OPTIMAL DISTRIBUTION OF CENTERS FOR RADIAL BASIS FUNCTION METHODS

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ABSTRACT. Both the approximation quality and the stability of radial basis function interpolation depend on the distribution of the center set. This paper considers the variation of centers for the purpose of improving the methods' performance. We first show that for radial basis function interpolation it is desirable to work with uniformly distributed centers, before we focus on the characterization and construction of center sets which achieve to maximize their uniformity.

1. INTRODUCTION

Radial basis functions provide powerful grid-free methods for multivariate interpolation to scattered data. For the purpose of briefly explaining the key features of the interpolation scheme, let $\Omega \subset \mathbb{R}^d$ be a non-empty, bounded, open domain and let $D_X(f) = (f(x_1), \ldots, f(x_N))^T \in \mathbb{R}^N$ be a given data vector containing values of an unknown function $f : \Omega \to \mathbb{R}$ sampled at a finite set $X = \{x_1, \ldots, x_N\} \subset \Omega$ of pairwise distinct *center* points. For a fixed *basis function* $\phi : [0, \infty) \to \mathbb{R}$, the interpolant $s_{f,X}$ to f at X is an element from the linear space

$$\mathcal{S}_{\phi,X} = \operatorname{span}\{\phi(\|\cdot - x\|) \, : \, x \in X\} + \Pi_m^d,$$

satisfying $D_X(s_{f,X}) = D_X(f)$, where $\|\cdot\|$ is the Euclidean norm on $\mathbb{R}^d$ and Π_m^d stands for the linear space of all d-variate real-valued polynomials of degree less than m.

Classical examples for radial basis functions are given by Duchon's *thin plate splines* [8], where $\phi(r) = r^2 \log(r)$, Hardy's *multiquadrics* [14], $\phi(r) = -(r^2 + c^2)^{1/2}$, *inverse Multiquadrics* $\phi(r) = (r^2 + c^2)^{-1/2}$, and *Gaussians* $\phi(r) = \exp(-cr^2)$, $c > 0$. Recent developments have provided compactly supported radial basis functions [5, 31, 34].

As observed by Schaback [24], there is an intimate relation between the stability and the approximation behaviour of the interpolation method: Roughly speaking, there is no commonly used radial basis function which allows us to combine good convergence rates with small condition numbers of the arising collocation matrices. For the purpose of understanding this dilemma, which was in [24] referred to as *uncertainty relation*, note that for a fixed basis function ϕ both the interpolation method's approximation quality and stability depend on the distribution of the point set X in the domain Ω:

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In view of stability, due to lower bounds on the spectral norm of the collocation matrix as proven in [1, 2, 19, 20], one desires that the center set's *separation distance*

$$q_X = \min_{\substack{x,y \in X \\ x \neq y}} \|x - y\|$$

is not too small. On the other hand, available bounds [16, 17, 35] on the error $\|f - s_{f,X}\|_{L_\infty(\Omega)}$, with the domain Ω satisfying an *interior cone condition*, require keeping the *fill distance*

$$h_{X,\Omega} = \sup_{y \in \Omega} \min_{x \in X} \|x - y\|$$

from X to Ω small.

However, it is obviously not possible to minimize $h_{X,\Omega}$ and to maximize q_X at the same time. Note that neither $h_{X,\Omega}$ nor q_X depends on the selected basis function ϕ. Nonetheless their values contribute, for all commonly used radial basis functions, significantly to the corresponding method's success. Further details on the impact of the two quantities $q_X, h_{X,\Omega}$ on radial basis function interpolation shall be provided by the following Section 2. For a comprehensive review on radial basis functions and their applications we refer the reader to the survey papers [4, 9, 21, 25, 26].

Inspired by the aforementioned uncertainty relation, this paper is, apart from numerical experiments in [3], the first to consider the variation of the center points for the purpose of improving the performance of radial basis function interpolation. To this end, we shall focus on the construction and characterization of *admissible* (a precise definition shall follow in Section 4) finite point sets, $X \subset \Omega$, which achieve, due to their geometry, to optimally balance $h_{X,\Omega}$ against q_X by maximizing their *uniformity* $\rho_{X,\Omega} = q_X / h_{X,\Omega}$. We shall say that such center sets are *optimally distributed* in the domain Ω.

Note that the results of this paper do also take direct impact on recent meshless Galerkin [32] and collocation methods [10, 12, 13] which are using radial basis functions for solving partial differential equations (see the papers [11, 30] for an up-to-date overview). In these applications, each center from the set X can be understood as a method parameter. The choice of the set X is therefore a non-trivial task. A successful method of this kind requires, for similar reasons as for interpolation, selecting a set X which achieves to balance between q_X and $h_{X,\Omega}$ by maximizing its uniformity $\rho_{X,\Omega}$.

Much of the results of this paper naturally relies on concepts from discrete computational geometry. Section 3 introduces the notation and provides one key result which yields the bound $\rho_{X,\Omega} \leq \sqrt{2(d+1)/d}$ to be proven in Section 4. This bound leads us to necessary and sufficient conditions for optimally distributed sets. It turns out that such point sets can be constructed by using regular simplices.

Finally, although for the sake of generality our discussion is mainly in arbitrary space dimension, the most constructive applications of this work are given for the special case $d = 2$. On the basis of our results, concrete examples for optimally distributed point sets in two dimensions are presented, mainly for the special case of the unit square, where $\Omega = [0, 1]^2 \subset \mathbb{R}^2$. The remaining Section 5 of the paper is devoted to numerical examples where the utility of optimally distributed point sets for radial basis function interpolation is shown.

