Minimization with differential inequality and equality constraints applied to complete Lyapunov functions

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Abstract

Meshfree collocation in reproducing kernel Hilbert spaces is an established method to solve generalized interpolation problems such as PDEs. It can be formulated as an optimization problem with equality constraints. In this paper, we consider optimization problems with both inequality and equality constraints for general linear operators, and develop a general theory of discretizing such problems. The unique solution of these discretized problems is obtained using quadratic optimization, and we show that the solutions of the discretized problems strongly converge to the unique solution of the original problem. The general theory is applied to compute complete Lyapunov functions for autonomous ordinary differential equations.

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1 Introduction

Meshfree collocation is an established method to solve (generalized) interpolation problems such as partial differential equations, see e.g. [25] for the general method and [18] for applications to the computation of Lyapunov functions. The framework for this method is a linear (differential) operator L, which acts on a Hilbert space H with inner product $\langle ., . \rangle_H$, consisting of functions $v\colon \Omega \subset \mathbb{R}^d \to \mathbb{R}$. We consider the problem

$$Lv(x) \quad = \quad r(x), \qquad x \in \Omega \tag{1}$$

for v, where r is a given function. Fixing a set of finitely many collocation points $X_\Omega = \{x_1, \ldots, x_N\} \subset \Omega$, we find an approximation by solving the generalized interpolation problem

$$\begin{aligned} \text{minimize} \quad & \|v\|_H \\ \text{subject to} \quad Lv(x_i) \quad &= \quad r(x_i) \text{ for } x_i \in X_\Omega. \end{aligned}$$

The solution of the generalized interpolation problem is given by

$$v^*(x) = \sum_{j=1}^{N} \beta_j v_{\lambda_j}(x),$$

where $\beta_j \in \mathbb{R}$ are coefficients and v_{λ_j} are the Riesz representers of the linear operators $\lambda_j = \delta_{x_j} \circ L \in H^*$; δ_{x_j} denotes the point evaluation at x_j. If H is a reproducing kernel Hilbert space with positive definite kernel $K\colon \Omega \times \Omega \to \mathbb{R}$, then the Riesz representer is given by $v_{\lambda_j}(x) = \lambda_j^y K(x, y)$, i.e.

$$v^*(x) = \sum_{j=1}^{N} \beta_j \lambda_j^y K(x, y).$$

Here, the superscript y denotes the evaluation of λ_j with respect to the variable y. The coefficient vector $\beta = (\beta_j)_{j=1,\ldots,N}$ is found by solving $A\beta = r$, where the vector $r = (r_j)_{j=1,\ldots,N}$ is given by $r_j = r(x_j)$ and $A = (a_{ij})_{i,j=1,\ldots,N}$ with $a_{ij} = \lambda_i^x \lambda_j^y K(x, y)$ is a positive definite matrix if all collocation points x_j are regular, i.e. $\lambda_j \neq 0$. Hence, the solution of the generalized interpolation problem can be computed by solving a system of N linear equations. The method can also be used to solve boundary value problems, using different operators for the boundary points. If (1) has a solution v, then there are error estimates on $Lv - Lv^*$ which involve the fill distance $h_{X_\Omega,\Omega} = \sup_{y\in\Omega} \inf_{x_i\in X_\Omega} \|y - x_i\|_2$, measuring how dense the collocation points are in Ω.

In this paper, we seek to generalize this approach by also considering linear inequalities. We consider again a reproducing kernel Hilbert space H

of functions $v\colon \Omega \to \mathbb{R}$ with positive definite kernel K as well as a linear operator L acting on H. We seek to solve a problem of the form

$$\begin{cases} Lv(x) &= r(x), \quad x \in \Gamma, \\ Lv(x) &\leq b(x), \quad x \in \Omega \setminus \Gamma, \end{cases}$$

where $\Gamma \subset \Omega$; both $\Gamma = \varnothing$ and $\Gamma = \Omega$ are possible, although the latter case is the classical interpolation problem. To obtain a unique solution, we consider the minimization problem

$$\begin{cases} \text{minimize} & \|v\|_H \\ \text{subject to} & Lv(x) = r(x), \quad x \in \Gamma, \\ & Lv(x) \leq b(x), \quad x \in \Omega \setminus \Gamma, \end{cases} \tag{2}$$

for v, where r and b are given functions. Fixing two sets of finitely many collocation points $X_\Gamma = \{x_1, \ldots, x_M\} \subset \Gamma$ and $X_\Omega = \{x_{M+1}, \ldots, x_{M+N}\} \subset \Omega \setminus \Gamma$, we discretize the problem, leading to

$$\begin{cases} \text{minimize} & \|v\|_H \\ \text{subject to} & Lv(x_i) = r(x_i), \quad x_i \in X_\Gamma, \\ & Lv(x_i) \leq b(x_i), \quad x_i \in X_\Omega. \end{cases} \tag{3}$$

It turns out that the solution of (3) is given by

$$v^*(x) = \sum_{j=1}^{M+N} \beta_j \lambda_j^y K(x, y),$$

where $\lambda_j = \delta_{x_j} \circ L$ and that the coefficients β_j can be calculated as the unique solution of a quadratic optimization problem. We will show the strong convergence in H of solutions of the discretized problems (3) to the (unique) solution of (2) if the fill distances of the collocation points go to zero. The discretized problem has already been studied in [14].

In the second part of the paper, we apply the results to an important problem from dynamical systems, namely the computation of complete Lyapunov functions for continuous-time dynamical systems given by an autonomous ODE.

A similar approach was used in [15], which deals with minimization problems with only inequality constraints and thus has to use a cost function including an integral, since otherwise the solution would be trivial. In this paper, we consider both inequality and equality constraints.

Let us give an overview over the paper: In Section 2 we state and prove our main result. In Section 3 we apply the general method to the problem of computing complete Lyapunov functions, present examples in Section 4 and end with conclusions in Section 5.

2 Minimization problem

We assume that $\Omega \subseteq \mathbb{R}^d$ is a bounded domain with Lipschitz boundary. Let $\Gamma \subset \Omega$; note that both $\Gamma = \varnothing$ and $\Gamma = \Omega$ are allowed, however, the latter case is the classical generalized interpolation. Further, let $L\colon H^\sigma(\Omega) \to H^{\sigma-m}(\Omega)$ be a linear, bounded operator, where $H^\sigma(\Omega)$ denotes, as usual, the L_2-Sobolev space of (fractional) order $\sigma > d/2 + m + 1$ with $m \in \mathbb{N}_0$.

Remark 2.1 *We call a point $x \in \mathbb{R}^d$* singular point of the linear operator *L, if $\delta_x \circ L = 0$ and* regular point of L *otherwise.*

Remark 2.2 *An example for L is a linear differential operator of order $m \in \mathbb{N}_0$ given by*

$$Lv = \sum_{|\alpha| \le m} c_\alpha D^\alpha v,$$

where all $c_\alpha \in C^{\sigma-m}(\overline{\Omega})$. Here, a singular point x is a point such that $c_\alpha(x) = 0$ for all $|\alpha| \le m$.

Note that the definition in Remark 2.1 in the context of differential operators was given in [18, Definition 3.2].

Let H be a reproducing kernel Hilbert space (RKHS) that consists of the functions $H^\sigma(\Omega)$. However, $H^\sigma(\Omega)$ is not necessarily equipped with the standard inner product, but in general with one inducing an equivalent norm. For a brief overview of reproducing kernel Hilbert spaces with the relevant definitions and theorems, see [15, Section 2]; a more detailed introduction can be found in [25, Chapters 10 and 16].

