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MINIMIZATION WITH DIFFERENTIAL INEQUALITY CONSTRAINTS APPLIED TO COMPLETE LYAPUNOV FUNCTIONS

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Abstract. Motivated by the desire to compute complete Lyapunov functions for nonlinear dynamical systems, we develop a general theory of discretizing a certain type of continuous minimization problems with differential inequality constraints. The resulting discretized problems are quadratic optimization problems, for which there exist efficient solution algorithms, and we show that their unique solutions converge strongly in appropriate Sobolev spaces to the unique solution of the original continuous problem. We develop the theory and present examples of our approach, where we compute complete Lyapunov functions for nonlinear dynamical systems.

A complete Lyapunov function characterizes the behaviour of a general dynamical system. In particular, the state space is divided into the chain-recurrent set, where the complete Lyapunov function is constant along solutions, and the part characterizing the gradient-like flow, where the complete Lyapunov function is strictly decreasing along solutions. We propose a new method to compute a complete Lyapunov function as the solution of a quadratic minimization problem, for which no information about the chain-recurrent set is required. The solutions to the discretized problems, which can be solved using quadratic programming, converge to the complete Lyapunov function.

1. Introduction

Let us first motivate the concept of complete Lyapunov functions, before we focus our attention on the minimization problem discussed in this paper.

We will consider a general autonomous ODE

$$\dot{x} = f(x), \text{ where } x \in \mathbb{R}^d. \tag{1}$$

A complete Lyapunov function (CLF) is a function $V\colon \mathbb{R}^d \to \mathbb{R}$, which is non-increasing along trajectories as well as strictly decreasing along trajectories outside the chain-recurrent set R, $V(R)$ is a nowhere dense subset of $\mathbb{R}$, and the level sets of V in R, $V^{-1}(r) \cap R \neq \emptyset$ for $r \in \mathbb{R}$, are the chain-transitive components of R, see [14, §6.4], [23, §4]. For the definition of the chain-recurrent set, see below.

We call a function that only fulfills the first property, namely that V is non-increasing along trajectories, a *CLF candidate*. If V is sufficiently smooth, e.g. C^1,

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then this can be expressed by $V'(x) \leq 0$, where $V'(x) = \nabla V(x) \cdot f(x)$ denotes the orbital derivative, i.e. the derivative along solutions of (1); hence, we will refer to any function fulfilling $V'(x) \leq 0$ for every x in a set $U \subseteq \mathbb{R}^d$ as a *CLF candidate* on U.

A CLF candidate V on the state-space of the ODE (1) is a CLF for the dynamical system defined by the solution to the ODE, if and only if it is strictly decreasing along solutions on the largest possible set. It can be shown that this condition is equivalent to V being strictly decreasing along solution trajectories in the complement of the *chain-recurrent set*, cf. [14, 23].

For defining the chain-recurrent set we need a little preparation. For convenience let us assume that the solution to the ODE (1) defines a dynamical system on the open set $U \subseteq \mathbb{R}^d$, i.e. that solutions $t \mapsto \phi(t,\xi)$ to the initial-value problems

$$\dot{\phi}(t,\xi) = f(\phi(t,\xi)), \quad \phi(0,\xi) = \xi \in U,$$

are unique and defined for all $t \in \mathbb{R}$ (complete), that $(t,\xi) \mapsto \phi(t,\xi)$ is continuous, and that $\phi(t,\xi) \in U$ for all $t \in \mathbb{R}$. For example, a sufficient condition for the uniqueness of solutions is that f is locally Lipschitz continuous and then completeness can always be achieved by considering the ODE (1) with f replaced by

$$\frac{f(x)}{\sqrt{1 + \|f(x)\|_2}} \cdot \frac{\operatorname{dist}(x, U^C)}{1 + \operatorname{dist}(x, U^C)},$$

where $\operatorname{dist}(x, U^C)$ is the distance of x to the complement of U and $\operatorname{dist}(x, \emptyset) := 1$, cf. e.g. [28] and the references therein or [30]. Note that this does not change the solution trajectories inside U, the movement of the system along solution trajectories is just slowed down to make it complete.

A point $\xi \in U$ is called *chain-recurrent* if for a constant $T > 0$ and any continuous function $\varepsilon : U \to (0, \infty)$ there exists an (ε, T)-chain, i.e. $(t_i, \eta_i) \in \mathbb{R} \times U$ for $i = 1, \ldots, N$, $N \in \mathbb{N}$, with $t_i \geq T$ and such that $\eta_0 = \eta_N = \xi$ and

$$\|\phi(t_i, \eta_{i-1}) - \eta_i\|_2 < \varepsilon(\phi(t_i, \eta_{i-1})) \text{ for all } i = 1, \ldots, N.$$

The set of all chain-recurrent points is called the *chain-recurrent set* [14]. Note that on noncompact state spaces it is necessary to use a function ε rather than constants, cf. [23, 24]. There is a fundamental difference between the flow on the chain-recurrent set and its complement. On the chain-recurrent set the dynamics are (almost) repetitive, whereas on its complement the flow is gradient-like, i.e. solutions pass through and are insensitive to infinitesimal perturbations. The dynamics in the gradient-like part are similar to a gradient system, i.e. a system (1) where the right-hand side $f(x) = \nabla W(x)$ is given by the gradient of a function $W : \mathbb{R}^d \to \mathbb{R}$.

A non-constant CLF (candidate) provides important information about the solutions of (1): the area of the phase space, where $V'(x) = 0$ contains the chain-recurrent set, and the area, where $V'(x) < 0$ holds, displays gradient-flow behaviour. Note that a constant function trivially satisfies the condition $V'(x) \leq 0$ and is a CLF candidate. Hence, the larger the area of the state space, where V is strictly decreasing, the more information about the system and its chain-recurrent set can be obtained from the CLF candidate.

The values and level sets of a CLF provide additional information about the dynamics and the long-term behaviour of the system, e.g. an asymptotically stable equilibrium is a local minimum of a CLF. Moreover, the (constant) values of a CLF on different connected components of the chain-recurrent set describe the dynamics in between them.

Summarizing, a smooth complete Lyapunov function satisfies

$$\begin{aligned} V'(x) &< 0 \text{ for } x \in G, \\ V'(x) &= 0 \text{ for } x \in R, \end{aligned}$$

where points in G display gradient-like flow and R denotes the chain-recurrent set.

The first proof of the existence of a prototype CLF for dynamical systems, a CLF candidate with negative orbital derivative on a maximal set, was given by Auslander [8] and later by Conley [14] for CLFs in the modern sense. Their proofs hold for flows on compact metric spaces. Conley considers each corresponding attractor-repeller pair and constructs a function which is 1 on the repeller, 0 on the attractor and decreasing in between. Then these, countably many, functions are weighted and summed up over all attractor-repeller pairs. Later, Hurley extended these ideas to more general spaces [22–25]. These Lyapunov functions, however, are merely continuous. The existence of smooth CLFs on compact state spaces was shown in [16] and, in a different context, the existence of smooth time-functions, which are closely related to CLFs, was established for cone-fields on noncompact state spaces in [10]. In [30] it was shown that such time-functions can be modified to CLFs for ODEs and thus the existence of C^∞ CLFs on noncompact state spaces was established.

Computational approaches to construct CLFs were proposed in [9, 20, 27]. The state space was subdivided into cells, defining a discrete-time system given by the multivalued time-T map between them, which was computed using the computer package GAIO [15]. Hence, an approximate complete Lyapunov function was constructed using graph algorithms [9]. This approach requires a high number of cells, even for low dimensions, and the approximation is good for the values of the CLF, but not necessarily for its orbital derivative. Moreover, no convergence result was obtained; we will present such a result in this paper.

In [11], a complete Lyapunov function was constructed as a continuous piecewise affine (CPA) function on a fixed simplicial complex. However, it is assumed that information on the location of local attractors is available, while such information is not needed in our approach.

In [3–5] CLF candidates were computed by approximately solving the ill-posed PDE

$$V'(x) = -1 \tag{2}$$

using meshfree collocation, in particular using Radial Basis Functions (RBFs). This was inspired by constructing classical Lyapunov functions for systems with an asymptotically stable equilibrium [17, 19]. However, (2) cannot be fulfilled at all points in the chain-recurrent set. Meshfree collocation still constructs an approximation, but the usual error estimates are not available, as they compare the approximation to the solution of the problem (2), which does not exist in our case. In practice, the method works well on the part of the state space where the flow is gradient-like and it is able to detect the chain-recurrent set as the area of the state space where the approximation fails.