2. Radial Basis Function Interpolation

Given a vector $D_X(f) \in \mathbb{R}^N$, $X = \{x_1, \ldots, x_N\}$, of real function values, for computing a solution $s_{f,X} \in \mathcal{S}_{\phi,X}$ of the interpolation problem $D_X(s_{f,X}) = D_X(f)$ the radial basis function interpolation scheme requires solving the linear system

$$\sum_{j=1}^{N} c_j \phi(\|x_k - x_j\|) + \sum_{\ell=1}^{Q} d_\ell p_\ell(x_k) = f(x_k) \qquad 1 \le k \le N$$

under constraints

$$\sum_{j=1}^{N} c_j p_\ell(x_j) = 0 \qquad 1 \le \ell \le Q, \tag{2.1}$$

where the functions $p_1, \ldots, p_Q$ are assumed to be a basis of Π_m^d, i.e. $Q = \binom{m-1+d}{d}$.

Due to Micchelli [18], the collocation matrix

$$\begin{pmatrix} A_{\phi,X} & P_X \\ P_X^T & 0 \end{pmatrix}$$

with $A_{\phi,X} = (\phi(\|x_j - x_k\|))_{1 \le j,k \le N}$ and $P_X = (p_\ell(x_k))_{1 \le k \le N; 1 \le \ell \le Q}$ of the above system is guaranteed to be nonsingular provided that

$$p(x_k) = 0 \quad 1 \le k \le N \qquad \Longrightarrow \qquad p \equiv 0 \quad \text{for all } p \in \Pi_m^d$$

holds true and ϕ is conditionally positive definite of order m on $\mathbb{R}^d$:

Definition 2.1. A continuous function $\phi : [0, \infty) \to \mathbb{R}$ is said to be `conditionally positive definite` of order m on $\mathbb{R}^d$, $\phi \in \mathtt{cpd}(m, d)$, iff the quadratic form $c^T A_{\phi,X} c$ is strictly positive for all possible choices of sets $X = \{x_1, \ldots, x_N\} \subset \mathbb{R}^d$ containing finitely many pairwise distinct centers and $c = (c_1, \ldots, c_N)^T \in \mathbb{R}^N \setminus \{0\}$ satisfying (2.1).

For $\phi \in \mathtt{cpd}(m, d)$, local error estimates for interpolation are dating back to [16, 17, 35]. For a fixed $x \in \Omega$, available estimates possess the form

$$|f(x) - s_{f,X}(x)| \le C P_{\phi,X}(x) \tag{2.2}$$

where C is a positive constant that solely depends on the function f, and the *power function* $P_{\phi,X}(x)$ is pointwise given by the norm of the error functional at x. Throughout this paper, C denotes a generic positive constant. The power function is well-known to possess the representation

$$P_{\phi,X}^2(x) = \phi(0) - 2u^T(x) R_{\phi,X}(x) + u^T(x) A_{\phi,X} u(x) \tag{2.3}$$

where the vector $u(x) = (u_1(x), \ldots, u_N(x))^T \in \mathbb{R}^N$ contains the *cardinal functions* $u_j : \mathbb{R}^d \to \mathbb{R}$, $1 \le j \le N$, satisfying $u_j(x_k) = \delta_{jk}$, $1 \le j, k \le N$, and $R_{\phi,X}(x) = (\phi(\|x - x_1\|), \ldots, \phi(\|x - x_N\|))^T$. For a fixed x, these functions can pointwise be evaluated by solving the linear system

$$\begin{pmatrix} A_{\phi,X} & P_X \\ P_X^T & 0 \end{pmatrix} \cdot \begin{pmatrix} u(x) \\ v(x) \end{pmatrix} = \begin{pmatrix} R_{\phi,X}(x) \\ S_m(x) \end{pmatrix} \tag{2.4}$$

where $v(x) = (v_1(x), \ldots, v_Q(x))^T$, $S_m(x) = (p_1(x), \ldots, p_Q(x))^T \in \mathbb{R}^Q$. Further details can be found in [35]. For recording the numerical results in Section 5, frequent point-evaluations of the power function were required. For reasons of computational efficiency we prefer to work with an alternative representation of the power function as given by the following

Theorem 2.2. *Let $\phi \in \mathtt{cpd}(m,d)$. The power function $P_{\phi,X}$ possesses the representation*

$$P^2_{\phi,X}(x) = \phi(0) - u^T(x)R_{\phi,X}(x) - v^T(x)S_m(x) \quad \text{for all } x \in \Omega. \tag{2.5}$$

For the special case $m = 0$, the power function can be bounded by

$$0 \leq P^2_{\phi,X}(x) \leq \phi(0) \qquad \text{for all } x \in \Omega. \tag{2.6}$$

Proof. If we expand the above system (2.4) as

$$\begin{aligned} A_{\phi,X}u(x) + P_X v(x) &= R_{\phi,X}(x) \\ P_X^T u(x) &= S_m(x) \end{aligned}$$

we obtain

$$u^T(x)A_{\phi,X}u(x) = u^T(x)R_{\phi,X}(x) - v^T(x)S_m(x)$$

and thus by using (2.3) we find the validity of (2.5). Additionally, from (2.4), (2.5) we deduce yet another representation of the power function by

$$P^2_{\phi,X}(x) = \phi(0) - \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}^T \cdot \begin{pmatrix} A_{\phi,X} & P_X \\ P_X^T & 0 \end{pmatrix} \cdot \begin{pmatrix} u(x) \\ v(x) \end{pmatrix}$$

which gives us

$$P^2_{\phi,X}(x) = \phi(0) - u^T(x)A_{\phi,X}u(x)$$

for the special case $m = 0$. But in this case, the matrix $A_{\phi,X}$ is positive definite which implies (2.6). □

Note that in the above error estimate (2.2) the function f is supposed to be an element of the *native function space* $\mathcal{F}_\phi$ which is entirely determined by the properties of ϕ. We do not want to expand all the details on $\mathcal{F}_\phi$ here but recommend Schaback's survey [26] and his two recent papers [27, 28] instead.