We consider the problem:

$$\begin{cases} \text{minimize} & \|v\|_H \\ \text{subject to} & Lv(x) = r(x), \qquad x \in \Gamma \\ & Lv(x) \le b(x), \qquad x \in \Omega \setminus \Gamma \end{cases} \tag{4}$$

with continuous functions $r, b\colon \Omega \to \mathbb{R}$. The main result of this section is that this problem has a unique solution v and, moreover, that it is the limit of a strongly convergent sequence of solutions of discretized problems. Those discretized problems can be formulated as finite dimensional quadratic programming problems.

Let us first consider the discretized problem: choose finite sets of regular points of the operator L (see Remark 2.1) $X_\Gamma = \{x_1, \ldots, x_M\} \subset \Gamma$ and $X_\Omega = \{x_{M+1}, \ldots, x_{M+N}\} \subset \Omega \setminus \Gamma$; again, $M = 0$ or $N = 0$ are allowed. Furthermore, let $\lambda_i \in H^*$ be given by $\lambda_i(v) = Lv(x_i)$, $i = 1, \ldots, M+N$, as well as $r_i = r(x_i)$, $i = 1, \ldots, M$ and $b_i = b(x_{M+i})$, $i = 1, \ldots, N$. We will deal with the discretized problems in Section 2.1. In Section 2.2 we will establish the strong convergence of the solutions of the discretized problems to the solution of (4), under the assumption that the fill distance of the discretization points goes to zero.

2.1 Discretized version

The discretized version was introduced and discussed in [14]. In this section we will recall the main results, see [14, Lemmas 5.1-5.3], and then expand by discussing the Karush-Kuhn-Tucker (KKT) conditions for this problem, which are first derivative tests for a solution in nonlinear programming to be optimal.

Proposition 2.3 *We consider the problem for $v \in H$*

$$\left\{ \begin{array}{llll} \textit{minimize} & \|v\|_H & & \\ \textit{subject to} & \lambda_i(v) = r_i, & & i = 1, \ldots, M \\ & \lambda_i(v) \leq b_i, & & i = M+1, \ldots, M+N \end{array} \right. \tag{5}$$

where $r_i, b_i \in \mathbb{R}$, H is a reproducing kernel Hilbert space with kernel K, inner product $\langle \cdot, \cdot \rangle_H$ and norm $\| \cdot \|_H$, and $\lambda_i \in H^*$, $i = 1, \ldots, M+N$ are linearly independent.

Then the unique minimizer of problem of (5) is of the form (6)

$$v^*(x) = \sum_{j=1}^{N} \beta_j \lambda_j^y K(x, y), \tag{6}$$

where the coefficient vector $\beta = (\beta_j)_{j=1,\ldots,N}$ is defined by the unique solution of the minimization problem

$$\left\{ \begin{array}{llll} & \beta^T A \beta & & \\ \textit{subject to} & B_1 \beta & = r & \in \mathbb{R}^M \\ \textit{and} & B_2 \beta & \leq b & \in \mathbb{R}^N. \end{array} \right. \tag{7}$$

Here, $A = \begin{pmatrix} B_1 \\ B_2 \end{pmatrix}$, $B_1 \in \mathbb{R}^{M \times (M+N)}$, $B_2 \in \mathbb{R}^{N \times (M+N)}$ and $a_{ij} = \lambda_i^x \lambda_j^y K(x, y)$.

Summarizing, the problem (5) has a unique solution that can be computed using the finite-dimensional quadratic optimization problem (7).

For the remainder of this subsection we study the relation between the inequality conditions and the corresponding coefficients β_j, $j = M+1, \ldots, M+N$ using KKT conditions, following [8].

Proposition 2.4 *Consider problem (7) and let $\beta^* \in \mathbb{R}^{M+N}$ be the solution.*

Then $\beta_i^* \leq 0$ for all $i = M+1, \ldots, M+N$.

Moreover, for each $i \in \{M+1, \ldots, M+N\}$, if $(B_2 \beta^*)_i < b_i$, then $\beta_i^* = 0$.

Proof: We denote the i-th row (or column) of the symmetric matrix A by a_i, $i = 1, \ldots, M+N$. The discrete problem (7) can be expressed as

$$\begin{array}{rlll} \min & F_0(\beta) & = \beta^T A \beta & \\ \text{such that} & H_i(\beta) & = a_i^T \beta - r_i & = 0 \text{ for } i = 1, \ldots, M \\ & F_i(\beta) & = a_i^T \beta - b_i & \leq 0 \text{ for } i = M+1, \ldots, M+N. \end{array}$$

Note that the functions F_i are convex, H_i are affine and they all are differentiable, and the refined Slater's condition is satisfied, since all constraint functions F_i, $i = M+1, \ldots, M+N$ are affine. Hence, the KKT conditions provide necessary and sufficient conditions for optimality, see e.g. [8, Chapter 5.5.3]. In more detail, β^* is a minimiser if and only if the KKT conditions hold. Here, μ and ν are the KKT multipliers; for problems with no inequality constraints, these would be Lagrange multipliers.

$$\begin{aligned}
H_i(\beta^*) &= 0 \text{ for } i = 1, \ldots, M \\
F_i(\beta^*) &\leq 0 \text{ for } i = M+1, \ldots, M+N \\
\mu_i &\geq 0 \text{ for } i = 1, \ldots, N \\
\mu_i F_{M+i}(\beta^*) &= 0 \text{ for } i = 1, \ldots, N \\
0 &= \nabla F_0(\beta^*) + \sum_{i=1}^{N} \mu_i \nabla F_{M+i}(\beta^*) + \sum_{i=1}^{M} \nu_i \nabla H_i(\beta^*).
\end{aligned}$$

These conditions become in our case

$$\begin{aligned}
a_i^T \beta^* &= r_i \text{ for } i = 1, \ldots, M \\
a_i^T \beta^* &\leq b_i \text{ for } i = M+1, \ldots, M+N \\
\mu_i &\geq 0 \text{ for } i = 1, \ldots, N \\
\mu_i (a_{M+i}^T \beta^* - b_{M+i}) &= 0 \text{ for } i = 1, \ldots, N \\
0 &= 2A\beta^* + \sum_{i=1}^{N} \mu_i a_{M+i} + \sum_{i=1}^{M} \nu_i a_i
\end{aligned} \tag{8}$$

The last equation can be equivalently written as

$$0 = A \left(2\beta^* + \begin{pmatrix} \nu \\ \mu \end{pmatrix} \right) \tag{9}$$

Since a_i are the columns of the (symmetric) matrix A. From (9) we can deduce, since A is non-singular, that

$$\beta^* = -\frac{1}{2} \begin{pmatrix} \nu \\ \mu \end{pmatrix}. \tag{10}$$

Since $\mu_i \geq 0$ for all $i = 1, \ldots, N$, this implies that $\beta_i^* \leq 0$ for all $i = M+1, \ldots, M+N$. From (8) it follows for each $i = 1, \ldots, N$ that if $a_{M+i}^T \beta^* < b_{M+i}$, then $\mu_i = 0$, i.e. $\beta_i^* = 0$. □

2.2 Convergence

We now consider again problem (4) and will show that it has a unique solution, which is the limit of solutions to the discretized problem.

Theorem 2.5 *Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with Lipschitz boundary. Let $\Gamma \subset \Omega$; note that $\Gamma = \varnothing$ and $\Gamma = \Omega$ are allowed.*

Let $L\colon H^\sigma(\Omega) \to H^{\sigma-m}(\Omega)$ be a linear, bounded operator, where $m \in \mathbb{N}_0$ and $\sigma > d/2 + m + 1$. Let $b, r : \Omega \to \mathbb{R}$ be continuous functions and $H = H^\sigma(\Omega)$ with norm $\|\cdot\|_H := \|\cdot\|_{k_\sigma}$ induced by the reproducing kernel $k_\sigma : \Omega \times \Omega \to \mathbb{R}$, given by $k_\sigma(x,y) = \Phi_\sigma(x-y)$, $x, y \in \Omega$, where Φ_σ is a suitable, positively definite function.