The method has been improved in several ways, for example, by using the information gained on the chain-recurrent set by an approximate solution to (2) for an iteration using a different right-hand side for the PDE. This process can then be further iterated. Although the method works well in examples, so far no proof has been given since the error estimates for meshfree collocation are always in terms of the difference to a solution, and (2) has no solution. To ensure that we consider an equation that has a solution, we need to know the location of the chain-recurrent set.

Since the definition of a CLF is based on inequalities rather than equations, in [18] the problem:

$$\begin{aligned} \text{minimize} \quad & \|V\|_H \\ \text{subject to} \quad & V'(x) \;=\; -1 \text{ for } x \in \Omega_-, \\ & V'(x) \;\le\; 0 \text{ for } x \in \Omega \setminus \Omega_-, \end{aligned}$$

was considered, where $\Omega \subseteq \mathbb{R}^d$ is the area under consideration, $\Omega_- \subseteq G$ lies in the gradient-like set and H is an appropriate reproducing kernel Hilbert space of functions. The advantage of this method is that a solution of this problem exists, and we only need to know a subset of the state space where the flow is gradient-like. In fact, the method was shown to work well, even if Ω_- consists of just one point, see [18]. The computation of an approximate solution was obtained as the norm-minimal solution in a reproducing kernel Hilbert space after discretization. Note that when choosing $\Omega_- = \emptyset$, which would require no information on the location of the chain-recurrent set, the norm-minimal solution is the constant solution $V \equiv 0$ and thus does not provide any information about the dynamics.

In this paper we do not require any information about the chain-recurrent set and consider a minimization problem, that has a unique solution. By choosing a suitable cost function we will ensure that a constant solution $V \equiv C$ cannot be the minimizer, but instead a negative orbital derivative is favoured over a zero orbital derivative. In particular, we will choose to minimize

$$\|V\|_H^2 + \int_\Omega V'(x)\, dx, \tag{3}$$

where $\Omega \subseteq \mathbb{R}^d$ is the area of the phase space under consideration, and H is a Sobolev space of functions $g\colon \Omega \to \mathbb{R}$. The constraint

$$V'(x) \le 0 \tag{4}$$

ensures that the function is a CLF candidate.

The reasons for the particular form of (3), where the orbital derivative enters linearly and the norm is quadratic, are twofold: on the one hand, this leads to a quadratic optimization problem (11), that can be solved efficiently. On the other hand, it turns out that the solution to this problem is a *non-constant* CLF candidate, if there exists a smooth, non-constant CLF, see Proposition 4.1.

Since the theory for our application only depends on the map $V \to V'$ being linear, we will consider a general minimization problem of the form (8), with V' replaced by LV for a general linear differential operator L and we will show that it has a unique solution. Moreover, we will propose a method to compute this solution: by discretizing the problem, we obtain a corresponding quadratic programming problem, which has itself a unique solution. We will show that the solutions of the discretized problems strongly converge to the solution of the original problem.

When discretizing with a sequence of finer and finer sets of points, we obtain a sequence of solutions of the quadratic programming problems, which converges strongly to the solution of the original minimization problem. This establishes an efficient method for computing an approximation to the original problem. The advantage compared to previous methods is that no information about the chain-recurrent set, or indeed about solutions of the ODE, is required and we can prove the strong convergence of the method. The advantage compared to methods mentioned earlier is that no triangulation of the space, or finite-dimensional subspace of the function space, needs to be considered; only scattered data points are required.

Let us give an overview over the contents: In Section 2 we recall reproducing kernel Hilbert spaces. In the main Section 3 we introduce the general version of the minimization problem, see (8). We first show that the discretized problem has a unique solution, which can be computed by solving a quadratic programming problem, and then we prove that the original problem has a unique solution, which is the limit of discretized problems. In Section 4 we apply the general theory to the problem of computing a complete Lyapunov function and in Section 5 we apply the method to a planar example and the three-dimensional Lorenz attractor; moreover, we discuss the numerically computed rate of convergence for one example.

2. Reproducing kernel Hilbert spaces

We start with a short introduction to reproducing kernel Hilbert spaces. Details and proofs can, for example, be found in [7]. We follow here mainly Chapters 10 and 16 of [32].

Definition 2.1. Let $\Omega \subseteq \mathbb{R}^d$. A Hilbert space $H = H(\Omega)$ of continuous functions $f : \Omega \to \mathbb{R}$ is called a *reproducing kernel Hilbert space*, abbreviated RKHS, if there is a function $K : \Omega \times \Omega \to \mathbb{R}$ with

(1) $K(\cdot, x) \in H$ for all $x \in \Omega$,
(2) $g(x) = \langle g, K(\cdot, x)\rangle_H$ for all $g \in H$ and all $x \in \Omega$.

The function K is called the *reproducing kernel* of H.

The reproducing kernel is called *positive definite*, if for any set of pairwise distinct points $\{x_1, \dots, x_N\} \subseteq \Omega$ the matrix $(K(x_i, x_j))_{i,j=1,\dots,N}$ is positive definite.

It is easy to see that the reproducing kernel of a RKHS is symmetric and uniquely determined by the Hilbert space. However, if it is possible to define a different inner product on the same space, equipping the space with an equivalent norm, then it is possible to have different reproducing kernels. Moreover, a Hilbert space $H(\Omega)$ is a RKHS if and only if point evaluations $\delta_x : H \to \mathbb{R}$, $f \mapsto \delta_x(f) = f(x)$ are continuous. The kernel is always positive semi-definite in the sense that the above mentioned matrices are symmetric and positive semi-definite. The kernel is positive definite if and only if all point evaluations δ_x, $x \in \Omega$ are linearly independent. Finally, if $K : \Omega \times \Omega \to \mathbb{R}$ is a positive definite kernel, then there exists a unique Hilbert space, for which K is the reproducing kernel. This space can be constructed by completing the linear space, which is spanned by the functions $K(\cdot, x)$, $x \in \Omega$.

In a RKHS, the Riesz representative of a functional $\lambda \in H^*$ is given by applying it to one argument of the kernel, i.e., for every $x \in \Omega$ we apply λ to $K(x, \cdot)$ and obtain a function we denote by $\lambda^y K(\cdot, y)$, where the superscript in λ^y indicates that the functional λ is applied to the second variable, i.e. we have

$$\lambda(f) = \langle f, \lambda^y K(\cdot, y)\rangle_H, \qquad f \in H, \lambda \in H^*, \tag{5}$$

see for example [32, Theorem 16.7]. This also means that we have for $\lambda, \mu \in H^*$ the identity

$$\lambda^x \mu^y K(x,y) = \langle \lambda^x K(\cdot, x), \mu^y K(\cdot, y)\rangle_H. \tag{6}$$

In this paper, we are particularly interested in Sobolev spaces $H = H^\sigma(\Omega)$. If $\sigma = k \in \mathbb{N}_0$ then $H^\sigma(\Omega)$ consists of all functions $u \in L_2(\Omega)$ having weak derivatives $D^\alpha u \in L_2(\Omega)$ up to order $|\alpha| \le k = \sigma$. The norm is defined in the usual way. If σ is not an integer, we use operator interpolation theory to define the space and norm, for details see for example [1, 13].

If $\Omega \subseteq \mathbb{R}^d$ is a bounded domain with a Lipschitz boundary, then there exists a continuous linear extension operator $E : H^\sigma(\Omega) \to H^\sigma(\mathbb{R}^d)$, i.e. E satisfies particularly $Eu|_\Omega = u$ and $\|Eu\|_{H^\sigma(\mathbb{R}^d)} \le C\|u\|_{H^\sigma(\Omega)}$ for all $u \in H^\sigma(\Omega)$ with a fixed constant $C > 0$ (see [13, 29]). One immediate consequence of the existence of such an extension operator is the Sobolev embedding theorem for $H^\sigma(\Omega)$, which states that $H^\sigma(\Omega) \subseteq C(\Omega) \cap L_\infty(\Omega)$ if $\sigma > d/2$. As this embedding is continuous, we have that $H^\sigma(\Omega)$ is a RKHS provided $\sigma > d/2$.

