Comparison of Different Radial Basis Functions in Dynamical Systems*

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Abstract: In this paper we study the impact of using different radial basis functions for the computation of complete Lyapunov function candidates using generalised interpolation. We compare the numerical well-posedness of the discretised problem, condition numbers of the collocation matrices, and the quality of the solutions for Wendland functions $\psi_{3,1}$ and $\psi_{5,3}$, Gaussians, Inverse quadratics and Inverse multiquadrics, and Matérn kernels $\psi_{(n+3)/2}$ and $\psi_{(n+5)/2}$.

1 INTRODUCTION

Radial basis functions (RBFs) are a standard tool for interpolation and generalised interpolation problems in high dimensions. One of the applications in the area of Dynamical Systems is the computation of Lyapunov functions (Giesl, 2007a; Giesl and Wendland, 2007), as well as complete Lyapunov function candidates (Argáez et al., 2017a; Argáez et al., 2017b; Argáez et al., 2018a; Argáez et al., 2018b). This is formulated as a generalised interpolation problem, approximately solving a suitable linear, first-order partial differential equation (PDE).

Let us explain the computation of complete Lyapunov function candidates for dynamical systems in more detail, where the dynamics are given by the autonomous ordinary differential equation (ODE) $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ with $\mathbf{x} \in \mathbb{R}^n$. Our initial method computes a complete Lyapunov function candidate V as the generalised interpolant to the linear, first-order PDE $\nabla V(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = -1$. Note, however, that the PDE is ill-posed, as it does not have a solution at certain points $\mathbf{x}$, namely in the chain-recurrent set, i.e. where the dynamics are repetitive or almost repetitive, which includes equilibria and periodic orbits. However, this apparent disadvantage of the method is used to obtain information on the location of the chain-recurrent set of the ODE. This information can then be used for further iterations to obtain complete Lyapunov function candidates localising the chain-recurrent set with more precision.

The RBFs that have mainly been used for the computation of complete Lyapunov function candidates are Wendland's RBFs. They are positive definite and polynomials on their compact support and their smoothness is fixed through a parameter. The corresponding reproducing kernel Hilbert space (RKHS), where the mesh-free collocation is performed and the norm of which is minimised, is norm-equivalent to a Sobolev space. Usually Wendland functions with low smoothness parameters are used and the method in (Argáez et al., 2017a; Argáez et al., 2017b; Argáez et al., 2018a; Argáez et al., 2018b) to compute complete Lyapunov functions candidates works very well. However, any sufficiently smooth RBF can be used. Indeed, in theory the smoother the RBFs, the better the convergence results, but in applications less smooth RBFs often work better, since they avoid numerical problems as shown in this paper.

A natural question is thus how the method works in practice with different RBFs. In this paper we systematically analyse several candidates for RBFs and compare three aspects relevant to the applicability. All the RBFs we analyse depend on a positive real parameter c and the influence of the value of the parameter must also be taken into account. Further, the density of the collocation points in the generalised interpolation problem plays a vital role. To make the analysis tractable we compute complete Lyapunov function candidates for a system with a known chain-

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recurrent set; two periodic orbits and one equilibrium. The three aspects we analyse are:

First, the collocation matrix generated for the discretised problem is symmetric and should in theory be positive definite. If it is not positive definite due to numerical issues, then it is not possible to compute a solution to the discretised problem and the method cannot work. We analyse the positive definiteness of the collocation matrix as a function of the RBF parameter $c > 0$ and the density of the collocation grid parameterised through $\alpha > 0$, cf. formula (9) below.

Second, the condition number of the collocation matrix is of great relevance to the method, in particular when iterating. Thus, we also analyse the condition number of the collocation matrix as a function of the RBF parameter $c > 0$ and the density of the collocation grid α.

Third, since we know the location of the chain-recurrent set, we analyse how well it is localised by the method using the different RBFs. Again the RBF parameter $c > 0$ and the density of the collocation grid α play a role. In general, one aims for a good localisation of the chain-recurrent set with as coarse a collocation grid as possible.

The RBFs we analyse, always with a scaling parameter $c > 0$, are the following, for references see, e.g., (Fasshauer, 2007; Wendland, 2005; Schaback, 1993; Buhmann, 2003).

Wendland $\psi_{3,1}$

$$\psi(r) = (1-cr)_+^4[4cr+1] \tag{1}$$

Recall that $x_+ := \max\{0,x\}$ and $x_+^k := (x_+)^k$. We consider $\mathbb{R}^2$, so $n = 2$, and the parameters for the Wendland function $\psi_{l,k}$ are chosen such that $l = \lfloor \frac{n}{2} \rfloor + k + 1 = k+2$; the corresponding RKHS is norm-equivalent to the Sobolev space $H^{k+(n+1)/2} = H^{5/2}$.

Wendland $\psi_{5,3}$

$$\psi(r) = (1-cr)_+^8[32(cr)^3+25(cr)^2+8cr+1] \tag{2}$$

The corresponding RKHS is norm-equivalent to the Sobolev space $H^{k+(n+1)/2} = H^{9/2}$.

Gaussians

$$\psi(r) = \exp\left(\frac{-r^2}{2c^2}\right) \tag{3}$$

Inverse multiquadric

$$\psi(r) = \frac{1}{\sqrt{1+(cr)^2}} \tag{4}$$

Inverse quadratic

$$\psi(r) = \frac{1}{1+(cr)^2} \tag{5}$$

Matérn $\psi_{(n+3)/2}$

$$\psi(r) = (1+cr)\exp(-cr) \tag{6}$$

Matérn kernels are well known in the statistics literature (Matern, 1986) and called Sobolev splines in (Schaback, 1993). We consider $\mathbb{R}^2$, so $n = 2$, and the parameter for the Matérn kernel ψ_β is chosen such that $\beta = \frac{n+3}{2} = \frac{5}{2}$; the corresponding RKHS is norm-equivalent to the Sobolev space $H^\beta = H^{\frac{5}{2}}$.

Matérn $\psi_{(n+5)/2}$

$$\psi(r) = \left(1+cr+\frac{1}{3}(cr)^2\right)\exp(-cr) \tag{7}$$

We consider $\mathbb{R}^2$, so $n = 2$, and the parameter for the Matérn kernel ψ_β is chosen such that $\beta = \frac{n+5}{2} = \frac{7}{2}$; the corresponding RKHS is norm-equivalent to the Sobolev space $H^\beta = H^{\frac{7}{2}}$.