Consider the optimization problem for $v \in H$

$$\begin{cases} \text{minimize} & \|v\|_H \\ \text{subject to} & Lv(x) = r(x), \qquad x \in \Gamma, \\ & Lv(x) \le b(x), \qquad x \in \Omega \setminus \Gamma. \end{cases} \tag{11}$$

Moreover, we assume the existence of $V_0 \in H^\sigma(\Omega)$ satisfying the constraints of (11) as well as

- *let $X_N^n = \{x_1^n, \ldots, x_{M_n+N_n}^n\} \subset \Omega$ be a set of pairwise distinct and regular points of L (cf. Remark 2.1) for all $n \in \mathbb{N}$. Set $X_\Gamma^n := \{x_1^n, x_2^n, \ldots, x_{M_n}^n\}$ and $X_\Omega^n := \{x_{M_n+1}^n, x_{M_n+2}^n, \ldots, x_{M_n+N_n}^n\}$.*
- *$X_\Gamma^n \subseteq \Gamma$ and $X_\Omega^n \subseteq \Omega \setminus \Gamma$.*
- *the fill distances $h_{X_\Gamma^n,\Gamma} = \sup_{x\in\Gamma} \min_{x_i \in X_\Gamma^n} \|x - x_i\|_2$ (if $\Gamma \neq \varnothing$) and $h_{X_\Omega^n,\Omega\setminus\Gamma} = \sup_{x\in\Omega\setminus\Gamma} \min_{x_i\in X_\Omega^n} \|x - x_i\|_2$ (if $\Omega \setminus \Gamma \neq \varnothing$) converge to 0 as $n \to \infty$.*

For $n \in \mathbb{N}$, we denote by v_n the (unique) solution v of the following problem

$$\begin{cases} \text{minimize} & \|v\|_H \\ \text{subject to} & Lv(x_i^n) = r(x_i^n), \qquad i = 1, \ldots, M_n, \\ & Lv(x_i^n) \le b(x_i^n), \qquad i = M_n+1, \ldots, M_n+N_n. \end{cases} \tag{12}$$

Then the optimization problem (11) has a unique solution v. Moreover, the solutions v_n of the optimization problems (12) converge strongly in H to v as $n \to \infty$.

Proof: We fix $n \in \mathbb{N}$ and observe that the optimization problem (12) is of the form (5). Indeed, since Ω has a Lipschitz boundary and $\sigma > d/2$, $H := H^\sigma(\Omega)$ is a RKHS. On $H^\sigma(\Omega)$, we choose an inner product $\langle\cdot,\cdot\rangle_H = \langle\cdot,\cdot\rangle_{H^\sigma(\Omega)} = \langle\cdot,\cdot\rangle_{k_\sigma}$ induced by $k_\sigma(x,y) = \Phi_\sigma(x-y)$, $x, y \in \Omega$, where k_σ is a reproducing kernel with positive definite function $\Phi_\sigma : \mathbb{R}^d \to \mathbb{R}$. In particular, we have $g(x) = \langle g, k_\sigma(\cdot, x)\rangle_H$ for all $g \in H$ and $x \in \Omega$, see [15, Definition 2.1].

Note that the functionals $\lambda_i = \delta_{x_i^n} \circ L$ lie in H^*, since L is a continuous map from $H^\sigma(\Omega)$ to $H^{\sigma-m}(\Omega)$ and $\sigma > d/2+m$. These functionals are also linearly independent, because x_i^n are regular points of L, cf. [18, Proposition 3.3]. Thus, the problem (12) is of the form (5) with those λ_i, $r_i = r(x_i^n)$ for $i = 1, \dots, M_n$, $b_i = b(x_i^n)$ for $i = M_n+1, \dots, M_n+N_n$ and $M = M_n$ as well as $N = N_n$.

We will show the strong convergence of the sequence $(v_n)_{n\in\mathbb{N}}$ of solutions of (12) to an element $v \in H$, which turns out to be the unique solution of (11).

Step 1 We can conclude from (11) that

$$\begin{aligned} LV_0(x_i^n) &= r(x_i^n), \quad i = 1, \dots, M_n \\ LV_0(x_i^n) &\le b(x_i^n), \quad i = M_n+1, \dots, M_n+N_n. \end{aligned}$$

This shows that V_0 satisfies the constraints of (12). Since v_n is the minimizer of this problem, we have

$$\|v_n\|_H \quad \le \quad \|V_0\|_H =: C_0. \tag{13}$$

This shows that the bounded sequence $\|v_n\|_H$ has a subsequence, which we again denote by $(v_n)_{n\in\mathbb{N}}$, that converges weakly to a function $v \in H$. Moreover, we have

$$\|v\|_H \le \liminf_{n\to\infty} \|v_n\|_H \le C_0. \tag{14}$$

For Steps 2-4, we denote by $(v_n)_{n\in\mathbb{N}}$ any fixed weakly convergent subsequence of the original sequence; we will show the convergence of the original sequence in Step 5.

Step 2 In this step, we will show $Lv(x) = r(x)$ for all $x \in \Gamma$ and $Lv(x) \le b(x)$ for all $x \in \Omega\setminus\Gamma$; recall that v is the weak limit of the (sub)sequence $(v_n)_{n\in\mathbb{N}}$.

Let $\lambda = \delta_x \circ L \in H^*$. Then the Riesz representer of λ is given by $\lambda^y k_\sigma(\cdot, y)$ and hence

$$|Lv(x) - Lv_n(x)| \quad = \quad |\lambda(v - v_n)| = |\langle v - v_n, \lambda^y k_\sigma(\cdot, y)\rangle_H| \longrightarrow 0, \tag{15}$$

since v_n converges weakly to v.

By a similar argumentation as above, the Sobolev space $H^{\sigma-m}(\Omega)$ is also a RKHS and we choose the inner product to be defined by a reproducing kernel of the form $k_{\sigma-m}(x,y) = \Phi_{\sigma-m}(x-y)$, where $\Phi_{\sigma-m}\colon \mathbb{R}^d \to \mathbb{R}$. The Sobolev embedding theorem implies $H^{\sigma-m}(\mathbb{R}^d) \subseteq W^1_\infty(\mathbb{R}^d) \cap C^1(\mathbb{R}^d)$ since $\sigma - m > d/2+1$. Thus, there exists $M > 0$ with $\|\nabla\Phi_{\sigma-m}(\xi)\|_2 \le M$ for all $\xi \in \mathbb{R}^d$.

Given $x, y \in \Omega$, we use the mean value theorem which implies the existence of $\xi \in \mathbb{R}^d$ on the line between 0 and $x - y$ to show that

$$\begin{aligned}
&|Lv_n(x) - Lv_n(y)| \\
&= \langle Lv_n, k_{\sigma-m}(\cdot, x) - k_{\sigma-m}(\cdot, y)\rangle_{H^{\sigma-m}(\Omega)} \\
&\leq \|Lv_n\|_{H^{\sigma-m}(\Omega)} \|k_{\sigma-m}(\cdot, x) - k_{\sigma-m}(\cdot, y)\|_{H^{\sigma-m}(\Omega)} \\
&= \|Lv_n\|_{H^{\sigma-m}(\Omega)} \left(k_{\sigma-m}(x, x) + k_{\sigma-m}(y, y) - 2k_{\sigma-m}(x, y)\right)^{1/2} \\
&\leq \sqrt{2} c_0 \|v_n\|_{H^{\sigma}(\Omega)} \left(\Phi_{\sigma-m}(0) - \Phi_{\sigma-m}(x - y)\right)^{1/2} \\
&\leq \sqrt{2} c_0 C_0 \|\nabla \Phi_{\sigma-m}(\xi)\|_2^{1/2} \|x - y\|_2^{1/2} \\
&\leq C_1 \|x - y\|_2^{1/2} \qquad (16)
\end{aligned}$$

for all $n \in \mathbb{N}$ by (13) and with $C_1 = \sqrt{2} c_0 C_0 M^{1/2}$. Note that we have also used that $L \colon H^{\sigma}(\Omega) \to H^{\sigma-m}(\Omega)$ is a bounded operator with norm c_0 and the identity

$$\lambda^x \mu^y k_{\sigma-m}(x, y) = \langle \lambda^x k_{\sigma-m}(\cdot, x), \mu^y k_{\sigma-m}(\cdot, y)\rangle_{H^{\sigma-m}(\Omega)}. \qquad (17)$$

Step 2a: equality constraints If $\Gamma \neq \varnothing$, then we will show $Lv(x) = r(x)$ for all $x \in \Gamma$. More precisely, we let $x \in \Gamma$ and $\varepsilon > 0$, and will show that $|Lv(x) - r(x)| < \varepsilon$.