In addition, we shall suppose that $\hat{\phi}$, the d-variate (generalized) Fourier transform of ϕ, has algebraic decay at infinity. More precise, for a specific number $s_\infty > 0$ it is required that

$$\gamma_1 \|\omega\|^{-d-s_\infty} \leq \hat{\phi}(\|\omega\|) \leq \gamma_2 \|\omega\|^{-d-s_\infty} \qquad \text{for } \|\omega\| \to \infty \tag{2.7}$$

holds true for suitable constants $\gamma_2 \geq \gamma_1 > 0$. Then, according to [29, 33] the power function can be bounded above in terms of the fill distance $h_{X,\Omega}$, provided that the domain Ω satisfies an interior cone condition.

Definition 2.3. We say that $\Omega \subset \mathbb{R}^d$ satisfies an `interior cone condition`, iff there exists an angle θ and a radius $r > 0$, such that for every $x \in \Omega$ there exists a unit vector $\xi(x)$ satisfying

$$C(x, \xi(x), \theta, r) = \left\{ x + \lambda y \,:\, y \in \mathbb{R}^d, \|y\|_2 = 1, y^T\xi(x) \geq \cos(\theta), \lambda \in [0,r] \right\} \subset \Omega,$$

i.e. the cone $C(x, \xi(x), \theta, r)$ is entirely contained in Ω.

For the rest of this paper, we shall assume that $\Omega \subset \mathbb{R}^d$ satisfies an interior cone condition.

Theorem 2.4. *Let $\phi \in \texttt{cpd}(m,d)$ satisfy (2.7), and let the domain $\Omega \subset \mathbb{R}^d$ be bounded and open. Then there exist constants h_0, C, such that for all finite sets of centers $X \subset \Omega$ with $h_{X,\Omega} \leq h_0$ and all $x \in \Omega$ the power function can be bounded by*

$$P_{\phi,X}(x) \leq C h_{X,\Omega}^{s_\infty/2}$$

yielding the error bound

$$\|f - s_{f,X}\|_{L_\infty(\Omega)} \leq C h_{X,\Omega}^{s_\infty/2}$$

for $f \in \mathcal{F}_\phi$. □

All of the requirements for ϕ which were mentioned so far in this text, in particular the decay condition (2.7), are for instance satisfied by the thin plate splines and Wendland's compactly supported radial basis functions (cf. [29]). Local error estimates of a form similar to (2.2) are also available for both meshless Galerkin methods [32] and collocation methods [12].

As to the stability of the interpolation process, estimates on the condition number of the collocation matrix are due to [1, 2, 19, 20] dominated by the magnitude of q_X. We close this section by quoting a corresponding result to be found in [29] (see also [24, 26]).

Theorem 2.5. *Let $\phi \in \texttt{cpd}(m,d)$ satisfy (2.7), and let $\lambda_{\min}^X$ denote the smallest nonvanishing eigenvalue of $A_{\phi,X}$. Then, for all $c \in \mathbb{R}^N \setminus \{0\}$ satisfying (2.1), $\lambda_{\min}^X$ can be bounded by*

$$\frac{c^T A_{\phi,X} c}{c^T c} \geq \lambda_{\min}^X \geq C \cdot q_X^{s_\infty}$$

where C solely depends on ϕ. □

3. Generalized Delaunay Triangulations and Regular Simplices

The discussion in the following Section 4 shall make use of standard tools from discrete computational geometry, such as Delaunay triangulations and their dual Voronoi diagrams. This section shall introduce the required notation, and it quotes one useful result concerning the optimality of regular simplices. For a comprehensive treatment of the subject see the textbook [22] and references therein.

For a fixed finite point set $X \subset \mathbb{R}^d$, the decomposition

$$\mathbb{R}^d = \bigcup_{x \in X} V_X(x)$$

of the d-dimensional Euclidean space into *Voronoi tiles*

$$V_X(x) = \left\{ y \in \mathbb{R}^d \ : \ \|y - x\| = \min_{z \in X} \|y - z\| \right\}$$

is referred to as the *Voronoi diagram* of X. Each Voronoi tile $V_X(x)$ is a non-empty, closed and convex polytope containing all points in space that are at least as close to x as to any other point from X.

Two different Voronoi tiles $V_X(x)$ and $V_X(y)$ are either disjoint or they share a common face, in which case x and y are said to be *Voronoi neighbours*. For each $x \in X$, all of its closest points from $X \setminus \{x\}$ are Voronoi neighbours of x . The vertices of the Voronoi tiles are called *Voronoi vertices*. There exist merely finitely many Voronoi vertices which we shall collect in the set $\mathcal{V}_X$.

By connecting all possible Voronoi neighbours, we obtain a graph whose vertex set is X. This graph defines a simplicial decomposition $\mathcal{D}(X)$ of the convex hull conv(X) which is usually referred to as the *Delaunay triangulation* of X. Such a triangulation exists for every finite set X. The triangulation $\mathcal{D}(X)$ will be unique provided that the points from X are in *general position*, i.e. no $d+2$ points from X are cospherical.

Due to a fundamental property of Delaunay triangulations, it is true for each simplex $T \in \mathcal{D}(X)$ that its circumsphere S_T contains no point from X in its interior. Moreover, the center c_T of S_T is a Voronoi vertex from $\mathcal{V}_X$.

Note that the function $d_X : \mathbb{R}^d \to \mathbb{R}$, which gives us by

$$d_X(y) = \min_{x \in X} \|y - x\|,$$

the distance from a single point $y \in \mathbb{R}^d$ to the set X has a local maximum at each Voronoi vertex [7]. In particular, the value $d_X(c_T)$ gives us the radius r_T of S_T. Moreover, for every simplex T which is *self-centered*, i.e. c_T is contained in the convex hull conv(V_T) of its vertex set V_T, we obtain $h_{V_T,T} = r_T$.