Remark 1.1. *Note that although all the RBFs studied are parameterised by a parameter $c > 0$, this parameter has different meanings for different RBFs and its numerical values cannot be directly compared.*

The paper is organised as follows: In the next section we give a brief description of the method to compute complete Lyapunov function candidates from (Giesl, 2007b) refined in (Argáez et al., 2017a; Argáez et al., 2017b; Argáez et al., 2018a; Argáez et al., 2018b), before we present our results in Section 3 and discuss them in Section 4.

In this paper we are only interested in the performance of different RBFs to obtain complete Lyapunov functions. Therefore, one iteration suffices.

2 USING RBFs TO COMPUTE COMPLETE LYAPUNOV FUNCTION CANDIDATES

The method used to compute complete Lyapunov function candidates using generalised interpolation with RBFs is described in detail in (Argáez et al., 2017a; Argáez et al., 2017b; Argáez et al., 2018a; Argáez et al., 2018b). Here we just give a brief overview. Given is a dynamical system, whose dynamics are defined by an ODE

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \quad \mathbf{f}: \mathbb{R}^n \to \mathbb{R}^n, \tag{8}$$

and we are interested in the qualitative behaviour of its solution $t \mapsto \phi(t,\xi)$ as a function of the initial value $\xi \in \mathbb{R}^n$; here $\phi(0,\xi) = \xi$ and $\dot{\phi}(t,\xi) = \mathbf{f}(\phi(t,\xi))$. The qualitative behaviour of the solutions is characterised by a so-called complete Lyapunov function for the system $V: \mathbb{R}^n \to \mathbb{R}$, which is non-increasing along all solution trajectories, and strictly decreasing where possible, cf. (Auslander, 1964; Conley, 1978; Hurley, 1998). A complete Lyapunov function candidate is a function, which fulfills the first property, namely that it is non-increasing along all solution trajectories. This can be expressed by a non-positive orbital derivative (derivative along solutions) $\nabla V(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) \leq 0$, if V is sufficiently smooth.

It was shown in (Argáez et al., 2018a) that it is advantageous to homogenise the solutions' speed while maintaining the same trajectories by substituting $\hat{\mathbf{f}}(\mathbf{x}) = \mathbf{f}(\mathbf{x})/\sqrt{\delta^2 + \|\mathbf{f}(\mathbf{x})\|^2}$ for $\mathbf{f}$ in (8), where $\delta > 0$ is a small parameter. We set $\delta^2 = 10^{-8}$ in our computations.

The computation of complete Lyapunov function candidates is then posed as a generalised interpolation problem and solved using a collocation method based on RBFs. The set of collocation points $X = \{\mathbf{x}_1, \ldots, \mathbf{x}_N\} \subset \mathbb{R}^n$ is a subset of a, possibly shifted, hexagonal grid

$$\left\{ \alpha \sum_{k=1}^{n} i_k \omega_k : i_k \in \mathbb{Z} \right\}, \text{ where} \tag{9}$$

$$\omega_k = \sum_{j=1}^{k-1} \varepsilon_j \mathbf{e}_j + (k+1)\varepsilon_k \mathbf{e}_k \text{ and } \varepsilon_k = \sqrt{\frac{1}{2k(k+1)}}.$$

In the formula $\mathbf{e}_j$ is the usual jth unit vector and the parameter $\alpha > 0$ is a measure of the density; small $\alpha > 0$ correspond to high density. Further, we require $\mathbf{f}(\mathbf{x}_i) \neq \mathbf{0}$ for any $\mathbf{x}_i \in X$ to obtain a positive definite collocation matrix. This hexagonal grid has been shown to minimise the condition numbers of the collocation matrices for a fixed fill distance (Iske, 1998).

Next we compute the generalised interpolant v to $v'(\mathbf{x}_i) := \nabla v(\mathbf{x}_i) \cdot \mathbf{f}(\mathbf{x}_i) = -p(\mathbf{x}_i)$ at all collocation points $\mathbf{x}_i \in X$; $v'(\mathbf{x}_i) := \nabla v(\mathbf{x}_i) \cdot \mathbf{f}(\mathbf{x}_i)$ is the so-called orbital derivative of the function v and is negative if v is decreasing along solution trajectories of the ODE (8). The generalised interpolant is known to be the norm-minimal function in the corresponding RKHS fulfilling the interpolation conditions $v'(\mathbf{x}_i) = -p(\mathbf{x}_i)$. It is computed by solving a system of linear equations with a collocation matrix.

For details we refer to (Argáez et al., 2017a; Argáez et al., 2018a; Argáez et al., 2018b) or (Giesl, 2007b, Chapter 3). In the first iteration we start with the right-hand side $p(\mathbf{x}_i) = 1$ for all $\mathbf{x}_i \in X$. Once we have computed the generalised interpolant v we evaluate $v'(\mathbf{x})$ on a grid $Y_{\mathbf{x}_i}$ along the flow at each collocation point $\mathbf{x}_i \in X$ and use this information to fix $p(\mathbf{x}_i)$ in the next iteration, cf. (Argáez et al., 2018b).

A complete Lyapunov function $V : \mathbb{R}^n \to \mathbb{R}$ for the ODE (8) fulfills $V'(\mathbf{x}) \leq 0$ for all $\mathbf{x} \in \mathbb{R}^n$ and $V'(\mathbf{x}) < 0$ whenever possible. The set of $\mathbf{x} \in \mathbb{R}^n$ where $V'(\mathbf{x}) = 0$ corresponds to (almost) recurrent motion and is called the chain-recurrent set. At points that are not in the chain-recurrent set the flow of the ODE is gradient-like, i.e. solutions flow through and do not return to a neighbourhood of the point. The method outlined above computes a complete Lyapunov function candidate v and can be used to localise the chain-recurrent set. There are different methods to do that; here we use the criterion that $\|\nabla v(\mathbf{x})\| \leq \gamma_+$ for some (small) parameter γ_+ (Argáez et al., 2021).

3 RESULTS

For all the tests we used the ODE

$$\mathbf{f}(x,y) = \begin{pmatrix} -x(x^2+y^2-1/4)(x^2+y^2-1)-y \\ -y(x^2+y^2-1/4)(x^2+y^2-1)+x \end{pmatrix}, \tag{10}$$

which has an asymptotically stable equilibrium at the origin and two circular periodic orbits centred at the origin; a repelling one with radius $1/2$ and an asymptotically stable one with radius 1. The chain-recurrent set of the system consists of these three components. With the method outlined in the last section one expects to obtain an estimate of the chain-recurrent set that covers the three components, i.e. the origin and the two circles centred at the origin with radius $1/2$ and 1, and preferably the estimate is reasonably tight.