By (15), there exists $N_1 \in \mathbb{N}$ such that for all $n \geq N_1$ we have

$$|Lv(x) - Lv_n(x)| < \frac{\varepsilon}{3}. \qquad (18)$$

Since r is continuous at $x \in \Gamma \subset \Omega$, there exists $\delta > 0$ such that

$$|r(x) - r(y)| < \frac{\varepsilon}{3} \qquad (19)$$

for all $y \in B_\delta(x)$.

Using that the fill distance satisfies $h_{X_\Gamma, \Gamma} \to 0$ as $n \to \infty$, there is $N_2 \in \mathbb{N}$ such that there exists $x_i^n \in X_\Gamma^n$ for all $n \geq N_2$ with

$$\|x - x_i^n\|_2 < \min\left(\frac{\varepsilon^2}{9C_1^2}, \delta\right). \qquad (20)$$

Let $n \geq \max(N_1, N_2)$. By (18), (16), (20), (19) and $Lv_n(x_i) = r(x_i^n)$, we have that

$$\begin{aligned}
|Lv(x) - r(x)| &\leq |Lv(x) - Lv_n(x)| + |Lv_n(x) - Lv_n(x_i^n)| \\
&\quad + |Lv_n(x_i^n) - r(x_i^n)| + |r(x_i^n) - r(x)| \\
&< \frac{\varepsilon}{3} + C_1 \frac{\varepsilon}{3C_1} + 0 + \frac{\varepsilon}{3} = \varepsilon.
\end{aligned}$$

Step 2b: inequality constraints If $\Omega\setminus\Gamma \neq \varnothing$, then we will show $Lv(x) \leq b(x)$ for all $x \in \Omega \setminus \Gamma$. More precisely, we let $x \in \Omega \setminus \Gamma$ and $\varepsilon > 0$, and will show that $Lv(x) - b(x) < \varepsilon$.

(15) implies the existence of $N_1 \in \mathbb{N}$ such that

$$|Lv(x) - Lv_n(x)| < \frac{\varepsilon}{3} \tag{21}$$

for all $n \geq N_1$. By the continuity of b at $x \in \Omega$, there exists a $\delta > 0$ such that

$$|b(x) - b(y)| < \frac{\varepsilon}{3} \tag{22}$$

for all $y \in B_\delta(x)$.

Using that the fill distance satisfies $h_{X_\Omega,\Omega\setminus\Gamma} \to 0$ as $n \to \infty$, there is $N_2 \in \mathbb{N}$ such that there exists $x_i^n \in X_\Omega^n$ for all $n \geq N_2$ with

$$\|x - x_i^n\|_2 < \min\left(\frac{\varepsilon^2}{9C_1^2}, \delta\right). \tag{23}$$

Let $n \geq \max(N_1, N_2)$. Then (21), (16), (23), and (22) as well as $Lv_n(x_i) \leq b(x_i^n)$ imply

$$\begin{aligned} Lv(x) - b(x) &= (Lv(x) - Lv_n(x)) + (Lv_n(x) - Lv_n(x_i^n)) \\ &\quad + (Lv_n(x_i^n) - b(x_i^n)) + (b(x_i^n) - b(x)) \\ &< \frac{\varepsilon}{3} + C_1\frac{\varepsilon}{3C_1} + 0 + \frac{\varepsilon}{3} \;=\; \varepsilon. \end{aligned}$$

Step 3 In Step 2 we have shown that $Lv(x) = r(x)$ holds for all $x \in \Gamma$ and $Lv(x) \leq b(x)$ holds for all $x \in \Omega \setminus \Gamma$. Hence, v satisfies the constraints of (12) for each $n \in \mathbb{N}$ and thus

$$\|v_n\|_H \leq \|v\|_H$$

since v_n is the minimizer of (12).

This implies $\limsup_{n\to\infty} \|v_n\|_H \leq \|v\|_H$ and, using (14), also

$$\lim_{n\to\infty} \|v_n\|_H = \|v\|_H,$$

and thus that v_n converges strongly to v.

Step 4 We first show that v is a minimizer. Let $V \in H$ satisfy the constraints of (11), i.e. V also satisfies satisfies the constraints of the discrete problem for every n. Hence,

$$\|v_n\|_H \leq \|V\|_H$$

and by the strong convergence, we can conclude $\|v\|_H \leq \|V\|_H$, which shows that v is a minimizer. The uniqueness of the minimizer $v \in H$ follows from the strict convexity of $\| \cdot \|_H$ and the fact that the constraints are affine.

Step 5: Original sequence We have shown that every weakly convergent subsequence of the original sequence $(v_n)_{n\in\mathbb{N}}$ (see Step 1) necessarily converges strongly to v, the unique solution of (11). Now we establish that the original sequence $(v_n)_{n\in\mathbb{N}}$ of solutions to (12) converges strongly to v. We argue by contradiction and assume that there exists $\varepsilon > 0$ and a subsequence $(v_{n_k})_{k\in\mathbb{N}}$ such that

$$\|v_{n_k} - v\|_H \geq \varepsilon \text{ for all } k \in \mathbb{N}. \tag{24}$$

$(v_{n_k})_{k\in\mathbb{N}}$ is bounded and thus has a weakly convergent subsequence. But we have shown that this subsequence converges weakly, and then strongly, to v, which is a contradiction to (24). □

3 Complete Lyapunov functions

We will now apply the general theory, developed in the previous section, to the problem of computing complete Lyapunov functions. Let us consider the general autonomous ODE

$$\dot{x} = f(x), \text{ where } x \in \mathbb{R}^d. \tag{25}$$

We are interested in the determination of the chain-recurrent set $\mathcal{R}$, which contains attractors and repellers, and the stability of its connected components via a complete Lyapunov function (CLF). A complete Lyapunov function is a function $V\colon \mathbb{R}^d \to \mathbb{R}$, which is non-increasing along solutions of (25) and even strictly decreasing along solutions outside the chain-recurrent set $\mathcal{R}$. Moreover, $V(\mathcal{R})$ is a subset of $\mathbb{R}$, which is nowhere dense, and the level sets of V in $\mathcal{R}$, $V^{-1}(r) \cap \mathcal{R} \neq \varnothing$ for $r \in \mathbb{R}$, are the chain-transitive components of $\mathcal{R}$, see [9, §6.4], [21, §4]. A CLF provides even more information about the dynamics and the long-term behaviour of the system through its values, e.g. an asymptotically stable equilibrium is a local minimum and the values on different connected components of the chain-recurrent set describe the dynamics between them.