The following theorem will provide one useful isoperimetric property of *regular simplices*. Recall that a simplex is said to be regular, iff all of its edge lengths are equal. Hence, for the special case $d = 2$, a regular simplex is an equilateral triangle.

Theorem 3.1. *Let T denote a nondegenerate d-dimensional simplex, V_T the set of its $d+1$ vertices, and r_T the radius of its circumsphere S_T. Furthermore let*

$$J_d = \sqrt{\frac{d}{2(d+1)}}.$$

Then we have

$$q_{V_T} \le r_T / J_d$$

where equality holds if and only if T is a regular simplex.

The above theorem is a well-known result from discrete computational geometry proven by Rankin [23] in the context of *spherical codes* (see also [7], Chapter 1, Section 2.6). The notation J_d for the reciprocal value of the uniformity $\rho_{V_{\Delta_d},\Delta_d}$ of a regular d-simplex Δ_d is dedicated to H. Jung [15] (cf. [6], Chapter 2, Section 11).

We remark one interesting aspect concerning the asymptotic behaviour of the numbers J_d: The sequence $\{J_d^{-1}\}_{d \ge 1}$ is strictly monotonically decreasing and $\lim_{d\to\infty} J_d^{-1} = \sqrt{2}$. This implies that the uniformity of the point sequence $\{V_{\Delta_d}\}_{d\ge 1}$ in Δ_d, $\Delta_d \subset \mathbb{R}^d$ being a regular simplex of unit edge length, can uniformly be bounded below by

$$\rho_{V_{\Delta_d},\Delta_d} > \sqrt{2} \quad \text{for all } d \ge 1.$$

In contrast, consider the corresponding sequence $\{V_{\square_d}\}_{d\ge 1}$ of the unit cubes' $\square_d = [0,1]^d \subset \mathbb{R}^d$ vertex set $V_{\square_d}$ for which we also find $q_{V_{\square_d}} = 1$, but $h_{V_{\square_d},\square_d} = \sqrt{d}/2$, which implies

$$\lim_{d\to\infty} \rho_{V_{\square_d},\square_d} = 0.$$

4. Optimal Distribution of Centers

Let $\Omega \subset \mathbb{R}^d$ be a compact domain satisfying an interior cone condition. Subject of the following considerations are finite point sets in Ω which are admissible in the following sense.

Definition 4.1. A finite point set $X \subset \Omega$ is said to be `admissible`, iff $\mathcal{V}_X \cap \Omega$ is non-empty. We shall collect all such sets in $\mathcal{X}_\Omega$.

In this section, we are aiming at the construction and characterization of point sets from $\mathcal{X}_\Omega$ which are optimally distributed in Ω.

Definition 4.2. A point set $X \in \mathcal{X}_\Omega$ is said to be `optimally distributed` in Ω, iff X maximizes the uniformity $\rho_{X,\Omega}$ among all point sets $Y \in \mathcal{X}_\Omega$ by satisfying

$$\rho_{X,\Omega} = \sup_{Y \in \mathcal{X}_\Omega} \rho_{Y,\Omega}.$$

We collect all point sets, which are optimally distributed in Ω, in $\mathcal{X}_\Omega^* \subset \mathcal{X}_\Omega$.

The following theorem gives us an upper bound on the uniformity of elements from $\mathcal{X}_\Omega$.

Theorem 4.3. *Let $X \in \mathcal{X}_\Omega$. Then, the uniformity of X in Ω can be bounded above by*

$$\rho_{X,\Omega} \leq J_d^{-1}.$$

Proof. Let $\mathcal{D}(X)$ be the Delaunay triangulation of the point set X. Then, the shortest distance between two distinct points from X is given by the length of the shortest edge in $\mathcal{D}(X)$, so that $q_X = \min_{T \in \mathcal{D}(X)} q_{V_T}$ holds true. Moreover, we have

$$h_{X,\Omega} = \max_{y \in \Omega} d_X(y) \geq \max_{v \in \mathcal{V}_X \cap \Omega} d_X(v) = \max_{\substack{T \in \mathcal{D}(X) \\ c_T \in \Omega}} r_T. \tag{4.1}$$

By using Theorem 3.1 we find

$$\rho_{X,\Omega} = \frac{q_X}{h_{X,\Omega}} \leq \frac{\min_{T \in \mathcal{D}(X)} q_{V_T}}{\max_{\substack{T \in \mathcal{D}(X) \\ c_T \in \Omega}} r_T} \leq \max_{\substack{T \in \mathcal{D}(X) \\ c_T \in \Omega}} \frac{q_{V_T}}{r_T} \leq J_d^{-1}. \tag{4.2}$$

□

In what follows we shall provide sufficient and necessary conditions for optimally distributed center sets. To this end, let us first notice the following simple

Remark 4.4. Let $X \in \mathcal{X}_\Omega$ be optimally distributed in Ω, such that $\rho_{X,\Omega} = J_d^{-1}$. Moreover, let $A \subset \mathbb{R}^d$ satisfy $X \subset A$ and $h_{X,\Omega} = h_{X,A}$. Then, the set X is also optimally distributed in A, provided that $\mathcal{V}_X \cap A$ is non-empty. Indeed, since the value of q_X is not affected we obtain $\rho_{X,A} = J_d^{-1}$.