In the following the collocation points are always the hexagonal grid from formula (9), shifted as in (Hafstein, 2017) and intersected with $[-1.5, 1.5]^2$. To localise the chain-recurrent set we evaluated v' on the dense regular grid $(\Delta x\mathbb{Z} \times \Delta y\mathbb{Z}) \cap [-1.5, 1.5]^2$ with $\Delta x = \Delta y = 0.02$. In all examples we analyse the chain-recurrent set of the complete Lyapunov function for different values of c and α. The different columns in the figures show combinations of α and c resulting in condition numbers 10^3, 10^6 and 10^{13}, respectively. Note that the condition number increases, while the error decreases, if we either decrease α (denser set of collocation points) or if we decrease c (larger overlap). The chain-recurrent set was approximated as the set of points $\mathbf{x}$ fulfilling $\|\nabla v'(\mathbf{x})\| \leq \gamma^+ = 0.2$ for all examples. Table 1 shows the parameters used for our computations.

3.1 Wendland $\psi_{3,1}$

We consider the Wendland function $\psi_{3,1}$ from (1) with scaling parameter $c > 0$. The collocation matrix is always positive definite for all choices of $c > 0$ (scaling parameter) and α (density of the hexagonal collocation grid) that we investigated, namely $0.1 \leq c \leq 10$ and $0.02 \leq \alpha \leq 1$. Figures 1 and 2 show the computed chain-recurrent set for system (10). All computations show very good approximations of the

Table 1: Different parameters for α and c used according to the radial basis functions. Parameters were chosen to reproduce similar condition numbers (cond.) in the corresponding collocation matrices.

	Wendland func. $\psi_{3,1}$		Wendland func. $\psi_{5,3}$	
Cond.	α	c	α	c
10^3	0.06	1	0.03	7
10^5	0.03	1	0.03	2.5
10^{13}	Not reached with our settings		0.03	0.2
	Gaussian function		Inverse Multiquadrics	
Cond.	α	c	α	c
10^3	0.12	0.1	0.14	4
10^5	0.39	0.6	0.51	0.4
10^{13}	0.05	0.1	0.55	0.1
	Inverse Quadratic		Matérn $\psi_{(n+3)/2}$	
Cond.	α	c	α	c
10^3	0.2	2.4	0.3	0.3
10^5	0.41	0.5	0.03	0.3
10^{13}	0.08	1.5	Not reached with our settings	
	Matérn $\psi_{(n+5)/2}$			
Cond.	α	c		
10^3	0.16	5.3		
10^5	0.07	2.9		
10^{13}	0.03	0.1		

chain-recurrent set, which consists of two circles of radii $1/2$ and 1 and a point at the origin. Iteration 1 is better than iteration 0. The upper figure with higher condition number produces a slightly clearer approximation of the chain-recurrent set than the lower figure.

3.2 Wendland $\psi_{5,3}$

We consider the Wendland function $\psi_{5,3}$ from (2) with scaling parameter $c > 0$. Again the collocation matrix is positive definite for all choices of $c > 0$ (scaling parameter) and α (density of the hexagonal collocation grid) that we investigated, namely $0.1 \leq c \leq 10$ and $0.02 \leq \alpha \leq 1$. Figures 3 (iteration 0) and 4 (iteration 1) show the approximation of the chain-recurrent set for system (10) using $\psi_{5,3}$. The lowest condition number (top) shows an over-estimation of the chain-recurrent set in iteration 1, the medium condition (middle) shows an under-estimation. The best result is given by the largest condition number in iteration 1, Figure 4 bottom.

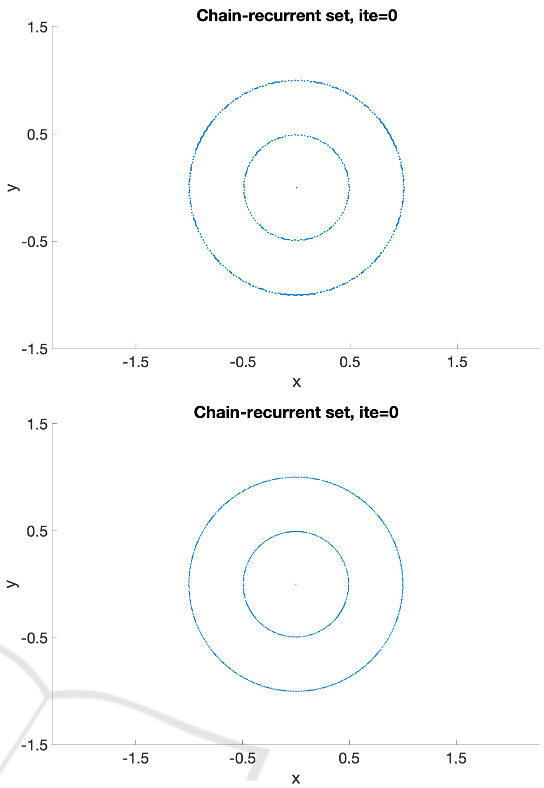

Figure 1: Chain-recurrent set from the approximation with Wendland function 3,1 in iteration 0 with collocation matrix with condition number 10^3 (upper) and 10^5 (lower).

3.3 Gaussian Radial Basis Functions

We consider the Gaussian RBF functions (3) with scaling parameter $c > 0$. Figure 15 shows that the collocation matrix is positive definite only for certain choices of $c > 0$ (scaling parameter) and α (density of the hexagonal collocation grid). Figures 5 and 6 show that the approximation of the chain-recurrent set is poor in all cases.

3.4 Inverse Multiquadrics

We consider the Inverse multiquadrics (4) with scaling parameter $c > 0$. In Figure 16 it can be seen the collocation matrix is positive definite only for certain choices of $c > 0$ (scaling parameter) and α (density of the hexagonal collocation grid). Figures 7 and 8 suggest that the best results are obtained with matrices whose condition number is small and even then the results are inferior to those of the Wendland functions.