Relaxing the assumptions on a CLF, we call a function V that is non-increasing along trajectories, a CLF candidate. If V is C^1, then this can be formulated as $V(x) \leq 0$, where $\dot{V}(x) = \nabla V(x) \cdot f(x)$ is the orbital derivative, i.e. the derivative along solutions of (25). A constant function is automatically a CLF candidate as it satisfies $\dot{V}(x) = 0 \leq 0$, however, it does not provide any insight into the dynamics. The larger the area, where

V is strictly decreasing, the more information the CLF candidate provides regarding the dynamics.

Several methods have been proposed to compute CLFs. In [24, 5, 20], a discrete-time dynamical system was defined by the dynamics between cells through a multivalued time-T map, computed using the software package GAIO [10]. A complete Lyapunov function was computed via graph algorithms [5]. The paper [7] proposed the construction of a complete Lyapunov function as continuous piecewise affine (CPA) function on a given simplicial complex, but required information on the location of local attractors. In [1, 2, 3], CLF candidates are computed by solving

$$\dot{V}(x) = -1 \tag{26}$$

with meshfree collocation, in particular using Radial Basis Functions (RBFs); however, note that (26) cannot be satisfied at all points in the chain-recurrent set, and thus the error estimates from meshfree collocation cannot be employed.

A modified problem with a different cost function, namely

$$\begin{array}{ll} \text{minimize} & \|V\|_H^2 + \int_\Omega \dot{V}(x)\,dx \\ \text{subject to} & \dot{V}(x) \le 0 \text{ for } x \in \Omega, \end{array}$$

was considered in [15] and the strong convergence of the discretized problems was shown. The solutions of this problem have values very close to 0, however, no information about the chain-recurrent set is required.

We now apply the theory of the previous section to the problem of computing a CLF (candidate). We consider the problem

$$\begin{cases} \text{minimize} & \|V\|_H \\ \text{subject to} & LV(x) = -1, \qquad x \in \Gamma \\ & LV(x) \le 0, \qquad x \in \Omega \setminus \Gamma \end{cases}$$

where Γ is a subset of the area of gradient-like flow. The inequality constraint guarantees that V is a complete Lyapunov function candidate, while the equality constraint ensures that $V \equiv 0$ is not the solution.

For the proof of Theorem 3.2, we require the existence of a complete Lyapunov function with prescribed orbital derivative, which is established in the following theorem from [17].

Theorem 3.1 *Let $\dot{x} = f(x)$ define a dynamical system on an open set $\Omega \subset \mathbb{R}^d$ with $f \in C^k(\Omega, \mathbb{R}^d)$, where $k \in \mathbb{N} \cup \{\infty\}$.*

Then for every compact set $\Gamma \subset \Omega \setminus \mathcal{R}$, where $\mathcal{R}$ denotes the chain-recurrent set, and every C^k-function $g\colon U \to (-\infty, 0)$ defined on a neighborhood $U \subset \Omega$ of Γ there exists a complete C^k-Lyapunov function $V_0\colon \Omega \to \mathbb{R}$ with

- *$\dot V_0(x) = g(x)$ for all $x \in \Gamma$ and*
- *$\dot V_0(x) < 0$ for all $x \in \Omega \setminus \mathcal{R}$.*

Now we can apply the theory of this paper to compute complete Lyapunov function candidates.

Theorem 3.2 *Consider the ODE*

$$\dot x \;=\; f(x) \tag{27}$$

with $f \in C^k(\mathbb{R}^d, \mathbb{R}^d)$ and $k > d/2 + 2$, $k \in \mathbb{N}$. Let $\Omega \subset \mathbb{R}^d$ be a bounded domain with Lipschitz boundary. Moreover, we choose $b \equiv 0$ and $r \in C^\sigma(\Omega, \mathbb{R})$ with $r(x) < 0$ for all $x \in \Omega$, e.g. $r \equiv -1$.

Let $\Gamma \neq \varnothing$ be a compact set with $\Gamma \subset \Omega \setminus \mathcal{R}$, where $\mathcal{R}$ is the chain-recurrent set.

Setting $\sigma = k$ and $\lambda_i = \delta_{x_i} \circ L$, $i = 1, \ldots, N$, where $LV = \dot V = \nabla V(x) \cdot f(x)$ is the orbital derivative, and using points $x_i^n \in \Omega$, which are pairwise distinct and no equilibria, i.e. $f(x_i^n) \neq 0$, this problem satisfies the assumptions of Theorem 2.5.

In particular, there is a function $V_0 \in H^\sigma(\Omega)$ satisfying the constraints of (11) and the points x_i^n are regular points of L.

Proof: The operator L is a differential operator of order $m = 1$ in the sense of Remark 2.2; note that $c_{e_i} = f_i \in C^{\sigma-1}(\overline{\Omega})$ with $\sigma = k > d/2 + 2 = d/2 + m + 1$. Hence, the singular points of L are precisely the equilibria of (27), see [18].

The existence of a function $V_0 \in H^\sigma(\Omega)$ satisfying the constraints of (11) follows from Theorem 3.1 with any neighborhood U of Γ and $g = r\big|_U$. Note that $V_0 \in C^k(\Omega) \subset H^\sigma(\Omega)$ since $\sigma = k$ and Ω is bounded. $\square$

In practice we can choose Γ as a very small set, even a one-point set with $x_0 \notin \mathcal{R}$ leads to good results. Since $\Gamma \neq \varnothing$, the solution of the minimization problem is not the trivial solution $v \equiv 0$; however, there is no guarantee that the areas where $\dot v = 0$ are not considerably larger than the chain-recurrent set $\mathcal{R}$. In particular, it is conceivable that connected components of the gradient-like set could be areas where $\dot v \equiv 0$. We will discuss strategies how to avoid this in practice below.

The following proposition provides a fast way to compute an approximation of the chain-recurrent set. Assuming that the limit v is not only a complete Lyapunov function candidate but a complete Lyapunov function, i.e. that $Lv(x) = 0$ if and only if x is in the chain-recurrent set, and also assuming that n is sufficiently large, Proposition 3.3 implies that if $x = x_i^n \in X_\Omega^n$, then $\beta_i^* < 0$ if x_i is in the chain-recurrent set, and $\beta_i^* = 0$ otherwise. This is the motivation for a criterion in Section 4 to distinguish between points in the chain-recurrent set and the gradient-flow part.

Proposition 3.3 *Let v be the solution of (11) with $r \equiv -1$ and $b \equiv 0$. Let $x = x_i^n \in X_\Omega^n \subset \Omega$ be a collocation point for all $n \in \mathbb{N}$ such that $Lv(x) < 0$; in particular, x is in the gradient-flow part.*

Then there exists $N \in \mathbb{N}$ such that for all discretizations $n \geq N$ we have

$$Lv_n(x_i^n) < 0$$

and $(\beta_i^n)^* = 0$, where $(\beta^n)^*$ is the solution of the corresponding problem (7).

Proof: By (15) we have $Lv_n(x) \to Lv(x) = -\varepsilon < 0$; hence, there is $N \in \mathbb{N}$ such that $Lv_n(x) \leq -\varepsilon/2 < 0$ for all $n \geq N$. By Proposition 2.4 we can conclude that $(\beta_i^n)^* = 0$ for all $n \geq N$. □

Corollary 3.4 *Let $G \subset \Omega \setminus \mathcal{R}$ be a subset of the gradient-like flow. Assume that the kernel is given by a Radial Basis Function with compact support $r > 0$. Further, let $\varnothing \neq G_0 \subset G$ be such that $\inf_{x \in G_0, y \notin G} \|x - y\|_2 \geq r$ and $\Gamma \cap G = \varnothing$, i.e. points in G satisfy the inequality constraints.*

Then there are necessarily points $x \in G_0$ such that $\dot{v}(x) = 0$.