Unfortunately, for general domains $\Omega \subseteq \mathbb{R}^d$, an explicit form of the reproducing kernel of $H^\sigma(\Omega)$ is usually unknown. To circumvent this problem, we will proceed as follows. We start on all of $\mathbb{R}^d$ and choose a reproducing kernel $K_\sigma : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$ that delivers an equivalent norm to the standard norm on $H^\sigma(\mathbb{R}^d)$. According to [32, Corollary 10.13], we can choose the kernel as a translation-invariant function $K_\sigma(x,y) = \Phi_\sigma(x-y)$ as long as $\Phi_\sigma : \mathbb{R}^d \to \mathbb{R}$ has a Fourier transform

$$\widehat{\Phi_\sigma}(\omega) = \int_{\mathbb{R}^d} \Phi_\sigma(x) e^{-ix^T\omega} dx$$

that decays like $(1 + \|\cdot\|_2^2)^{-\sigma}$, i.e. there are two constants $c_1, c_2 > 0$ such that

$$c_1(1 + \|\omega\|_2^2)^{-\sigma} \le \widehat{\Phi_\sigma}(\omega) \le c_2(1 + \|\omega\|_2^2)^{-\sigma}, \qquad \omega \in \mathbb{R}^d. \tag{7}$$

It is also often possible to choose the function Φ_σ to be radial, i.e. $\Phi_\sigma = \phi_\sigma(\|\cdot\|_2)$ with a function $\phi_\sigma : [0,\infty) \to \mathbb{R}$. For example, Wendland's compactly supported radial basis function $\psi_{l,k} : [0,\infty) \to \mathbb{R}$, see [31], with $l = \lfloor \frac{d}{2} \rfloor + k + 1$, $k \in \mathbb{N}$, define a translation-invariant reproducing kernel by $K_\sigma(x,y) = \Phi_\sigma(x-y) = \psi_{l,k}(\|x-y\|_2)$; the corresponding RKHS is norm equivalent to $H^\sigma(\mathbb{R}^d)$ with $\sigma = k + \frac{d+1}{2}$.

Next, given a bounded domain $\Omega \subseteq \mathbb{R}^d$ with a Lipschitz boundary, we can define the kernel $k_\sigma : \Omega \times \Omega \to \mathbb{R}$ by setting $k_\sigma := K_\sigma|\Omega \times \Omega$. As the restriction of a positive definite kernel, k_σ is a positive definite kernel itself and it is hence the reproducing kernel of a Hilbert space $H(\Omega)$. We now have the following result.

Lemma 2.2. *Assume $\Phi_\sigma \in L_1(\mathbb{R}^d) \cap C(\mathbb{R}^d)$ has a Fourier transform $\widehat{\Phi_\sigma}$ satisfying (7) with $\sigma > d/2$. Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with a Lipschitz boundary. Let $k_\sigma : \Omega \times \Omega \to \mathbb{R}$ be defined by $k_\sigma(x,y) = \Phi_\sigma(x-y)$, $x, y \in \Omega$. Then, there exists an inner product $\langle \cdot, \cdot \rangle_{k_\sigma} : H^\sigma(\Omega) \times H^\sigma(\Omega) \to \mathbb{R}$ on $H^\sigma(\Omega)$ such that k_σ is the reproducing kernel of $H^\sigma(\Omega)$ with respect to this inner product. The norm $\|\cdot\|_{k_\sigma}$ induced by this inner product is equivalent to the standard norm on $H^\sigma(\Omega)$, i.e. there are constants $C_1, C_2 > 0$ such that*

$$C_1\|u\|_{k_\sigma} \le \|u\|_{H^\sigma(\Omega)} \le C_2\|u\|_{k_\sigma}, \qquad u \in H^\sigma(\Omega).$$

Proof. For $\sigma \in \mathbb{N}$, this is Corollary 10.48 from [32]. For real $\sigma > d/2$ this follows then by interpolation theory. $\square$

3. Minimization problem

Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with Lipschitz boundary and $\sigma > d/2+m+1$, where $m \in \mathbb{N}$. Let L be a linear differential operator of order m defined by

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

where $v \in H^\sigma(\Omega)$ and all $c_\alpha \in C^{\sigma-m}(\overline{\Omega})$. Let H be a RKHS that consists of the functions $H^\sigma(\Omega)$, but not necessarily equipped with the same inner product. We consider the problem:

$$\text{(8)} \qquad \begin{cases} \text{minimize} & \|v\|_H^2 + \int_\Omega Lv(x)\,dx \\ \text{subject to} & Lv(x) \leq b(x), x \in \Omega \end{cases}$$

with a continuous function $b\colon \Omega \to \mathbb{R}$. We will show that this minimization problem has a unique solution v and that this solution can be approximated arbitrarily closely by considering a discretized version and an associated finite dimensional quadratic programming problem.

We will first consider the discretized version: subdivide the set Ω into finitely many, pairwise disjoint measurable sets $\Omega_i \subseteq \Omega$, $i = 1,\ldots,N$, with $\bigcup_{i=1}^N \Omega_i = \Omega$ and $w_i := |\Omega_i| \neq 0$. Furthermore, choose points $x_i \in \Omega_i$ and define $\lambda_i \in H^*$ by $\lambda_i(v) = Lv(x_i)$ for $i = 1,\ldots,N$. Finally, let $b_i = b(x_i)$, $i = 1,\ldots,N$. The connection between (8) and the optimization problem (9) below is that for this choice of functionals λ_i and weights w_i the second term in the cost function in (9) is arbitrarily close to the integral $\int_\Omega Lv(x)\,dx$ if the w_i are small enough. We will discuss the discretized problem in Section 3.1 and the strong convergence of its solution to the solution of (8) in Section 3.2.

3.1. **Discretized problem.** We consider a general Hilbert space H with inner product $\langle\cdot,\cdot\rangle_H$ and the associated norm $\|\cdot\|_H$. Let $\lambda_i \in H^*$ be linearly independent, $b_i \in \mathbb{R}$ and $w_i > 0$ for all $i = 1,\ldots,N$, $N \in \mathbb{N}$. Consider the problem for $v \in H$:

$$\text{(9)} \qquad \begin{cases} \text{minimize} & \|v\|_H^2 + \sum_{i=1}^N \lambda_i(v) w_i, \\ \text{subject to} & \lambda_i(v) \leq b_i,\ i = 1,\ldots,N. \end{cases}$$

The goal of this section is to show that (9) has a unique solution which can be determined by solving a quadratic programming problem. We start by showing that the solution is unique if it exists.

Lemma 3.1. *Problem* (9) *has at most one solution in H.*

Proof. First assume that $s \in H$ is a minimizer and $v \in H$ satisfies the constraints of (9).

We show that

$$m := 2\langle s, v-s\rangle_H + \sum_{j=1}^N \lambda_j(v-s) w_j \geq 0.$$

For a contradiction, assume that $m < 0$, in particular that $v \neq s$, and set

$$\alpha := \min\left(\frac{-m}{2\|v-s\|_H^2}, 1\right) > 0.$$

Note that $t = \alpha v + (1-\alpha)s$ satisfies the constraints and we have

$$\begin{aligned}
\|t\|_H^2 + \sum_{j=1}^N \lambda_j(t) w_j &= \|s + \alpha(v-s)\|_H^2 + \sum_{j=1}^N \lambda_j(s + \alpha(v-s)) w_j \\
&= \|s\|_H^2 + 2\alpha\langle s, v-s\rangle_H + \alpha^2\|v-s\|_H^2 \\
&\quad + \sum_{j=1}^N \lambda_j(s) w_j + \alpha \sum_{j=1}^N \lambda_j(v-s) w_j \\
&= \|s\|_H^2 + \sum_{j=1}^N \lambda_j(s) w_j + \alpha(\alpha\|v-s\|_H^2 + m) \\
&< \|s\|_H^2 + \sum_{j=1}^N \lambda_j(s) w_j,
\end{aligned}$$

because

$$\alpha\|v-s\|_H^2 + m \le \frac{m}{2} < 0.$$

Thus s is not a minimizer in contradiction to the initial assumptions.