The above observation naturally asks for the construction of *maximal* extensions of Ω, in which the set $X \in \mathcal{X}_\Omega^*$ is optimally distributed. This leads us to

Theorem 4.5. *Let $X \in \mathcal{X}_\Omega$ be optimally distributed in Ω, such that $\rho_{X,\Omega} = J_d^{-1}$. Furthermore, let $h \equiv h_{X,\Omega}$, and let*

$$B = \bigcup_{x \in X} B_h(x),$$

where $B_h(x) = \{z \in \mathbb{R}^d : \|z - x\| \leq h\}$ denotes the closed ball around $x \in \mathbb{R}^d$ with radius $h > 0$. Then, the following three statements are true.

(a) *Ω is a subset of B, i.e. $\Omega \subset B$;*
(b) *X is optimally distributed in B with $\rho_{X,B} = J_d^{-1}$;*
(c) *X is optimally distributed in any intermediate subset A, $\Omega \subset A \subset B$, with $\rho_{X,A} = J_d^{-1}$.*

Proof. Obviously, the inclusion $\Omega \subset B$ holds true. Indeed, for every single $y \in \Omega$ we find $d_X(y) \leq h$ which implies $y \in B_h(x)$ for a specific $x \in X$, and thus $y \in B$. Therefore, statement (a) is true.

As to (c), observe that $h_{X,\Omega} = h_{X,A}$ for $\Omega \subset A \subset B$. According to the above Remark 4.4, we find that X is optimally distributed in A with $\rho_{X,A} = J_d^{-1}$. Since (b) is a special case of (c), this completes our proof. □

Before we shall turn to the construction of optimally distributed center sets we provide the following necessary condition.

Theorem 4.6. *Let $X \in \mathcal{X}_\Omega$ be optimally distributed in Ω, such that $\rho_{X,\Omega} = J_d^{-1}$. Then, every simplex $T \in \mathcal{D}(X)$ whose circumcircle's center c_T lies in Ω is regular.*

Proof. From (4.1) we conclude $h_{X,\Omega} \geq r_T$, and therefore, like in (4.2), we obtain

$$\rho_{X,\Omega} \leq q_{V_T}/r_T \leq J_d^{-1}.$$

But then, $\rho_{X,\Omega} = J_d^{-1}$ particularly implies $q_{V_T}/r_T = J_d^{-1}$. According to Theorem 3.1, the simplex T is then regular. □

The above result suggests to use regular simplices for the construction of optimally distributed point sets. We further discuss this by providing the following

Theorem 4.7. *Let X be a finite point set, such that every simplex of its Delaunay triangulation $\mathcal{D}(X)$ is regular. Then, the set X is optimally distributed in its convex hull* conv(X).

Proof. Without loss of generality let the edge lengths of the simplices be normalized, such that $q_T = 1$ holds for every $T \in \mathcal{D}(X)$. Under this assumption and by using

$$h_{V_T,T} = J_d \quad \text{for every } T \in \mathcal{D}(X)$$

we find for $\Omega = \text{conv}(X)$ the identity

$$h_{X,\Omega} = \max_{y\in\Omega} d_X(y) = \max_{T\in\mathcal{D}(X)} \max_{y\in T} d_X(y) = \max_{T\in\mathcal{D}(X)} h_{V_T,T} = J_d$$

which, in combination with Theorem 4.3, completes our proof. □

The following theorem shows that the construction of optimally distributed point sets by using regular simplices does not necessarily require the involvement of Delaunay triangulations.

Theorem 4.8. *Let $\{T_j\}_{j=1}^m$ be a finite set of regular simplices of equal size, and let*

$$X = \bigcup_{j=1}^m V_{T_j}$$

denote its vertices. If

$$h_{X,T_j} = h_{V_{T_j},T_j} \qquad \text{for } 1 \leq j \leq m \tag{4.3}$$

holds, then the point set X is optimally distributed in

$$\Omega = \bigcup_{j=1}^m T_j.$$

Proof. Without loss of generality, we assume that $q_{V_{T_j}} = 1$ for all $1 \leq j \leq m$. This implies

$$h_{V_{T_j},T_j} = J_d \qquad \text{for } 1 \leq j \leq m$$

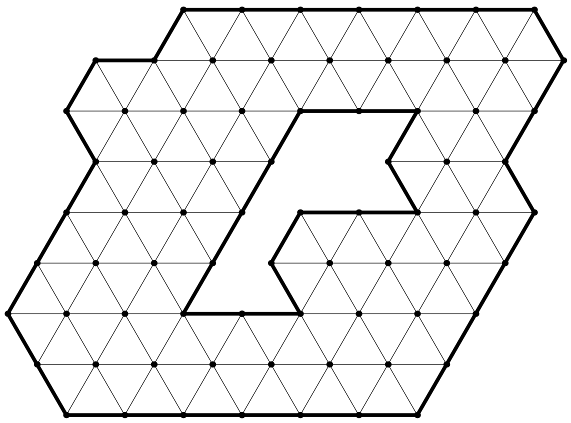
and therefore by using (4.3) we obtain

$$h_{X,\Omega} = \max_{y\in\Omega} d_X(y) = \max_{1\leq j\leq m} \max_{y\in T_j} d_X(y) = \max_{1\leq j\leq m} h_{V_{T_j},T_j} = J_d.$$

□

For the special case of two dimensions, Figure 1 displays one possible example for a set of equilateral triangles, whose vertices are optimally distributed in the triangles' union Ω.

FIGURE 1. A set of equilateral triangles, whose vertices are optimally distributed in the triangles' union Ω.