Proof: Assume, in contradiction to the statement, that $\dot{v}(x) < 0$ holds for all $x \in G_0$. Then Proposition 3.3 implies that $(\beta_i^n)^* = 0$ holds and, because of the form of v and the support radius, this shows that $v(x) \equiv 0$ for all $x \in G_0$, which is a contradiction. □

The corollary thus shows that if the support radius is small, and we provide limited information through a small area Γ with equality constraints, then the outcome is only a Lyapunov function candidate with large areas satisfying $\dot{v}(x) = 0$ although they are part of the gradient-like flow. The lesson to learn is thus to include points in Γ which are not too far apart with respect to the support radius r, see Example 3.5.

The numerical examples in the next section will show, however, that when choosing the support radius sufficiently large, the limit v is a valid complete Lyapunov function and is able to characterize the chain-recurrent set very well, while if the support radius is too small, we miss areas.

Example 3.5 *Consider the system $\dot{x} = 1$ for $x \in [-2, 2]$; this system would admit a complete Lyapunov function which is strictly decreasing in the entire space $[-2, 2]$, e.g. the function $v(x) = c - x$ with any $c \in \mathbb{R}$. However, when choosing $X_\Gamma = \{-1, 1\}$ and thus approximating a function with $\dot{v}(\pm 1) = -1$ and $\dot{v}(x) \leq 0$ for all $x \in [-2, 2]$ on a grid of points $X_\Omega = \alpha\mathbb{Z} \cap [-2, 2] \setminus \{\pm 1\}$ with $\alpha = 0.01$ and the Wendland function $\psi_{3,2}$ with support radius $1/c = 1/2$ we obtain a function which is only strictly decreasing in a small neighborhood around ± 1, while being constant with $\beta_i < 0$ in large parts, see Figure 1. In this case, the algorithm converges to a candidate complete*

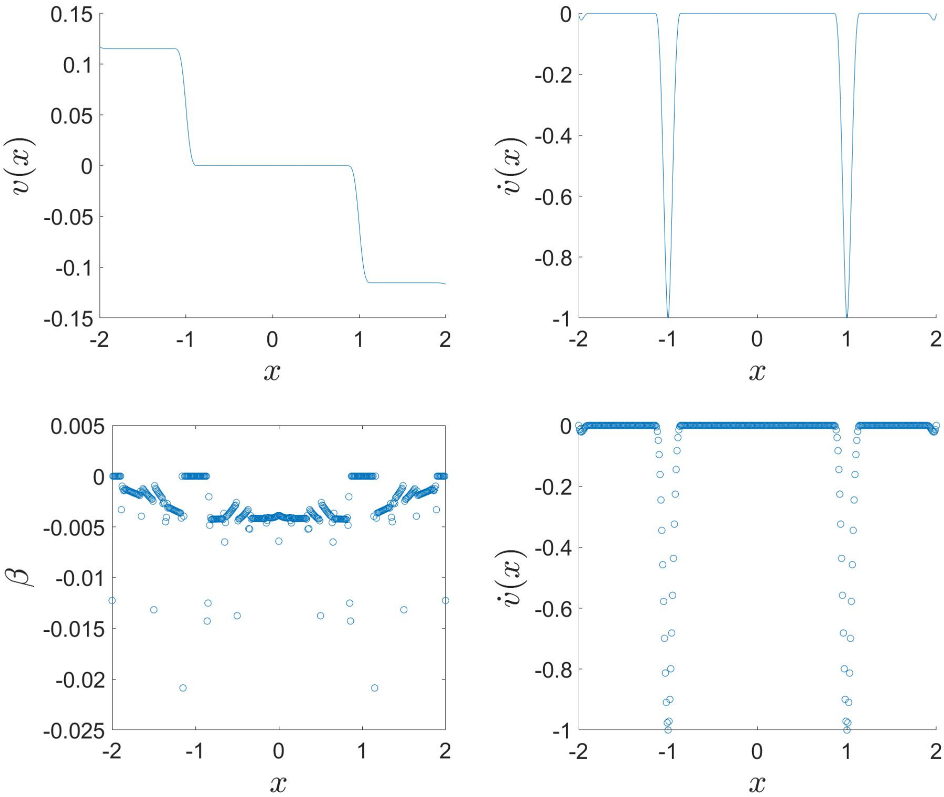

Figure 1: We use the algorithm for the system $\dot{x} = 1$ with only two points $\Gamma = \{-1, 1\}$ with equality condition $\dot{v}(\pm 1) = -1$ and support radius $1/c = 1/2$ of the Radial Basis function. Top left: $v(x)$, top right $\dot{v}(x)$. The function v is constant apart from small neighborhoods around ± 1. Bottom left: the values β_i at each collocation point, bottom right: the values $\dot{v}(x_i)$ at each collocation point. The coefficients β_i are only zero around ± 1 and at the boundary of the interval; in the areas where they are strictly negative, the function is constant.

Lyapunov function, which is not strictly decreasing in the entire gradient-flow part.

However, if we increase the support radius to $1/c = 1/0.3$, then the function is decreasing at all points apart from zero and the boundary; note that the coefficients β_i are mostly zero, see Figure 2. Hence, to converge to a complete Lyapunov function, we require a sufficiently large support radius.

We can use the method in two steps: we fix a set of points X and start with an initial distribution of $X = X_\Gamma \cup X_\Omega$ with $X_\Gamma \cap X_\Omega = \varnothing$, usually with a small number of points in X_Γ with equality constraints. In the second step we potentially move points from X_Ω to X_Γ (so changing the set Γ), by using

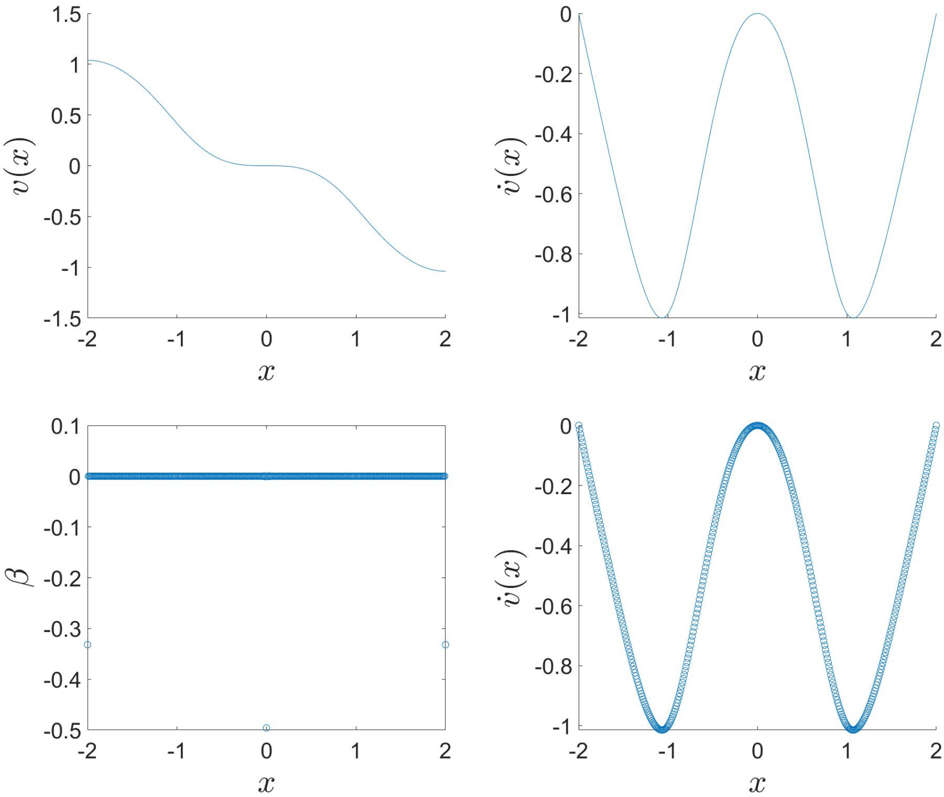

Figure 2: We use the algorithm for the system $\dot{x} = 1$ with only two points $\Gamma = \{-1, 1\}$ with equality condition $\dot{v}(\pm 1) = -1$ and support radius $1/c = 1/0.3$ of the Radial Basis function. Top left: $v(x)$, top right $\dot{v}(x)$. The function v is strictly decreasing apart from 0 and the boundary. Bottom left: the values β_i at each collocation point, bottom right: the values $\dot{v}(x_i)$ at each collocation point. The coefficients β_i are mostly zero apart from at 0 and at the boundary of the interval; this is a consequence of the proof of Proposition 3.3.

the following criterion:

1. If $\beta_i > -10^{-9}$ (i.e. close to 0), then the point x_i is placed into the set X_Γ, enforcing the condition $\dot{v}(x) = -1$.