Now assume $s_1, s_2 \in H$ are minimizers. Then by the above argument we have

$$2\langle s_1, s_2 - s_1\rangle_H + \sum_{j=1}^N \lambda_j(s_2 - s_1) w_j \ge 0$$

and

$$2\langle s_2, s_1 - s_2\rangle_H + \sum_{j=1}^N \lambda_j(s_1 - s_2) w_j \ge 0.$$

This implies

$$\begin{aligned}
0 &\le 2\|s_1 - s_2\|_H^2 \\
&= -2\langle s_1, s_2 - s_1\rangle_H - 2\langle s_2, s_1 - s_2\rangle_H \\
&= -2\langle s_1, s_2 - s_1\rangle_H - 2\langle s_2, s_1 - s_2\rangle_H \\
&\quad - \sum_{j=1}^N \lambda_j(s_2 - s_1) w_j - \sum_{j=1}^N \lambda_j(s_1 - s_2) w_j \\
&\le 0,
\end{aligned}$$

which shows $s_1 = s_2$. □

Now let H be a RKHS with a positive definite reproducing kernel K, see Definition 2.1. We show that then the solution s^* to (9) lies in a finite-dimensional subspace of H, spanned by the Riesz representers of the λ_j, namely $\lambda_j^y K(x,y)$, see Lemma 3.3. The proof uses a similar property for generalized interpolation problems, see [32, Theorem 16.1].

In particular, we will show that the solution s^* to (9) is of the form

$$s^*(x) = \sum_{j=1}^N \beta_j \lambda_j^y K(x,y), \tag{10}$$

where the coefficient vector $(\beta_1, \dots, \beta_N) = \beta \in \mathbb{R}^N$ is the unique solution to the quadratic optimization problem for $\beta \in \mathbb{R}^N$:

$$\text{(11)} \qquad \begin{cases} \text{minimize} & \beta^T A \beta + c^T \beta \\ \text{subject to} & A\beta \le b. \end{cases}$$

Here the matrix $A = (a_{ij})_{i,j=1,\dots,N}$ is defined by

$$a_{ij} = \lambda_i^x \lambda_j^y K(x,y), \quad i,j = 1,\dots,N,$$

the vector $c = (c_j)_{j=1,\dots,N}$ is defined by $c = A^T w = Aw$, i.e. by

$$c_j = \sum_{i=1}^N a_{ij} w_i, \quad j = 1,\dots,N,$$

and the inequality $A\beta \le b$ is to be read componentwise. Since the functionals λ_i are linearly independent, the matrix A is symmetric and positive definite. Note that since problem (11) is a quadratic programming problem, it can be solved efficiently.

We first show that the problem (11) has a unique solution.

Lemma 3.2. *Problem* (11) *has a unique solution.*

Proof. We can rewrite problem (11), using the variable $r = A\beta$ instead of β, as a minimization problem for $r \in \mathbb{R}^N$

$$\text{(12)} \qquad \begin{cases} \text{minimize} & r^T A^{-1} r + w^T r \\ \text{subject to} & r \le b. \end{cases}$$

Since the objective function is a quadratic form with positive definite matrix A^{-1}, it is strictly convex and thus problem (12) has a unique solution, if its (convex) feasibility set is not empty. Since $r = b$ is feasible, the proposition follows. □

Now we show that the minimizer of (9) is of the form s^*, see (10), where the coefficients β are uniquely defined as the solution of the minimization problem (11).

Lemma 3.3. *Let H be a RKHS with positive definite reproducing kernel K. Then there exists a unique minimizer of the problem* (9) *in H and it is of the form* (10), *where the coefficients $\beta = (\beta_1, \dots, \beta_N)$ are uniquely defined as the solution of the minimization problem* (11).

Proof. Define s^* by (10), where the coefficient β is uniquely defined as the solution of the minimization problem (11), see Lemma 3.2. Let $s \in H$ be any fixed function satisfying the constraints in (9). We will show that

$$\|s^*\|_H^2 + \sum_{j=1}^N \lambda_j(s^*) w_j \le \|s\|_H^2 + \sum_{j=1}^N \lambda_j(s) w_j,$$

from which the result follows.

The function s satisfies

$$\lambda_i(s) =: t_i \le b_i, \; i = 1,\dots,N,$$

for certain values $(t_i)_{i=1,\dots,N} = t \in \mathbb{R}^N$. Now consider the generalized interpolation problem for $v \in H$, using the parameters $t = (t_j)$:

$$\begin{cases} \text{minimize} & \|v\|_H^2 + \sum_{j=1}^N t_j w_j \\ \text{subject to} & \lambda_j(v) = t_j, \; j = 1,\dots,N. \end{cases}$$

Since the term $\sum_{j=1}^N t_j w_j$ in the objective function is a constant independent of v, we can equivalently consider the generalized interpolation problem for $v \in H$

$$\left\{ \begin{array}{ll} \text{minimize} & \|v\|_H^2 \\ \text{subject to} & \lambda_j(v) = t_j,\ j = 1, \dots, N. \end{array} \right.$$

By classical arguments, see [32, Theorem 16.1], the unique minimizer of this problem is given by

$$\tilde{s}(x) = \sum_{j=1}^N \tilde{\beta}_j \lambda_j^y K(x, y),$$

where $A\tilde{\beta} = t$ and $\lambda_j(\tilde{s}) = t_j$, $j = 1, \dots, N$. But then

$$\|\tilde{s}\|_H^2 + \sum_{j=1}^N \lambda_j(\tilde{s}) w_j \quad \leq \quad \|s\|_H^2 + \sum_{j=1}^N \lambda_j(s) w_j, \tag{13}$$

because $\|\tilde{s}\|_H^2 \leq \|s\|_H^2$ and $\sum_{j=1}^N \lambda_j(\tilde{s}) w_j = \sum_{j=1}^N t_j w_j = \sum_{j=1}^N \lambda_j(s) w_j$.

Now both s^* and $\tilde{s}$ are of the form (10) and the coefficients β, $\tilde{\beta}$ both satisfy the constraints of problem (11), namely

$$A\tilde{\beta} = t \leq b \quad \text{and} \quad A\beta \leq b. \tag{14}$$

Hence, both s^* and $\tilde{s}$ are of the form (10) and satisfy the constraints (9).

Note that we have

$$\begin{aligned} \|s^*\|_H^2 &= \left\langle \sum_{i=1}^N \beta_i \lambda_i^x K(\cdot, x), \sum_{j=1}^N \beta_j \lambda_j^y K(\cdot, y) \right\rangle_H \\ &= \sum_{i,j=1}^N \beta_i \beta_j \langle \lambda_i^x K(\cdot, x), \lambda_j^y K(\cdot, y) \rangle_H \\ &= \beta^T A \beta \end{aligned}$$

by (6).

Therefore, the coefficients β of s^* minimize

$$\beta^T A \beta + c^T \beta = \|s^*\|_H^2 + \sum_{j=1}^N \lambda_j(s^*) w_j$$

by assumption, so that

$$\begin{aligned} \|s^*\|_H^2 + \sum_{j=1}^N \lambda_j(s^*) w_j &\leq \|\tilde{s}\|_H^2 + \sum_{j=1}^N \lambda_j(\tilde{s}) w_j \\ &\leq \|s\|_H^2 + \sum_{j=1}^N \lambda_j(s) w_j \end{aligned}$$

due to (13) and we have shown that s^* is a minimizer of (9).

By Lemma 3.1 the problem (9) has no more than one minimizer and hence s^* is the unique minimizer. □

3.2. **Convergence.** We come back to the original problem (8) and show that it has a unique solution, which is the limit of solutions to the discretized problem. Let us first define singular and regular points of a linear differential operator of the form used in Theorem 3.5.

Remark 3.4. A point $x \in \mathbb{R}^d$ is called singular point of the linear differential operator L, if $\delta_x \circ L = 0$, i.e. $c_\alpha(x) = 0$ for all $|\alpha| \leq m$, and regular point of L otherwise, see [19, Definition 3.2].