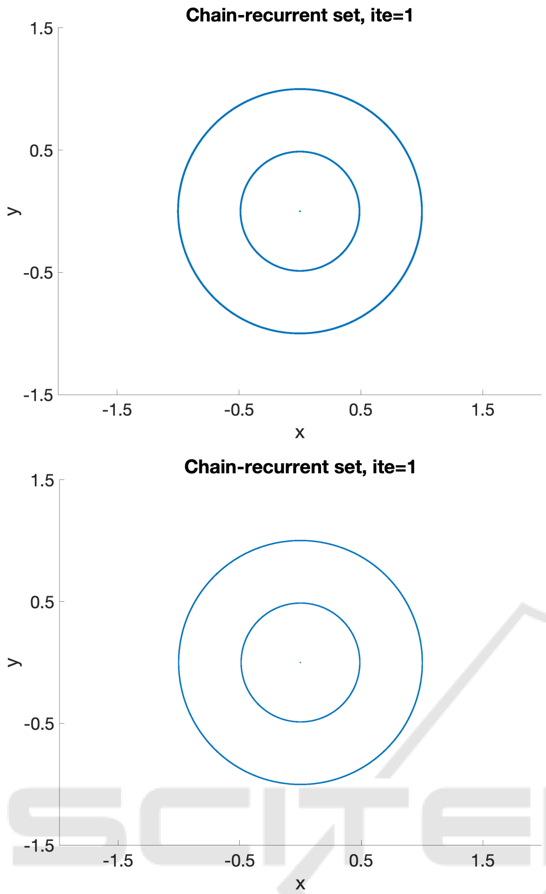

Figure 2: Chain-recurrent set from the approximation with Wendland function 3,1 in iteration 1 with collocation matrix with condition number 10^3 (upper) and 10^5 (lower).

3.5 Inverse Quadratic

We consider the Inverse quadratics (5) with scaling parameter $c > 0$. In Figure 17 we see that the collocation matrix is positive definite only for certain choices of c and α. Figures 9 and 10 show, similar to the Inverse multiquadrics, that better results are obtained for matrices with small condition number. But even then the approximation of the chain-recurrent set is poor and inferior to the case of Wendland functions.

3.6 Matérn $\psi_{(n+3)/2}$

We consider the Matérn kernel $\psi_{(n+3)/2}$ from (6) with scaling parameter $c > 0$. The collocation matrix is positive definite for all choices of c and α that we investigated, namely $0.1 \leq c \leq 10$ and $0.02 \leq \alpha \leq 1$. Figures 11 and 12 show good estimates for the larger condition number, while the smaller condition number delivers an over-estimation in iteration 0 and a completely wrong result in iteration 1.

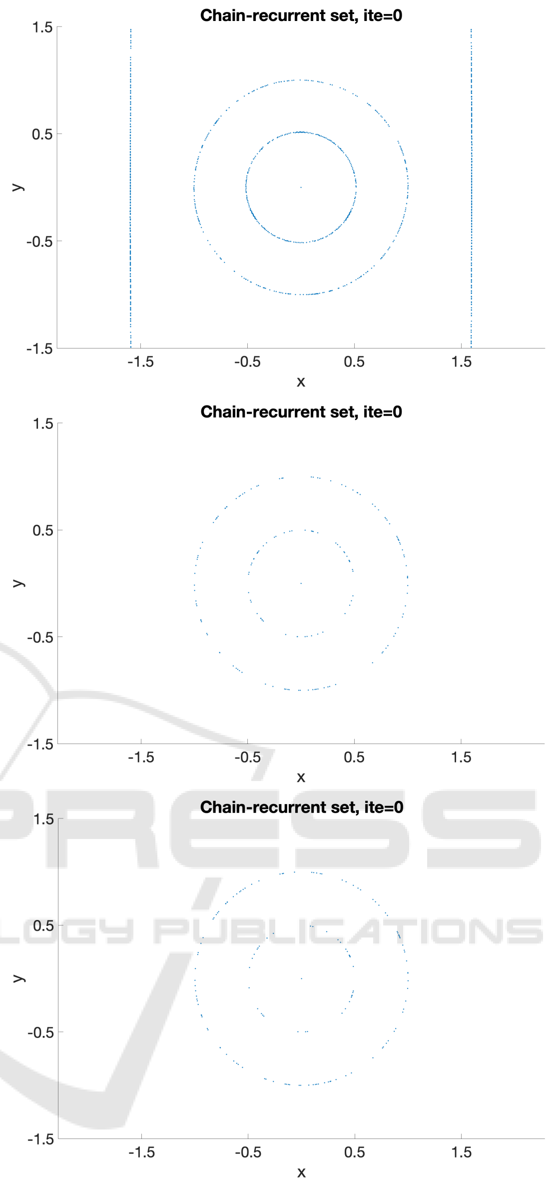

Figure 3: Chain-recurrent set from the approximation with Wendland function 5,3 in iteration 0 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

3.7 Matérn $\psi_{(n+5)/2}$

We consider the Matérn kernel $\psi_{(n+5)/2}$ from (7). The collocation matrix is positive definite for all choices of c and α that we investigated, namely $0.1 \leq c \leq 10$ and $0.02 \leq \alpha \leq 1$. Figures 13 and 14 show better approximations of the chain-recurrent set than with Matérn $\psi_{(n+3)/2}$, in particular in iteration 0. The lower the condition number, the better the results, with some gaps in the circles for large condition numbers.

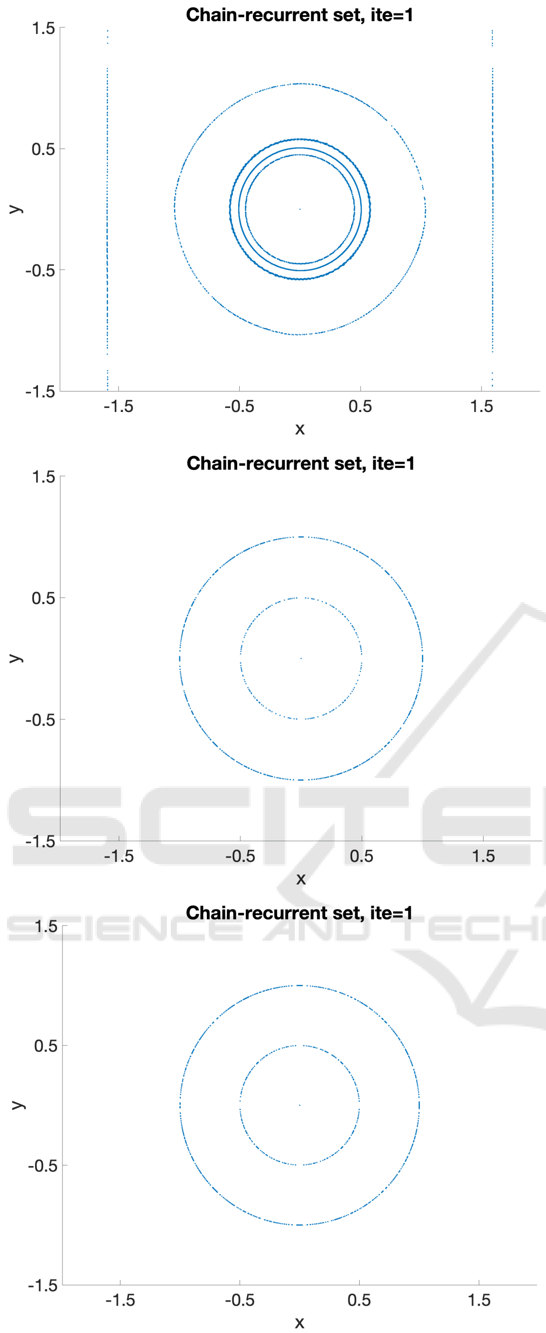

Figure 4: Chain-recurrent set from the approximation with Wendland function 5,3 in iteration 1 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

3.8 Comparison of All the Functions

In Figure 18 all the radial basis functions used are plotted for the parameter $c = 1$. The Wendland functions have a compact support and fall more rapidly than the other functions.