2. Otherwise, the point x_i remains in X_Ω.

We will see in the examples that the initial step identifies the chain-recurrent set and its complement well, and then computes a suitable complete Lyapunov function in the second step. The final result does not depend significantly on the initial distribution of X into X_Γ and X_Ω.

4 Examples

In this section we present case studies of 2- and 3-dimensional systems. Given a set $\Omega \subset \mathbb{R}^d$, we consider the collocation points on a hexagonal grid $X = \left\{\alpha \sum_{k=1}^{d} i_k w_k, i_k \in \mathbb{Z}\right\} \cap \Omega$ with fineness parameter α, where in dimension $d = 2$ we have, e.g. $w_1 = (1, 0)$ and $w_2 = \left(\frac{1}{2}, \frac{\sqrt{3}}{2}\right)$. For higher dimensions see, e.g., [12, Chapter 6] and references therein. As kernel we use $K(x, y) = \psi_{l,k}(c\|x-y\|_2)$, where $\psi_{l,k}$ is a Wendland function, $l = \lfloor \frac{d}{2} \rfloor + k + 1$, and $c > 0$ corresponds to the support radius through $r = 1/c$.

4.1 Two orbit system

We consider the system

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} -x(x^2 + y^2 - 1/4)(x^2 + y^2 - 1) - y \\ -y(x^2 + y^2 - 1/4)(x^2 + y^2 - 1) + x \end{pmatrix} = f(x, y). \tag{28}$$

It has an asymptotically stable equilibrium at the origin, a periodic orbit $\Omega_1 = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 1/4\}$, which is repelling, and a periodic orbit $\Omega_2 = \{(x, y) \in \mathbb{R}^2 \mid x^2 + y^2 = 1\}$, which is asymptotically stable. We set $\Omega = [-1.2, 1.2]^2$ and the fineness parameter $\alpha = 0.05$. We split the set X as described above into X_Γ (equality constraints) and X_Ω (inequality constraints) and use the Wendland function $\psi_{4,2}$ with parameter $c = 1$.

In this example, we consider different sets Γ for the equality constraints. In more detail, we define the sets $I := [0.15, 0.25] \times [-0.05, 0.05]$, $M := [0.65, 0.75] \times [-0.05, 0.05]$, and $O := [1.05, 1.15] \times [-0.05, 0.05]$. The set I (inner) is inside the periodic orbit Ω_1, the set M (middle) is between the periodic orbits Ω_1 and Ω_2, and the set O (outer) is outside of both the periodic orbits.

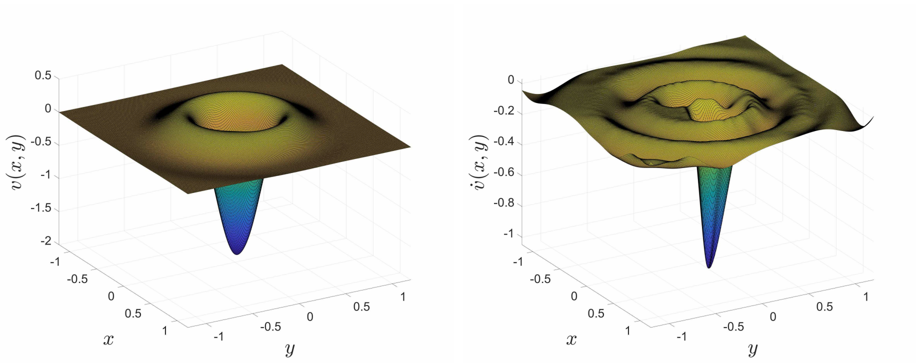

Figure 3: The CLF $v(x, y)$ (left) as well as $\dot{v}(x, y)$ (right). We have used $\dot{v}(x) = -1$ for $x \in I$ and $v(x) \leq 0$ for $x \in X \setminus I$.

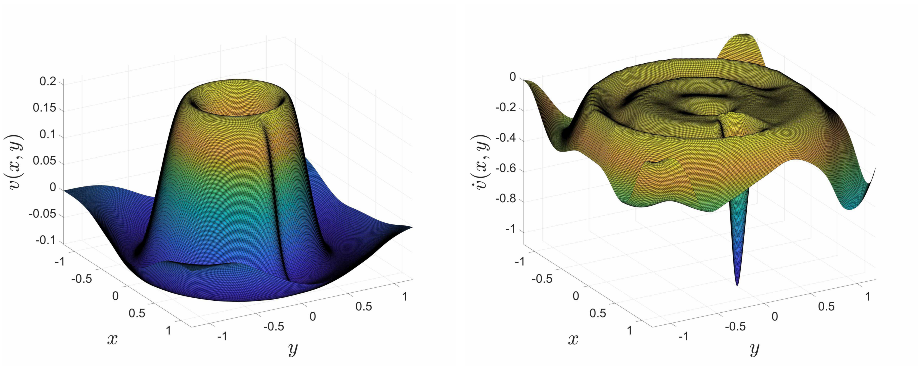

Figure 4: The CLF $v(x,y)$ (left) as well as $\dot{v}(x,y)$ (right) when using the conditions $\dot{v}(x) = -1$ for $x \in M$ and $\dot{v}(x) \leq 0$ for $x \in X \setminus M$.

In Figure 3 we depict the computed CLF candidate together with its orbital derivative $\dot{v}$, when we use the conditions $\dot{v}(x) = -1$ for the collocation points $x \in I$ and for all other collocation points $x \in X \setminus I$ we use the condition $\dot{v}(x) \leq 0$. Figures 4 and 5 show the corresponding results when using the conditions $\dot{v}(x) = -1$ for the collocation points $x \in M$ and $x \in O$, respectively and for all other collocation points $\dot{v}(x) \leq 0$. In Figure 6 we depict the computed CLF candidate together with its orbital derivative $\dot{v}$, when we use the conditions $\dot{v}(x) = -1$ for the collocation points $x \in I \cup M \cup O$ and for all other collocation points $x \in X \setminus (I \cup M \cup O)$ we use the condition $\dot{v}(x) \leq 0$.

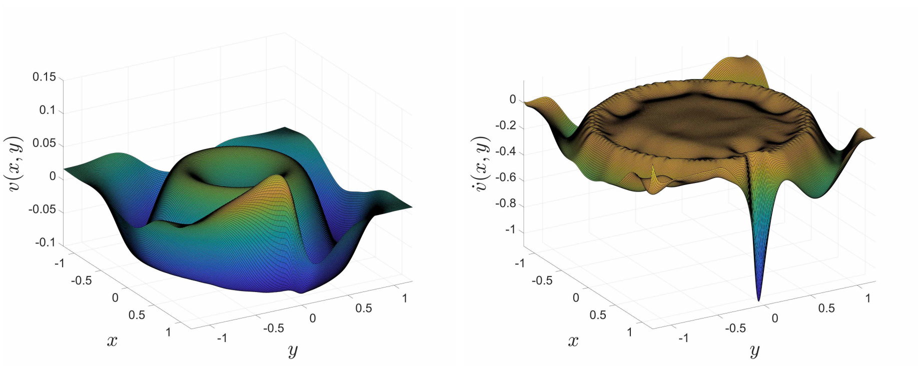

Figure 5: The CLF $v(x,y)$ (left) as well as $\dot{v}(x,y)$ (right) when using the conditions $\dot{v}(x) = -1$ for $x \in O$ and $\dot{v}(x) \leq 0$ for $x \in X \setminus O$.