Theorem 3.5. *Let $\Omega \subseteq \mathbb{R}^d$ be a bounded domain with Lipschitz boundary. Let L be a linear differential operator of order $m \in \mathbb{N}$ defined by*

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

where all $c_\alpha \in C^{\sigma-m}(\overline{\Omega})$ and $\sigma > d/2 + m + 1$. Let $b : \Omega \to \mathbb{R}$ be a continuous function and $H = H^\sigma(\Omega)$ with norm given by an appropriate reproducing kernel; see Lemma 2.2. Consider the optimization problem for $v \in H$

$$\left\{ \begin{array}{ll} \textit{minimize} & \|v\|_H^2 + \int_\Omega Lv(x)\, dx \\ \textit{subject to} & Lv(x) \leq b(x), \forall x \in \Omega, \end{array} \right. \tag{15}$$

and the sequence of optimization problems: Let $\Omega_1^n, \ldots, \Omega_{N_n}^n \subseteq \Omega$, $n \in \mathbb{N}$, be measurable sets with

- $|\Omega_i^n| > 0$ *for all* $i = 1, \ldots, N_n$,
- $\bigcup_{i=1}^{N_n} \Omega_i^n = \Omega$ *for all* $n \in \mathbb{N}$,
- $\Omega_i^n \cap \Omega_j^n = \emptyset$ *for all* $i \neq j$ *and all* $n \in \mathbb{N}$,
- $d_n := \max_{i=1,\ldots,N_n} d_i^n \longrightarrow 0$ *as* $n \to \infty$, *where* $d_i^n = \operatorname{diam} \Omega_i^n = \sup_{x,y \in \Omega_i^n} \|x - y\|$.

For $n \in \mathbb{N}$ and $i = 1, \ldots, N_n$ let $x_i^n \in \Omega_i^n$ be regular points of L, see Remark 3.4. Set $X^n := \{x_1^n, x_2^n, \ldots, x_{N_n}^n\}$. For each fixed $n \in \mathbb{N}$ let v_n be the unique solution of the minimization problem for $v \in H$

$$\left\{ \begin{array}{ll} \textit{minimize} & \|v\|_H^2 + \sum_{i=1}^{N_n} Lv(x_i^n)|\Omega_i^n| \\ \textit{subject to} & Lv(x_i^n) \leq b(x_i^n), \; i = 1, \ldots, N_n. \end{array} \right. \tag{16}$$

Furthermore, assume that there exists a $V_0 \in H^\sigma(\Omega)$ that satisfies the constraints of (15).

Then the optimization problem (15) *has a unique solution v and the solutions v_n of the optimization problems* (16) *converge strongly in H to v as $n \to \infty$.*

Proof. We start by showing that for a fixed $n \in \mathbb{N}$, the optimization problem (16) is just the optimization problem (9). To this end, we first note that, because of $\sigma > d/2$ and because of Ω having a Lipschitz boundary, $H := H^\sigma(\Omega)$ is indeed a RKHS. Moreover, using Lemma 2.2, we can choose an inner product on $H^\sigma(\Omega)$ and a reproducing kernel k_σ which is given by a positive definite function $\Phi_\sigma : \mathbb{R}^d \to \mathbb{R}$ as $k_\sigma(x, y) = \Phi_\sigma(x - y)$, $x, y \in \Omega$. The norm induced by this inner product is equivalent to the standard norm on $H^\sigma(\Omega)$, and we will use this inner product and its induced norm as the inner product and norm on $H^\sigma(\Omega)$, denoting $\langle \cdot, \cdot \rangle_H = \langle \cdot, \cdot \rangle_{H^\sigma(\Omega)} = \langle \cdot, \cdot \rangle_{k_\sigma}$. As L maps $H^\sigma(\Omega)$ continuously to $H^{\sigma-m}(\Omega)$ and as $\sigma > d/2 + m$ implies $H^{\sigma-m}(\Omega) \subseteq C(\Omega) \cap L_\infty(\Omega)$ by the Sobolev embedding theorem, the functionals $\lambda_i = \delta_{x_i^n} \circ L$ indeed belong to H^*. Moreover, as the points

x_i^n are regular points of the differential operator, they are also linearly independent, see [19, Proposition 3.3]. Hence, for a fixed $n \in \mathbb{N}$, problem (16) is indeed (9) with these λ_i, $w_i = |\Omega_i^n| > 0$, $b_i = b(x_i^n)$, $i = 1, \ldots, N_n$ and $N = N_n$.

For the rest of the proof we will use the notation $\lambda_{i,n} := \delta_{x_i^n} \circ L$, $w_{i,n} := |\Omega_i^n|$, and $b_{i,n} := b(x_i^n)$. We will now show, in several steps, that the sequence $(v_n)_{n\in\mathbb{N}}$ of solutions of (16) converges strongly to an element $v \in H$, which is the unique solution of (15).

Step 1. Since $\sigma - m > d/2$, we have by the Sobolev embedding theorem that the function $V_0 \in H^\sigma(\Omega)$ satisfies $LV_0 \in H^{\sigma-m}(\Omega) \subseteq L_\infty(\Omega) \cap C(\Omega)$. In particular, there is a constant c such that $|LV_0(x)| \le c$ for all $x \in \Omega$.

Since $c_\alpha \in C^0(\overline{\Omega})$, there is a constant $C > 0$ such that

$$\max_{x\in\overline{\Omega}} \sum_{|\alpha|\le m, |\beta|\le m} (-1)^{|\beta|} c_\alpha(x) c_\beta(x) D^{\alpha+\beta}\Phi_\sigma(0) \le C^2,$$

where $k_\sigma(x,y) = \Phi_\sigma(x-y)$ denotes the translation-invariant reproducing kernel of $H^\sigma(\Omega)$ introduced above. From (6) it follows that

$$\begin{aligned} \|\lambda_{i,n}^y k_\sigma(\cdot,y)\|_H^2 &= \lambda_{i,n}^x \lambda_{i,n}^y k_\sigma(x,y) \\ &= \sum_{|\alpha|\le m, |\beta|\le m} c_\alpha(x_i^n) c_\beta(x_i^n) D_1^\alpha D_2^\beta k_\sigma(x_i^n, x_i^n) \\ &= \sum_{|\alpha|\le m, |\beta|\le m} (-1)^{|\beta|} c_\alpha(x_i^n) c_\beta(x_i^n) D^{\alpha+\beta}\Phi_\sigma(0) \\ &\le C^2. \end{aligned}$$

By (5) we have $\lambda_{i,n}(v) = \langle v, \lambda_{i,n}^y k_\sigma(\cdot,y)\rangle_H$ and hence

$$\begin{aligned} -\sum_{i=1}^{N_n} \lambda_{i,n}(v_n) w_{i,n} &= -\sum_{i=1}^{N_n} w_{i,n} \langle v_n, \lambda_{i,n}^y k_\sigma(\cdot,y)\rangle_H \\ &\le \sum_{i=1}^{N_n} |\Omega_i^n| \|v_n\|_H \|\lambda_{i,n}^y k_\sigma(\cdot,y)\|_H \\ &\le |\Omega| \|v_n\|_H C \\ &\le \frac{1}{2}(\|v_n\|_H^2 + |\Omega|^2 C^2), \end{aligned}$$

that is

$$-|\Omega|^2 C^2 - \|v_n\|_H^2 \le 2 \sum_{i=1}^{N_n} Lv_n(x_i^n) w_{i,n}. \tag{17}$$

Next, we can conclude from (15) that

$$\lambda_{i,n}(V_0) = LV_0(x_{i,n}) \le b(x_i^n) = b_{i,n}.$$

Hence, V_0 satisfies the constraints of (9). Using that v_n is the minimizer of that problem as well as (17) we have

$$\begin{aligned}
-|\Omega|^2 C^2 + \|v_n\|_H^2 &\leq 2\left(\|v_n\|_H^2 + \sum_{i=1}^{N_n} Lv_n(x_i^n) w_{i,n}\right)\\
&\leq 2\left(\|V_0\|_H^2 + \sum_{i=1}^{N_n} LV_0(x_i^n) w_{i,n}\right)\\
&\leq 2\left(\|V_0\|_H^2 + c|\Omega|\right).
\end{aligned}$$

Thus,

$$\|v_n\|_H \leq C_0 := \sqrt{|\Omega|^2 C^2 + 2\left(\|V_0\|^2 + c|\Omega|\right)} \tag{18}$$

is bounded for all n and, because bounded sets in Hilbert spaces are relatively compact in the weak topology, there is a subsequence of $(v_n)_{n\in\mathbb{N}}$, which we again denote by $(v_n)_{n\in\mathbb{N}}$, that weakly converges to a function $v \in H$. From

$$\|v\|_H^2 = \langle v, v - v_n\rangle_H + \langle v, v_n\rangle_H \leq \langle v, v - v_n\rangle_H + \|v\|_H \|v_n\|_H$$

it follows that

$$\|v\|_H \leq \liminf_{n\to\infty} \|v_n\|_H \leq C_0. \tag{19}$$

Step 2. Now we use the kernel representation to show that $Lv(x) \leq b(x)$ for all $x \in \Omega$, where v is the weak limit of the (subsequence) $(v_n)_{n\in\mathbb{N}}$.