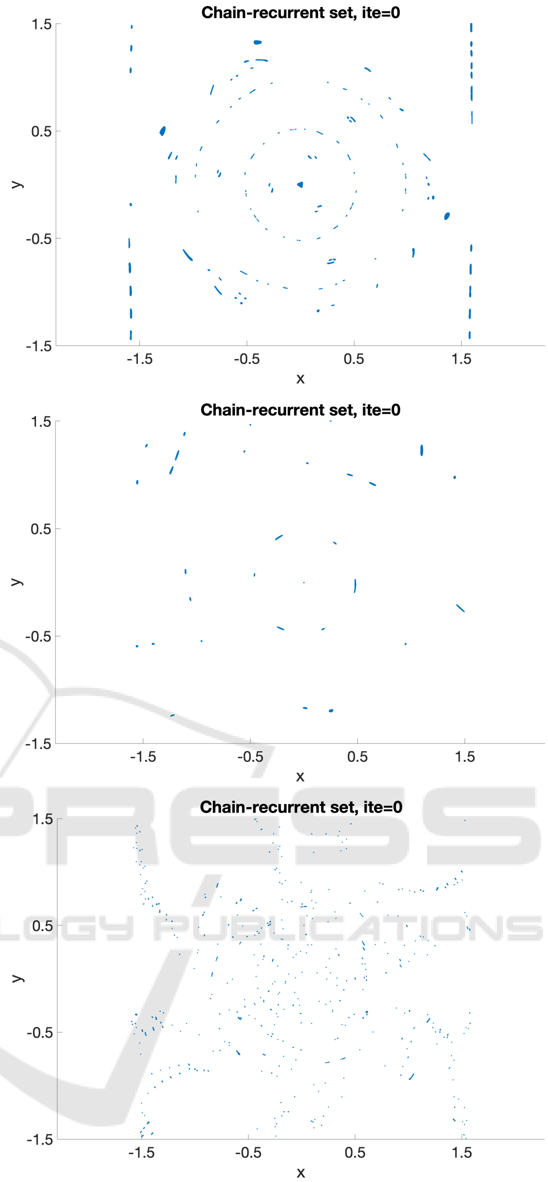

Figure 5: Chain-recurrent set from the approximation with the Gaussians in iteration 0 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

4 DISCUSSION

The results from our numerical investigation can be summarized as follows: The Wendland and Matérn functions share a similar behaviour concerning the area in the α vs. c plane for positive definite matrices: most of the combinations of different α and c parameters numerically produce positive definite matrices. The other radial basis functions (RBFs), namely Gaussians, Inverse multiquadrics and Inverse quadrat-

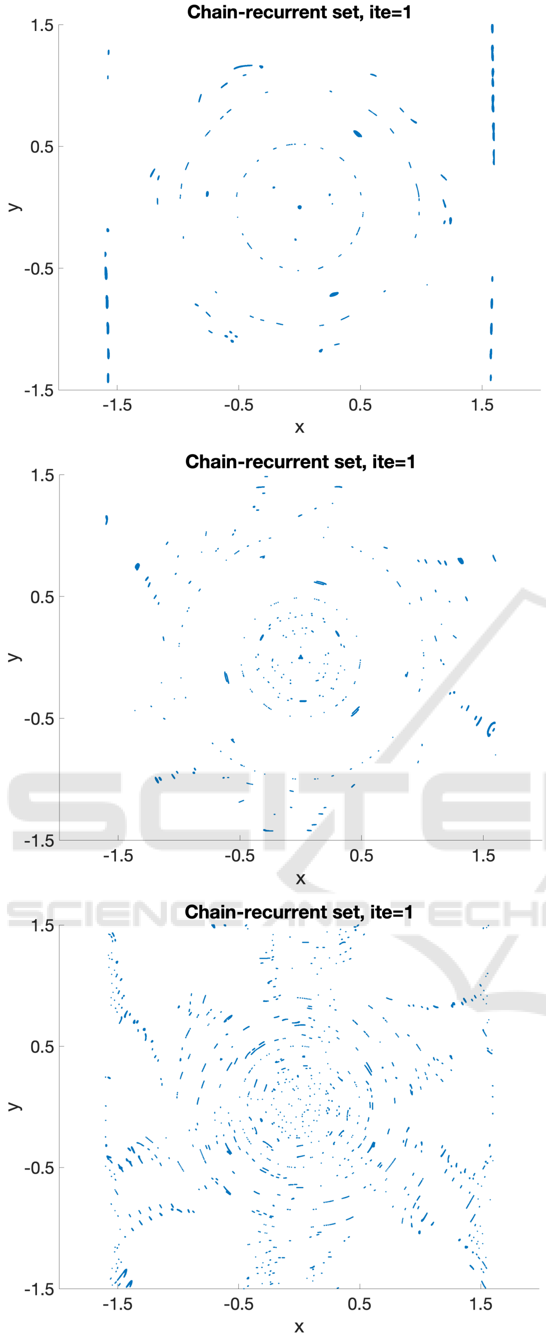

Figure 6: Chain-recurrent set from the approximation with the Gaussians in iteration 1 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

ics, have a limited region of parameter values leading to (numerically) positive definite collocation matrices.