In all four cases, the computed function captures the main features of a CLF very well, in particular, the points where the orbital derivative is negative as well as the minima and maxima: the equilibrium at the origin is a local minimum, the repelling periodic orbit Ω_1 at radius $1/2$ is a local maximum and the stable periodic orbit Ω_2 at radius 1 is a local minimum.

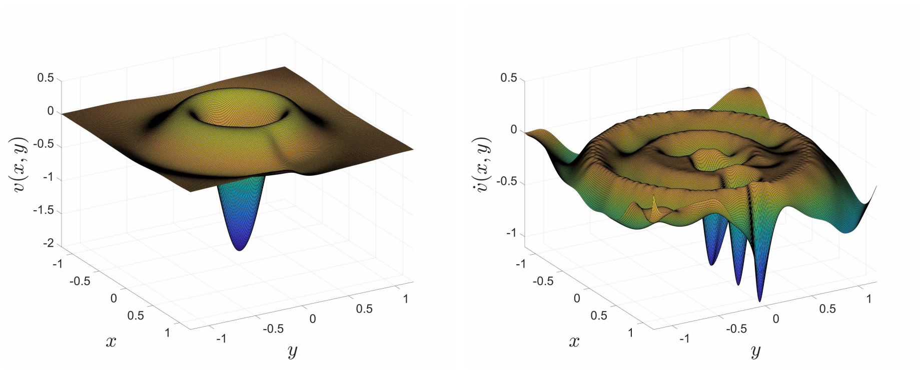

Figure 6: The CLF $v(x, y)$ (left) as well as $\dot{v}(x, y)$ (right) when using the conditions $\dot{v}(x) = -1$ for $x \in I \cup M \cup O$ and $\dot{v}(x) \leq 0$ for $x \in X \setminus (I \cup M \cup O)$.

However, there are differences in the values of v.

Complete Lyapunov functions provide information about many features of the system, including the chain-recurrent set, as well as the stability and basins of attraction of its connected components [4, 9, 21, 22, 23, 6]. However, note that although Theorem 2.5 asserts the convergence of our method to a true CLF candidate, when the number of collocation points is increased, methods that are designated to compute the chain-recurrent set directly might be more efficient for this purpose [11, 24, 5, 19]. One way to estimate the chain-recurrent set is to look at where the orbital derivative fails to be negative. To study the orbital derivative in more detail, we use two approaches. To estimate the chain-recurrent set, in this example consisting of the equilibrium at the origin and the periodic orbits Ω_1 and Ω_2, we triangulate the area $[-1.2, 1.2]^2$ into small triangles, more exactly we triangulate the area into $2 \cdot 1000 \cdot 1000 = 2 \cdot 10^6$ congruent triangles, and then interpolate the computed CLF by a CPA (continuous piecewise affine) CLF. For the CPA interpolation we have exact verifiable conditions to assert that the orbital derivative is negative, see [16]. As can be seen in Figure 7, the general shape of the chain recurrent set is approximately obtained. However, there is a lot of noise.

Another way, if we assume that the computed function is close to a CLF, is to use the KKT conditions and approximate the chain-recurrent set with those collocation points in $x_i \in X_\Omega$, where the condition $\dot{v}(x_i) \leq 0$ is used, and where $\beta_i < 0$, which implies $\dot{v}(x_i) = 0$ by Proposition 3.3. This is shown in Figure 8 and shows a similar result; however, note that this only requires to check that $\beta_i < 0$ and is thus much faster than the previous computation using CPA functions on triangulations.

Numerically, we have used the criterion $\beta_i \leq -10^{-5}$ to ensure that $\beta_i < 0$. The choice of the parameter 10^{-5} is not important, as the transition from small to large β is very sharp. As an example, we use $\alpha = 0.05$ and

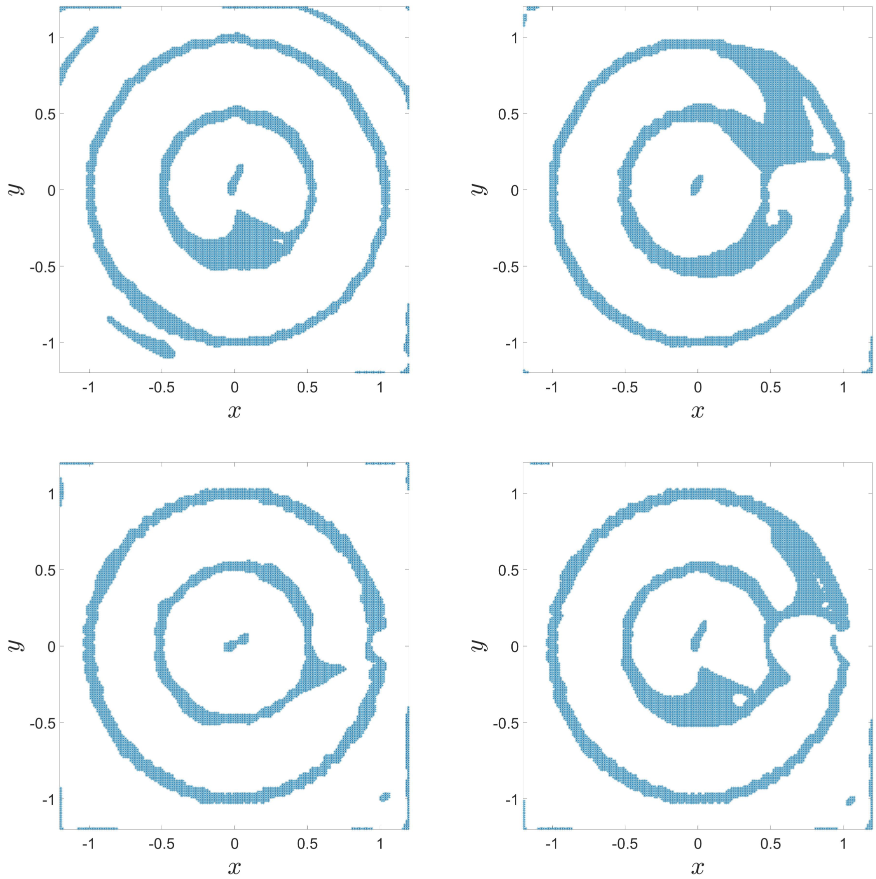

Figure 7: The area where the orbital derivative of the CPA interpolation of the computed CLF candidate fails to have a negative orbital derivative, when using the condition $\dot{v}(x) = -1$ for $x \in I$ and $v(x) \leq 0$ for $x \in X \setminus I$ (upper left), $\dot{v}(x) = -1$ for $x \in M$ and $v(x) \leq 0$ for $x \in X \setminus M$ (upper right), $\dot{v}(x) = -1$ for $x \in O$ and $v(x) \leq 0$ for $x \in X \setminus O$ (lower left), and $\dot{v}(x) = -1$ for $x \in I \cup M \cup O$ and $v(x) \leq 0$ for $x \in X \setminus (I \cup M \cup O)$ (lower right).

thus have $|X| = 1,232$ collocation points. If we order the coefficients $|\beta_i|$ in ascending order and plot $\log_{10}(|\beta|)$ for points 320 to 335 we obtain Figure 9, which shows that any value between 10^{-1} and 10^{-7} would give similar results.

Second step

Now we perform the second step, described in the previous section: after the initial computation, we use the same collocation points X, but move