First note that we have for $\lambda = \delta_x \circ L \in H^*$, as $\lambda^y k_\sigma(\cdot, y)$ is the Riesz representative of λ, that

$$|Lv(x) - Lv_n(x)| = |\lambda(v - v_n)| = \langle v - v_n, \lambda^y k_\sigma(\cdot, y)\rangle_H \longrightarrow 0, \tag{20}$$

as v_n converges weakly to v.

Next, as $\sigma - m > d/2$ and as $\Omega \subseteq \mathbb{R}^d$ has a Lipschitz boundary, the Sobolev space $H^{\sigma-m}(\Omega)$ is also a RKHS and, again following Lemma 2.2, we may assume that the inner product is chosen in such a way that the reproducing kernel has the form $k_{\sigma-m}(x, y) = \Phi_{\sigma-m}(x - y)$ with $\Phi_{\sigma-m}\colon \mathbb{R}^d \to \mathbb{R}$. Since we even have $\sigma - m > d/2+1$, the Sobolev embedding theorem even gives $H^{\sigma-m}(\mathbb{R}^d) \subseteq W^1_\infty(\mathbb{R}^d) \cap C^1(\mathbb{R}^d)$, which means in particular, that there is an $M > 0$ such that $\|\nabla\Phi_{\sigma-m}(\xi)\|_2 \leq M$ for all $\xi \in \mathbb{R}^d$.

Furthermore, we have for $x, y \in \Omega$ that there is a $\xi \in \mathbb{R}^d$ on the line segment between 0 and $x - y$ such that, using that $L\colon H^\sigma(\Omega) \to H^{\sigma-m}(\Omega)$ is a bounded operator with constant c_0,

$$\begin{aligned}
|Lv_n(x) - Lv_n(y)| &= \langle Lv_n, k_{\sigma-m}(\cdot, x) - k_{\sigma-m}(\cdot, y)\rangle_{H^{\sigma-m}(\Omega)}\\
&\leq \|Lv_n\|_{H^{\sigma-m}(\Omega)} \|k_{\sigma-m}(\cdot, x) - k_{\sigma-m}(\cdot, y)\|_{H^{\sigma-m}(\Omega)}\\
&= \|Lv_n\|_{H^{\sigma-m}(\Omega)} \left(k_{\sigma-m}(x, x) + k_{\sigma-m}(y, y) - 2k_{\sigma-m}(x, y)\right)^{1/2}\\
&\leq \sqrt{2} c_0 \|v_n\|_{H^\sigma(\Omega)} \left(\Phi_{\sigma-m}(0) - \Phi_{\sigma-m}(x - y)\right)^{1/2}\\
&\leq \sqrt{2} c_0 C_0 \|\nabla\Phi_{\sigma-m}(\xi)\|_2^{1/2} \|x - y\|_2^{1/2}\\
&\leq C_1 \|x - y\|_2^{1/2} \qquad (21)
\end{aligned}$$

for all $n \in \mathbb{N}$ by (18) and with $C_1 = \sqrt{2} c_0 C_0 M^{1/2}$.

We will now show that the fill distance

$$h_{X^n,\Omega} = \sup_{x\in\Omega} \min_{j=1,\ldots,N_n} \|x - x_j^n\|_2$$

satisfies

$$\lim_{n\to\infty} h_{X^n,\Omega} = 0. \tag{22}$$

Fix $n \in \mathbb{N}$. For a point $x \in \Omega$, there is an $i \in \{1, \ldots, N_n\}$ with $x \in \Omega_i^n$. We have

$$\min_{j=1,\ldots,N_n} \|x - x_j^n\|_2 \le \|x - x_i^n\|_2 \le \sup_{y,z\in\Omega_i^n} \|y - z\|_2 = d_i^n \le d_n.$$

Hence, we also have

$$h_{X^n,\Omega} = \sup_{x\in\Omega} \min_{j=1,\ldots,N_n} \|x - x_j^n\|_2 \le d_n.$$

This shows the statement, since $d_n \to 0$ as $n \to \infty$.

We will show that for all $x \in \Omega$ we have $Lv(x) \le b(x)$. Indeed, we fix $x \in \Omega$ and will show that for all $\varepsilon > 0$ we have $Lv(x) - b(x) < \varepsilon$.

Fix $\varepsilon > 0$. By (20), there is an $N_1 \in \mathbb{N}$ such that for all $n \ge N_1$ we have

$$|Lv_n(x) - Lv(x)| < \frac{\varepsilon}{3}. \tag{23}$$

Since b is continuous at x, there exists a $\delta > 0$ such that

$$|b(x) - b(y)| < \frac{\varepsilon}{3} \tag{24}$$

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

By (22) there is an $N_2 \in \mathbb{N}$ such that for all $n \ge N_2$ there exists $x_i^n \in X^n$ with

$$\|x - x_i^n\|_2 < \min\left(\frac{\varepsilon^2}{9C_1^2}, \delta\right). \tag{25}$$

For $n \ge \max(N_1, N_2)$ we have by (23), (21), (25), and (24) as well as $Lv_n(x_i) \le b(x_i^n)$, that

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

This shows the statement.

Step 3. Since $Lv(x) \le b(x)$ holds for all $x \in \Omega$, as shown in Step 2, v satisfies the constraints of (16) and thus

$$\|v_n\|_H^2 + \sum_{i=1}^{N_n} Lv_n(x_i^n) w_{i,n} \le \|v\|_H^2 + \sum_{i=1}^{N_n} Lv(x_i^n) w_{i,n}$$

since v_n is the minimizer of (16).

We will show that for every $\varepsilon > 0$ there exists an $N_0 \in \mathbb{N}$ such that

$$\left| \sum_{i=1}^{N_n} Lv_n(x_i^n) w_{i,n} - \sum_{i=1}^{N_n} Lv(x_i^n) w_{i,n} \right| < \varepsilon \tag{26}$$

for all $n \ge N_0$. This implies that $\limsup_{n\to\infty} \|v_n\|_H^2 \le \|v\|_H^2$ holds. Together with (19) this then shows

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

and from

$$\|v - v_n\|_H^2 = \|v_n\|_H^2 - \|v\|_H^2 + 2\langle v, v - v_n\rangle_H$$

it follows that v_n converges strongly to v.

Fix $\varepsilon > 0$. To show (26), we define $\mu(v) := \int_\Omega Lv(x)\,dx$. We have $\mu \in H^*$ since

$$|\mu(v)| \le \int_\Omega 1 \cdot Lv(x)\,dx \le |\Omega|^{1/2}\|Lv\|_{H^{\sigma-m}(\Omega)} \le |\Omega|^{1/2}c_0\|v\|_{H^\sigma(\Omega)}.$$

But then

$$\int_\Omega (Lv_n(x) - Lv(x))\,dx = \langle v_n - v, \mu^y k_\sigma(\cdot, y)\rangle_{H^\sigma(\Omega)} \to 0$$

since v_n converges weakly to v in $H = H^\sigma(\Omega)$. Hence, there is an $N_1 \in \mathbb{N}$ such that for all $n \ge N_1$ we have

$$\left|\int_\Omega (Lv_n(x) - Lv(x))\,dx\right| < \varepsilon/3. \tag{27}$$

Then we have

$$\begin{aligned}
\left|\int_\Omega Lv_n(x)\,dx - \sum_{j=1}^{N_n} w_{j,n}Lv_n(x_j^n)\right| &= \left|\sum_{j=1}^{N_n}\int_{\Omega_j^n} Lv_n(x)\,dx - \sum_{j=1}^{N_n}\int_{\Omega_j^n} Lv_n(x_j^n)\,dx\right| \\
&\le \sum_{j=1}^{N_n}\int_{\Omega_j^n} |Lv_n(x) - Lv_n(x_j^n)|\,dx \\
&\le C_1\sum_{j=1}^{N_n}\int_{\Omega_j^n} \|x - x_j^n\|_2^{1/2}\,dx \qquad \text{by (21)} \\
&\le C_1\sum_{j=1}^{N_n} d_n^{1/2}\int_{\Omega_j^n} dx \\
&= C_1 d_n^{1/2}|\Omega|. \qquad (28)
\end{aligned}$$

Note that the same estimate holds for v instead of v_n, since (21) holds with the same constant by (19).