Summarizing, the best results, both in terms of positive definite matrices and the accuracy of the

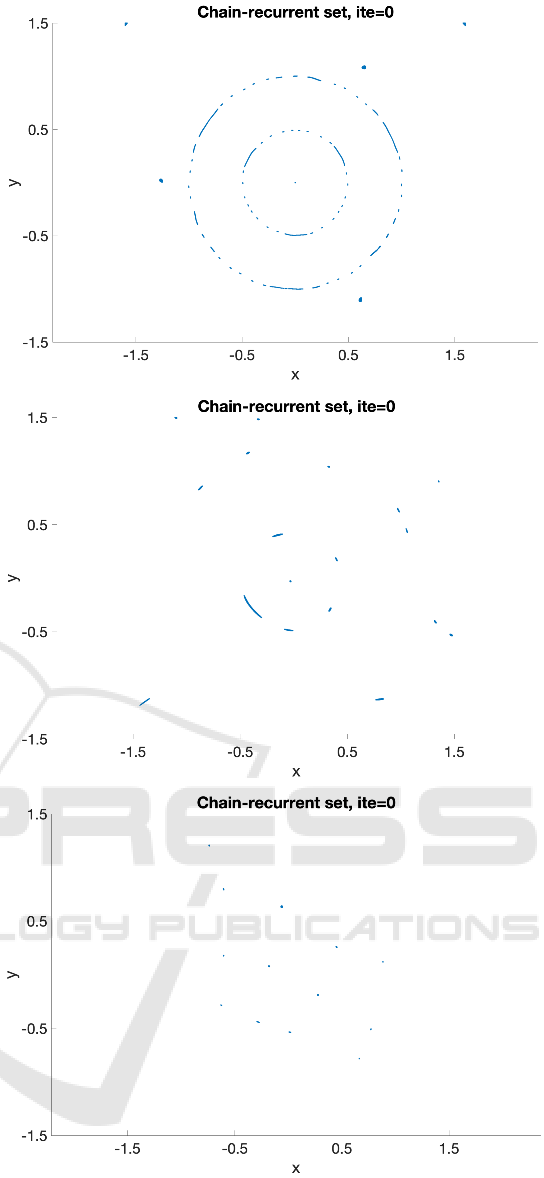

Figure 7: Chain-recurrent set from the approximation with the Inverse multiquadrics in iteration 0 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

chain-recurrent sets, were obtained for Wendland functions and Matérn kernels. These are kernels with a low degree of smoothness. For the smoother kernels, the matrices become numerically problematic quickly, i.e. not positive definite, when using denser collocation grids, while at the same time the localisation of the chain-recurrent set is poor.

This is a somewhat surprising result, since theoretical error estimates suggest that using smoother RBFs results in faster convergence; however, numerically, the collocation matrices quickly become non-positive

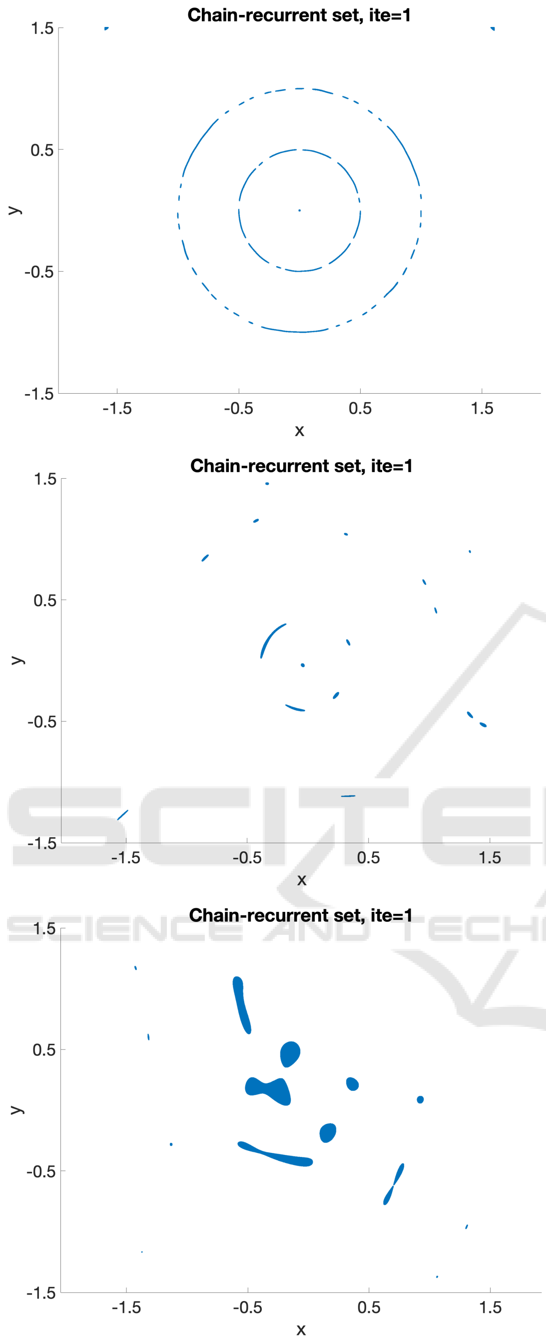

Figure 8: Chain-recurrent set from the approximation with the Inverse multiquadrics in iteration 1 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

definite. Our study confirms that Wendland functions are a good choice as RBFs for our application in Dynamical Systems to compute complete Lyapunov function candidates, and are preferable to Gaussians, Inverse quadratics and Inverse multiquadrics. Moreover, the Matérn kernels are also promising RBFs for our application and their use should be explored further.

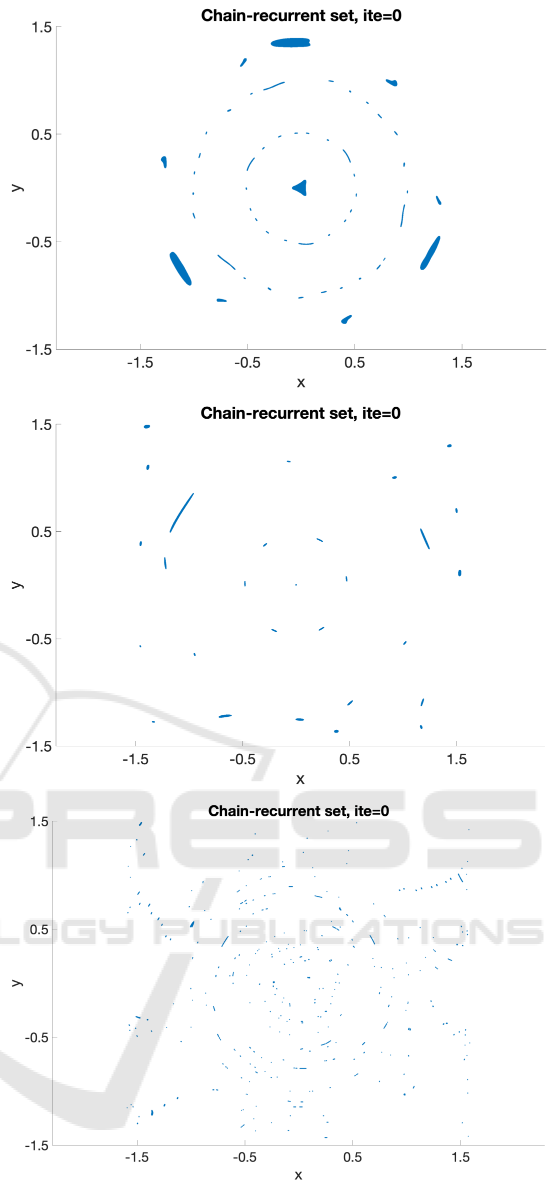

Figure 9: Chain-recurrent set from the approximation with the Inverse quadratics in iteration 0 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