Finally, let us turn to concrete examples for optimally distributed point sets in two dimensions. In the following discussion, we restrict ourselves to the unit square, i.e. $\Omega = [0,1]^2 \subset \mathbb{R}^2$. For the construction of optimally distributed point sets in $[0,1]^2$ we shall use the *hexagonal lattice*

$$\mathcal{H}_2 = \{jv_1 + kv_2 \,:\, j,k \in \mathbb{Z}\} \subset \mathbb{R}^2.$$

This particular infinite point set is generated by

$$v_1 = (1,0) \quad \text{and} \quad v_2 = (1/2, \sqrt{3}/2).$$

Moreover, every triangle of its (infinite) Delaunay triangulation $\mathcal{D}(\mathcal{H}_2)$ is equilateral (and thus a regular 2-simplex). We find $q_{\mathcal{H}_2} = 1$ for its separation distance, $h_{\mathcal{H}_2,\mathbb{R}^2} = J_2 = 1/\sqrt{3}$ for its fill distance to $\mathbb{R}^2$, and thus $\rho_{\mathcal{H}_2,\mathbb{R}^2} = \sqrt{3}$.

Lemma 4.9. *Let $n \geq 1$, $k_n = \lfloor \frac{2n}{\sqrt{3}} \rfloor$, $h_n = \frac{\sqrt{3}}{2n}$, and $v_n = (0, y_n)$, where $y_n = (1 - k_n \cdot h_n)/2$. Moreover, let*

$$X_n = (v_n + 1/n \cdot \mathcal{H}_2) \cap [0,1]^2.$$

Then, the following three statements on X_n are true.

(a) *X_n is optimally distributed in the strip*

$$S_n = \{(x,y) \,:\, 0 \leq x \leq 1; y_n \leq y \leq 1 - y_n\} \subset [0,1]^2;$$

(b) *$q_{X_n} = 1/n$, $h_{X_n,S_n} = 1/(\sqrt{3}n)$, and $\rho_{X_n,S_n} = \sqrt{3}$;*

(c) *The size of X_n is*

$$\#X_n = \begin{cases} (m+1)(n+1) + mn & \text{if } k_n = 2m \text{ is even} \\ (m+1)(2n+1) & \text{if } k_n = 2m+1 \text{ is odd.} \end{cases}$$

In the above definition of k_n, the symbol $\lfloor x \rfloor$, $x \in \mathbb{R}$, denotes the unique integer m satisfying $m \le x < m+1$.

Proof. Note that (b) implies (a) provided that $X_n \subset S_n$ holds true. Indeed, since $J_2^{-1} = \sqrt{3}$, this would be a simple conclusion from Theorem 4.3.

Therefore, we first discuss the inclusion $X_n \subset S_n$. To this end, observe that for every point $(x,y) \in X_n$ we obtain the representation

$$y = y_n + h_n \cdot k, \qquad 0 \le k \le k_n \tag{4.4}$$

for its second component with some integer k, whose range is limited as indicated above by the requirement $0 \le y \le 1$. Therefore, X_n is contained in the strip $S_n = [0,1] \times [y_n, y_n + h_n \cdot k_n]$.

Next, we prove (b). Obviously, $q_{X_n} = 1/n$ holds true. In order to show $h_{X_n,S_n} = 1/(\sqrt{3}n)$, let $\mathcal{D}(X_n)$ denote the Delaunay triangulation of X_n (cf. Figure 2). Observe that each triangle $T \in \mathcal{D}(X_n)$ is either congruent to the equilateral triangle T_e with vertex set

$$V_{T_e} = \{(0,y_n), (1/n, y_n), (1/(2n), y_n + h_n)\},$$

or it is congruent to the boundary triangle T_b whose vertex set is given by

$$V_{T_b} = \{(0,y_n), (0, y_n + 2h_n), (1/(2n), y_n + h_n)\}.$$

In either case, we obtain $h_{V_T,T} = h_{V_{T_e},T_e} = h_{V_{T_b},T_b} = 1/(\sqrt{3}n)$, and therefore

$$h_{X_n,\mathrm{conv}(X_n)} = \max_{T \in \mathcal{D}(X_n)} h_{V_T,T} = 1/(\sqrt{3}n). \tag{4.5}$$

Now note that $S_n = \mathrm{conv}(X_n)$, whenever k_n is even in which case the set X_n comprises the two points $(0, 1-y_n), (1, 1-y_n)$. If k_n is odd, then we obtain the inclusion $\mathrm{conv}(X_n) \subset S_n$, with the difference set $S_n \setminus \mathrm{conv}(X_n)$ containing two boundary triangles, T_l and T_r, whose vertex sets are given by

$$\begin{aligned} V_{T_l} &= \{(0, 1-y_n), (1/(2n), 1-y_n), (0, 1-y_n-h_n)\} \\ V_{T_r} &= \{(1, 1-y_n), (1-1/(2n), 1-y_n), (1, 1-y_n-h_n)\}, \end{aligned}$$

cf. Figure 2. In this case, since

$$h_{V_{T_l},T_l} = h_{V_{T_r},T_r} = 1/(\sqrt{3}n)$$

we obtain, like in (4.5), $h_{X_n,S_n} = 1/(\sqrt{3}n)$. This together with $q_{X_n} = 1/n$ implies $\rho_{X_n,S_n} = \sqrt{3}$ in either case as stated in (b).

Finally, let us turn to the remaining statement (c). To this end, recall the representation (4.4) for $(x,y) \in X_n$. Let us for the moment fix k in (4.4). If k is even, we see that X_n comprises $n+1$ points of the form $(\ell/n, y_n + h_n \cdot k)$, $0 \le \ell \le n$. If k is odd, X_n comprises n points of the form $((1+2\ell)/(2n), y_n + h_n \cdot k)$, $0 \le \ell \le n-1$. Altogether, we obtain

$$\#X_n = \sum_{\substack{0 \le k \le k_n \\ k \text{ even}}} (n+1) + \sum_{\substack{0 \le k \le k_n \\ k \text{ odd}}} n,$$

which implies (c). $\square$

Theorem 4.10. *For $n \geq 1$, let X_n be as in Lemma 4.9. Then, the set X_n is optimally distributed in the unit square $[0,1]^2$ with $\rho_{X_n,[0,1]^2} = \sqrt{3}$ if and only if*

$$\frac{2n}{\sqrt{3}} - \lfloor \frac{2n}{\sqrt{3}} \rfloor \leq \frac{2}{3}. \tag{4.6}$$

