data structure efficiently answering the range search query.

As future work, we expect to build new data structures for partitioning data in convex hulls using efficient cell-based searching procedures. The new code should allow us to further reduce CPU times, making it suitable and applicable in several fields of applied mathematics and scientific computing.

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