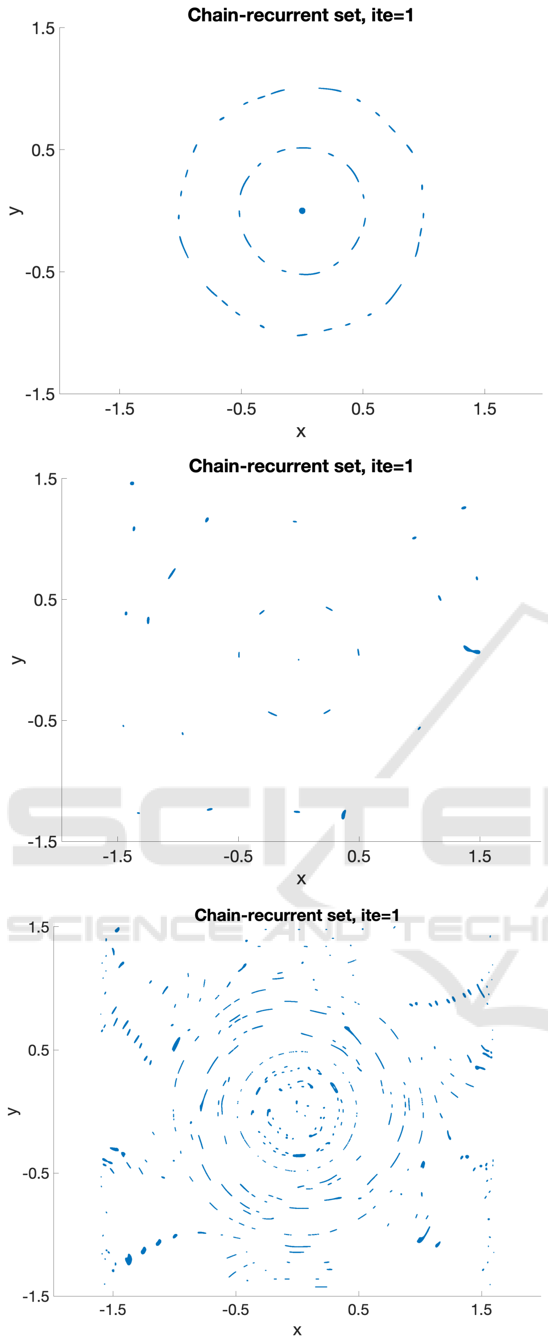

Figure 10: Chain-recurrent set from the approximation with the Inverse quadratics in iteration 1 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

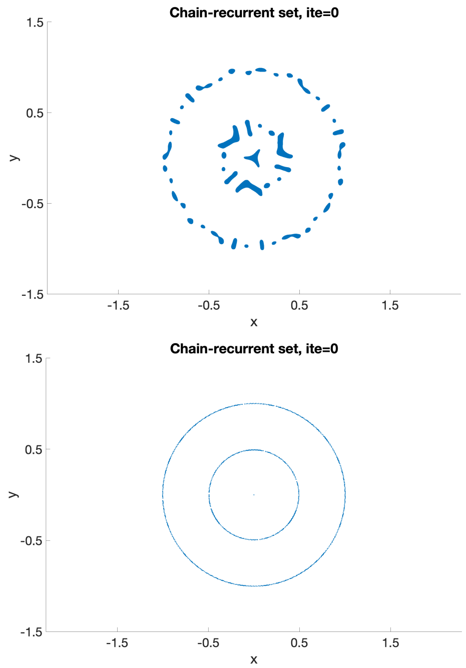

Figure 11: Chain-recurrent set from the approximation with Matérn $\psi_{(n+3)/2}$ kernels in iteration 0 with collocation matrix with condition number 10^3 (upper) and 10^5 (lower).

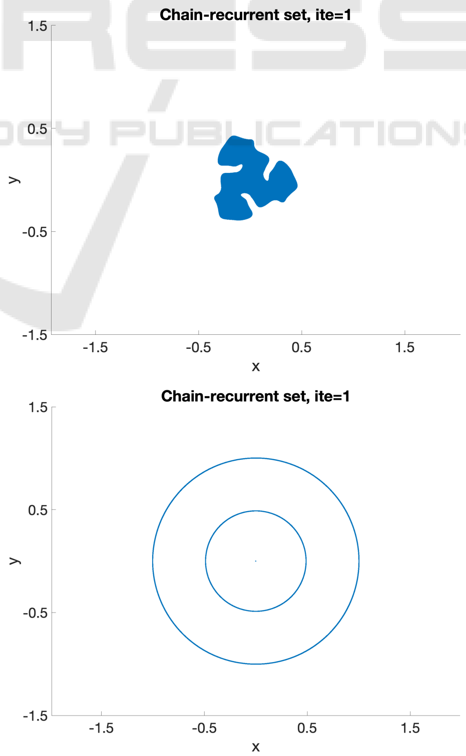

Figure 12: Chain-recurrent set from the approximation with Matérn $\psi_{(n+3)/2}$ kernels in iteration 1 with collocation matrix with condition number 10^3 (upper) and 10^5 (lower).