Proof. Due to Lemma 4.9, the set X_n is optimally distributed in $S_n \subset [0,1]^2$. According to Theorem 4.5, X_n is also optimally distributed in $[0,1]^2$, if and only if

$$\max_{y \in [0,1]^2 \setminus S_n} d_{X_n}(y) \leq h_{X_n,S_n} = 1/(\sqrt{3}n) \tag{4.7}$$

holds true. Note that the maximum in (4.7) is attained at the n boundary points

$$((1+2\ell)/(2n), 0), \qquad 0 \leq \ell \leq n-1,$$

and, depending on the parity of k_n, also at either the n points $((1+2\ell)/(2n), 1)$, $0 \leq \ell \leq n-1$, or the $n+1$ points $(\ell/n, 1)$, $0 \leq \ell \leq n$.

For $x^* = (1/(2n), 0)$ we obtain

$$d_{X_n}(x^*) = \|x^* - v_n\| = \sqrt{y_n^2 + 1/(4n^2)}.$$

In combination with (4.7), this leads us to the requirement

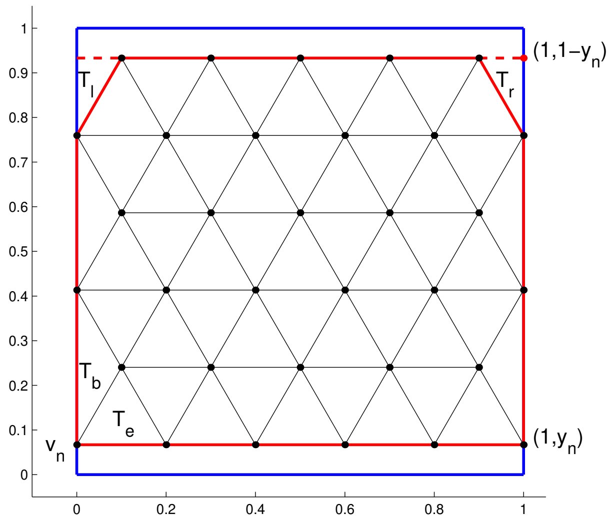
$$y_n \leq 1/(2\sqrt{3}n).$$

Recalling the definition of y_n, we see that this is equivalent to (4.6). □

We remark that, e.g., all of the numbers $n = 1, 2, 3, 4, 7, 8, 9, 10$ satisfy (4.6), whereas for $n = 5, 6$ this inequality does not hold. Therefore, the point set X_5 displayed in Figure 2 is not optimally distributed in the unit square (although it is optimally distributed in S_5).

The optimally distributed points sets $X_2, X_3, X_4 \in \mathcal{X}^*_{[0,1]^2}$ are displayed in the first column of Figure 3.

FIGURE 2. The point set $X_5 \subset [0,1]^2$, and its Delaunay triangulation.



5. Numerical Results

The purpose of this section is to illustrate the utility of optimally distributed points sets for radial basis function methods. To this end, we considered studying the behaviour of radial basis function interpolation on three different sequences of subsets from $\mathcal{X}_{[0,1]^2}$:

- $\{X_n\}_n$;
- $\{Y_n\}_n$, where $Y_n \subset [0,1]^2$ is a perturbation of X_n with $\max_{y \in Y_n} d_{X_n}(y) \leq 0.2 q_{X_n}$;
- $\{Z_n\}_n$, where $Z_n \subset [0,1]^2$ is a perturbation of X_n with $\max_{y \in Y_n} d_{X_n}(y) \leq 0.4 q_{X_n}$.

Figure 3 shows the point sets Y_2, Y_3, Y_4 (second column) and Z_2, Z_3, Z_4 (third column). Moreover the three graphs of the corresponding fill distances $h_{X_n,[0,1]^2}$, $h_{Y_n,[0,1]^2}$, $h_{Z_n,[0,1]^2}$, and separation distances $q_{X_n}, q_{Y_n}, q_{Z_n}$, $2 \leq n \leq 4$, are displayed in Figure 4.

For the four radial basis functions which were mentioned in the introduction, using the parameter $c = 0.2$ for multiquadrics, $c = 0.4$ for inverse Multiquadrics, and $c = 8.0$ for Gaussians, and all of the subsets X_n, Y_n, Z_n, $2 \leq n \leq 4$, we have approximated the power function's Čebyšev-norm $\|P_{\phi,X}\|_{L_\infty(\Omega)}$, and we computed the spectral condition number $\kappa_2(A_{\phi,X}) = \|A_{\phi,X}\|_2 \cdot \|A_{\phi,X}^{-1}\|_2$ of the corresponding collocation matrices. The Figures 5,6 reflect our results, particularly the impact of the fill distance $h_{X,\Omega}$ on $\|P_{\phi,X}\|_{L_\infty(\Omega)}$, and of the separation distance q_X on $\kappa_2(A_{\phi,X})$. Note that in the numerical examples, for all $2 \leq n \leq 4$, the optimally distributed set $X_n \in \mathcal{X}^*_{[0,1]^2}$, is superior over the comparable two sets $Y_n, Z_n \in \mathcal{X}_{[0,1]^2}$ in terms of both its better approximation behaviour and its smaller spectral condition number:

$$
\begin{array}{rcll}
\kappa_2(A_{\phi,X_n}) & \leq & \min\left(\kappa_2(A_{\phi,Y_n}), \kappa_2(A_{\phi,Z_n})\right), & 2 \leq n \leq 4, \\
\|P_{\phi,X_n}\|_{L_\infty(\Omega)} & \leq & \min\left(\|P_{\phi,Y_n}\|_{L_\infty(\Omega)}, \|P_{\phi,Z_n}\|_{L_\infty(\Omega)}\right), & 2 \leq n \leq 4.
\end{array}
$$

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FIGURE 3. The point sets $X_2, X_3, X_4 \subset \mathcal{X}^*_{[0,1]^2}$, $Y_2, Y_3, Y_4 \subset \mathcal{X}_{[0,1]^2}$ and $Z_2, Z_3, Z_4 \subset \mathcal{X}_{[0,1]^2}$.