Since $d_n \to 0$ as $n \to \infty$ there is $N_2 \in \mathbb{N}$ such that for all $n \ge N_2$ we have $d_n < \frac{\varepsilon^2}{9C_1^2|\Omega|^2}$.

For $n \ge N_0 := \max(N_1, N_2)$ we have

$$\begin{aligned}
\left|\sum_{i=1}^{N_n} Lv_n(x_i^n)w_{i,n} - \sum_{i=1}^{N_n} Lv(x_i^n)w_{i,n}\right| &\le \left|\sum_{i=1}^{N_n} Lv_n(x_i^n)w_{i,n} - \int_\Omega Lv_n(x)\,dx\right| \\
&\quad + \left|\int_\Omega Lv_n(x)\,dx - \int_\Omega Lv(x)\,dx\right| \\
&\quad + \left|\int_\Omega Lv(x)\,dx - \sum_{i=1}^{N_n} Lv(x_i^n)w_{i,n}\right| \\
&< \varepsilon
\end{aligned}$$

by (28) and (27), which shows (26).

Step 4. Finally, we seek to show that v is the unique minimizer. First, let us show that v is a minimizer. Assume that $V \in H$ is any function satisfying the constraints of (15). For every n, V also satisfies the constraints of the discrete problem, so we have

$$\|v_n\|_H^2 + \sum_{i=1}^{N_n} Lv_n(x_i^n) w_{i,n} \leq \|V\|_H^2 + \sum_{i=1}^{N_n} LV(x_i^n) w_{i,n}.$$

As $n \to \infty$, this becomes

$$\|v\|_H^2 + \int_\Omega Lv(x)\, dx \quad \leq \quad \|V\|_H^2 + \int_\Omega LV(x)\, dx \tag{29}$$

as $\|v_n\|_H \to \|v\|_H$ due to the strong convergence, $\sum_{i=1}^{N_n} Lv_n(x_i^n) w_{i,n} \to \int_\Omega Lv(x)\, dx$ using (27) and (28) and $\sum_{i=1}^{N_n} LV(x_i^n) w_{i,n} \to \int_\Omega LV(x)\, dx$ similar to (28). Equation (29) shows that v is a minimizer.

To show that there is not more than one minimizer, we first assume that $s \in H$ is a minimizer and $v \in H$ satisfies the constraints of (15) and show that

$$2\langle s, v - s\rangle_H + \int_\Omega L(v - s)(x)\, dx \quad \geq \quad 0. \tag{30}$$

Indeed, assume that $2\langle s, v - s\rangle_H + \int_\Omega L(v - s)(x)\, dx < 0$. Let $\alpha \in [0, 1]$. Note that $t = \alpha v + (1 - \alpha)s$ satisfies the constraints and we have

$$\begin{aligned}
\|t\|_H^2 + \int_\Omega Lt(x)\, dx \quad &= \quad \|s + \alpha(v - s)\|_H^2 + \int_\Omega L[s + \alpha(v - s)](x)\, dx \\
&= \quad \|s\|_H^2 + 2\alpha\langle s, v - s\rangle_H + \alpha^2\|v - s\|_H^2 \\
&\qquad + \int_\Omega Ls(x)\, dx + \alpha \int_\Omega L(v - s)(x)\, dx \\
&< \quad \|s\|_H^2 + \int_\Omega Ls(x)\, dx
\end{aligned}$$

for a suitable $\alpha > 0$. This is a contradiction to s being a minimizer.

Now let $s_1, s_2 \in H$ be minimizers. Then by (30) we have

$$2\langle s_1, s_2 - s_1\rangle_H + \int_\Omega L(s_2 - s_1)(x)\, dx \geq 0$$

and

$$2\langle s_2, s_1 - s_2\rangle_H + \int_\Omega L(s_1 - s_2)(x)\, dx \geq 0.$$

This implies

$$\begin{aligned}
0 \quad &\leq \quad 2\|s_1 - s_2\|_H^2 \\
&= \quad -2\langle s_1, s_2 - s_1\rangle_H - 2\langle s_2, s_1 - s_2\rangle_H \\
&= \quad -2\langle s_1, s_2 - s_1\rangle_H - 2\langle s_2, s_1 - s_2\rangle_H \\
&\qquad - \int_\Omega L(s_2 - s_1)(x)\, dx - \int_\Omega L(s_1 - s_2)(x)\, dx \\
&\leq \quad 0
\end{aligned}$$

which shows $s_1 = s_2$.

Hence, every weakly convergent subsequence of the original sequence $(v_n)_{n\in\mathbb{N}}$ necessarily converges strongly to the unique minimizer v of (15). It now follows that the original sequence $(v_n)_{n\in\mathbb{N}}$ of the solutions to the problems (16) converges strongly to v. For a contradiction assume this is not the case and there exists an $\varepsilon > 0$ and a subsequence $(v_{n_k})_{k\in\mathbb{N}}$ such that

$$\|v_{n_k} - v\|_H \geq \varepsilon \text{ for all } k \in \mathbb{N}. \tag{31}$$

Since $(v_{n_k})_{k\in\mathbb{N}}$ is bounded it has a weakly convergent subsequence and as we have shown above this subsequence must necessarily converge weakly, and then strongly, to v. This is a contradiction to (31). □

Remark 3.6. The assumption that there exists a function $V_0 \in H^\sigma(\Omega)$ that satisfies the constraints of (15) is obviously satisfied if the equation $Lv(x) = b(x)$ has a solution in $H^\sigma(\Omega)$. This will, for example, be the case in our application to compute complete Lyapunov functions in the next section.

4. Computing complete Lyapunov functions

For our application to compute complete Lyapunov functions we choose $b \equiv 0$ as well as $\lambda_i = \delta_{x_i} \circ L$, $i = 1, \ldots, N$, where $Lv = v' = f \cdot \nabla v$ denotes the operator of the orbital derivative, which is of order $m = 1$. Moreover, we assume that all points x_i are pairwise distinct and satisfy $f(x_i) \neq 0$, i.e. they are no equilibria of (1). This implies that they are regular points of L, see [19].

There exists a function V_0 satisfying the constraints

$$LV_0(x) = V_0'(x) \leq 0;$$

in fact, the constant function $V_0(x) \equiv 0$ is such a function. Hence, Theorem 3.5 shows that in our situation there exists a unique minimizer v, which is a CLF candidate, satisfying $v'(x) \leq 0$ for all $x \in \Omega$, and it is the limit of the functions v_n, obtained by solving a sequence of quadratic programming problems.

However, the minimizer could be itself a constant function and would then not deliver any information about the dynamics of the system.

We will show that if there exists a smooth CLF, which is not constant on Ω, then the minimizer is also not constant. By [30] this is the case, unless Ω is a subset of the chain-recurrent set.

Proposition 4.1. *Assume that the system* (1) *has a non-constant CLF candidate* $V_0 \in H^\sigma(\Omega) =: H$ *with* $\sigma > d/2 + 2$ *on a bounded domain* Ω *with a Lipschitz boundary and there exists a point* $x_0 \in \Omega$ *with* $V'(x_0) < 0$*. Then the minimizer* $v \in H$ *of the problem*

$$\begin{cases} \textit{minimize} & \|v\|_H^2 + \int_\Omega v'(x)\,dx \\ \textit{subject to} & v'(x) \leq 0 \;\forall x \in \Omega, \end{cases} \tag{32}$$

is a non-constant CLF candidate, which has not vanishing orbital derivative on all of Ω*.*

Proof. We prove the proposition by showing that there is a constant $c > 0$ such that the objective function for the CLF candidate cV_0 is strictly negative.

Since V_0 is a CLF candidate, so is cV_0 for all $c > 0$. Define $a = \|V_0\|_H^2$ and $b = \int_\Omega V_0'(x)\,dx$. We have $a > 0$ and $b < 0$, since V_0 is C^1 and satisfies $V_0'(x_0) < 0$.