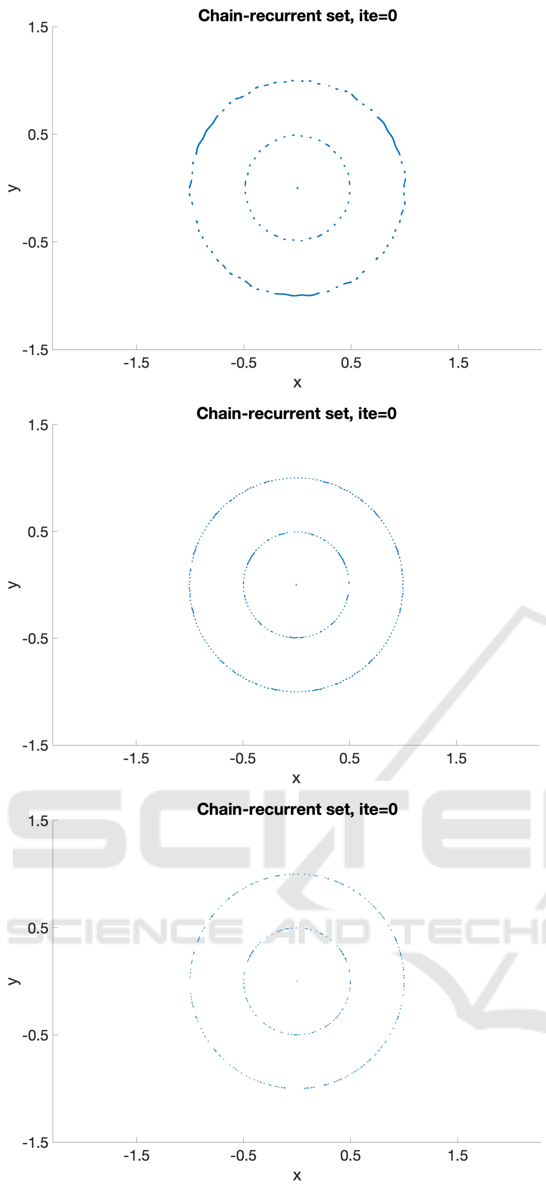

Figure 13: Chain-recurrent set from the approximation with Matérn $\psi_{(n+5)/2}$ kernels in iteration 0 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

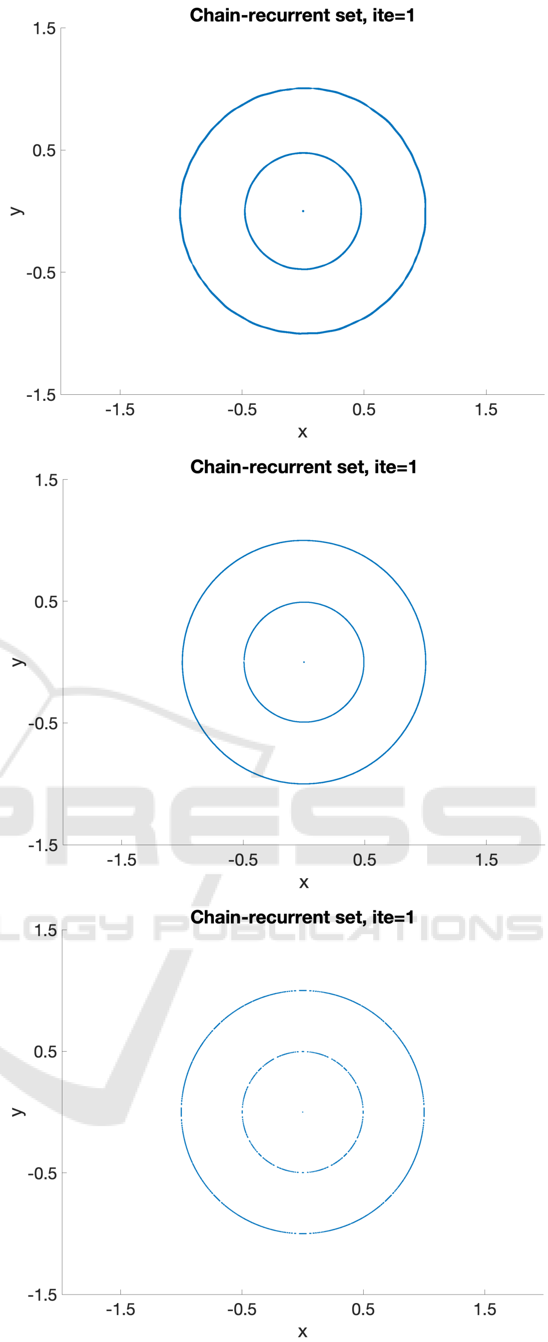

Figure 14: Chain-recurrent set from the approximation with Matérn $\psi_{(n+5)/2}$ kernels in iteration 1 with collocation matrix with condition numbers 10^3 (top), 10^5 (middle), and 10^{13} (bottom).

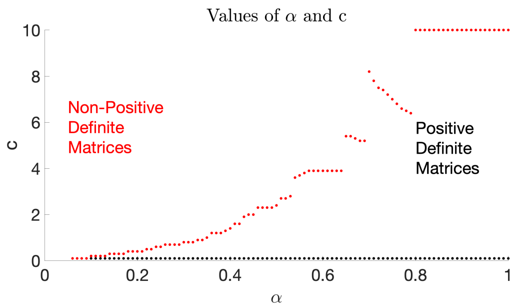

Figure 15: Gaussian RBF: c vs α, for a given α the collocation matrix is positive definite on the c interval between the black and the red dot.

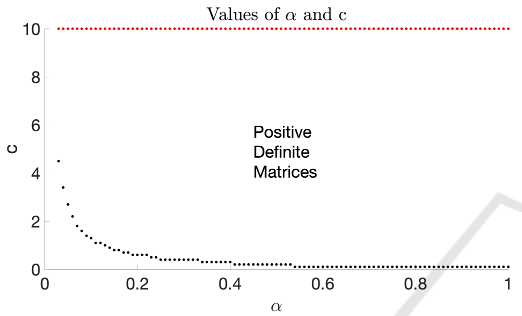

Figure 16: Inverse multiquadrics: c vs α, for a given α the collocation matrix is positive definite on the c interval between the black and the red dot.

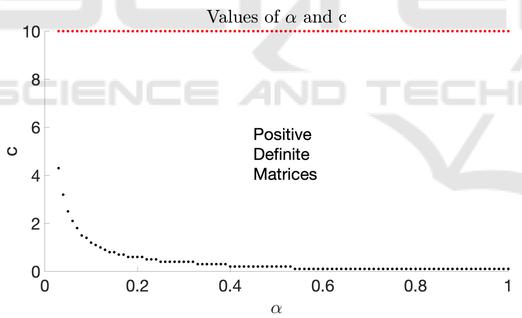

Figure 17: Inverse quadratic RBF: c vs α, for a given α the collocation matrix is positive definite on the c interval between the black and the red dot.

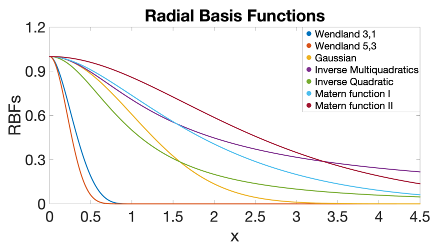

Figure 18: Comparison of all the radial basis functions used with parameter $c = 1$.

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