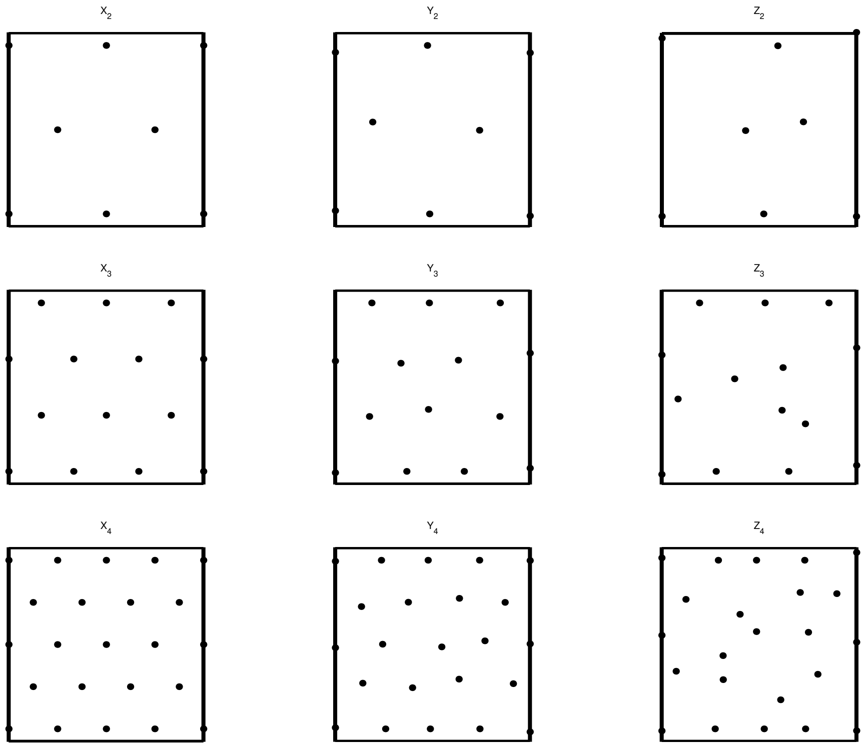

FIGURE 4. The fill and separation distances of the point sets X_n (green), Y_n (blue), and Z_n (red).

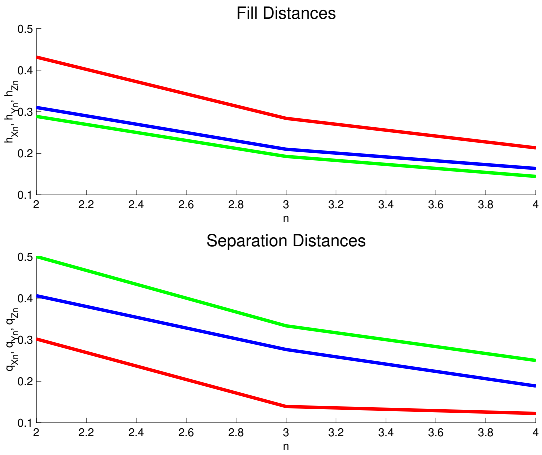

FIGURE 5. The condition numbers of the matrices A_{ϕ,X_n} (green), A_{ϕ,Y_n} (blue), and A_{ϕ,Z_n} (red), $2 \le n \le 4$, for different radial basis functions.

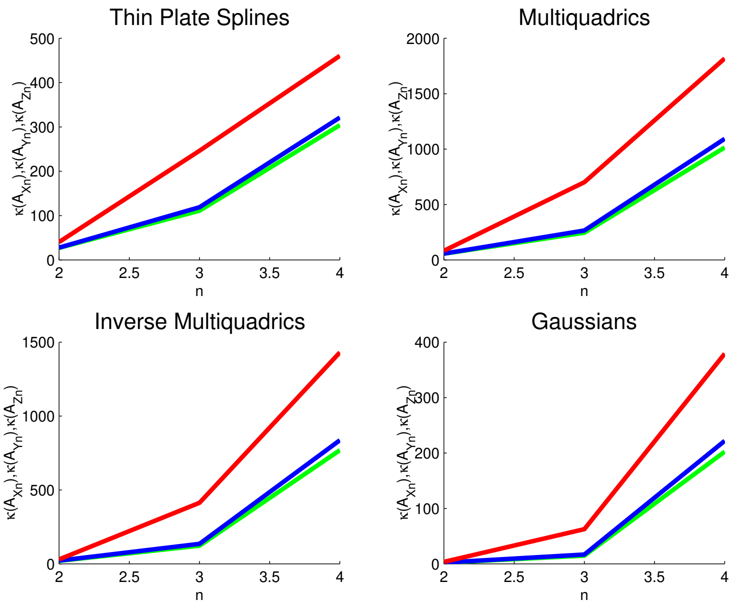

FIGURE 6. The power functions' Čebyšev-norm $\|P_{\phi,X_n}\|_{L_\infty(\Omega)}$ (green), $\|P_{\phi,Y_n}\|_{L_\infty(\Omega)}$ (blue), $\|P_{\phi,Z_n}\|_{L_\infty(\Omega)}$ (red), $2 \le n \le 4$, for different radial basis functions.