We have

$$\begin{aligned} g(c) &:= \|cV_0\|_H^2 + \int_\Omega cV_0'(x)\,dx \\ &= ac^2 + bc \\ &= a\left(c + \frac{b}{2a}\right)^2 - \frac{b^2}{4a}, \end{aligned}$$

which is a quadratic function in c with minimum $-\frac{b^2}{4a} < 0$, which is attained at $c = -\frac{b}{2a} > 0$. □

Remark 4.2. Note that considering the problem

$$\text{(33)} \qquad \begin{cases} \text{minimize} & \|w\|_H^2 + R\int_\Omega w'(x)\,dx \\ \text{subject to} & w'(x) \le 0\ \forall x \in \Omega, \end{cases}$$

where $R > 0$, results in a scaled minimizer $w(x) = Rv(x)$ compared to problem (32). Therefore one can use the parameter $R > 0$ to obtain a scaled CLF candidate for the system, however, it results in the same estimate of the chain-recurrent set.

More precisely, if $v \in H$ is the solution of (32), then $w(x) = Rv(x)$ is the solution of (33).

Indeed, first of all, both problems have a unique minimizer. Further, if $v'(x) \le 0$, then $w'(x) \le 0$ holds for all $x \in \Omega$. Lastly, we show that if w is not the minimizer of (33), then v is not the minimizer of (32): assume that there is $u \in H$ with

$$\|u\|_H^2 + R\int_\Omega u'(x)\,dx < \|w\|_H^2 + R\int_\Omega w'(x)\,dx.$$

Define $\tilde{u}(x) = \frac{u(x)}{R}$. Then we have

$$\begin{aligned} R^2\|\tilde{u}\|_H^2 + R^2\int_\Omega \tilde{u}'(x)\,dx &< R^2\|v\|_H^2 + R^2\int_\Omega v'(x)\,dx, \text{ i.e.} \\ \|\tilde{u}\|_H^2 + \int_\Omega \tilde{u}'(x)\,dx &< \|v\|_H^2 + \int_\Omega v'(x)\,dx, \end{aligned}$$

which shows that v is not the minimizer.

5. Examples

For the computations we use a finite set of points $X = \{x_1, \ldots, x_N\} \subseteq \mathbb{R}^d$. The set X is chosen as a subset of the following (shifted) hexagonal grid with fineness-parameter $\alpha_{\text{Hexa-basis}} \in \mathbb{R}^+$:

$$\text{(34)} \quad \alpha_{\text{Hexa-basis}}\left\{\frac{\omega_d}{2} + \sum_{k=1}^d i_k\omega_k : i_k \in \mathbb{Z}\right\}, \qquad \text{where}$$

$$\begin{aligned} \omega_1 &= (2\varepsilon_1, 0, 0, \ldots, 0) \\ \omega_2 &= (\varepsilon_1, 3\varepsilon_2, 0, \ldots, 0) \\ \vdots\ &\quad \vdots \\ \omega_d &= (\varepsilon_1, \varepsilon_2, \varepsilon_3, \ldots, (d+1)\varepsilon_d) \text{ and} \\ \varepsilon_k &= \sqrt{\frac{1}{2k(k+1)}}, \quad k \in \mathbb{N}. \end{aligned}$$

This hexagonal grid optimally balances the opposing aims of a small fill distance and a large separation distance of points to keep the condition numbers of the collocation matrices as small as possible [26]. The singular points of L are equilibria, i.e. points x satisfying $f(x) = 0$, and, therefore, all such points are removed from the set X.

The method was implemented on a UNIX system using C++ and the quadratic optimization problems were solved using a quadratic program solver provided by P. Perry `https://github.com/patperry/qp`. We will publish its implementation as a further update to LyapXool – a software package for computing complete Lyapunov functions [2, 6].

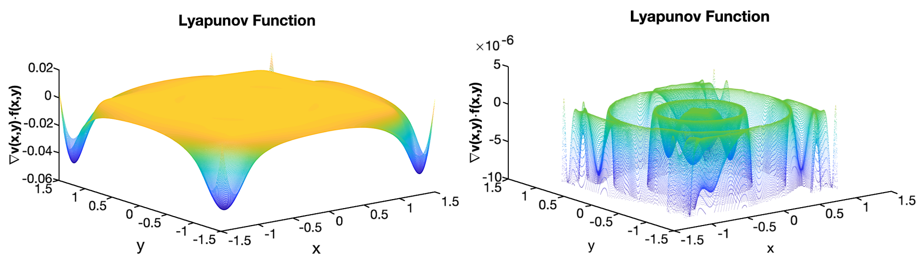

FIGURE 1. The orbital derivative $v'(x, y)$ of the complete Lyapunov function candidate v computed by our method for system (35). $v'(x, y)$ is approximately zero on the chain-recurrent set (origin and the two periodic orbits, circle with radii 0.5 and 1) and negative elsewhere. Both figures depict $v'(x, y)$, but on the right one we have zoomed in on the z-axis (interval $\left[-10^{-5}, 5 \times 10^{-6}\right]$), so that one can better identify the approximation to the chain-recurrent set, i.e. where $v'(x, y) \approx 0$.

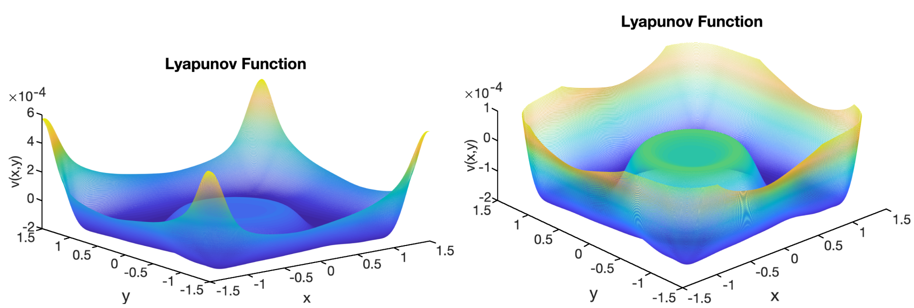

FIGURE 2. The complete Lyapunov function candidate $v(x, y)$ computed by our method for system (35). v has a minimum at the asymptotically stable equilibrium at the origin, a local maximum at the unstable periodic orbit (circle with radius 0.5) and a local minimum at the asymptotically stable periodic orbit (circle with radius 1). Both figures depict $v(x, y)$, but on the right one we have zoomed in on the z-axis (interval $\left[-2 \times 10^{-4}, 5 \times 10^{-4}\right]$), so that one can better identify the shape of v.

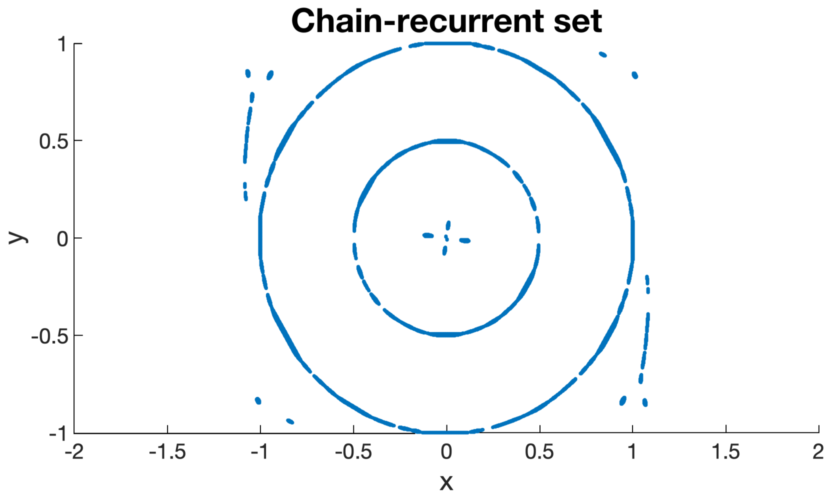

FIGURE 3. Approximation of the chain-recurrent set as the set $\{(x, y) \in \mathbb{R}^2 \mid v'(x, y) \geq 0\}$ for system (35). The chain-recurrent set consists of the asymptotically stable equilibrium at the origin, the unstable periodic orbit (circle with radius 0.5) and the asymptotically stable periodic orbit (circle with radius 1).

5.1. **Two periodic orbits.** We consider the system

$$\begin{pmatrix} \dot{x} \\ \dot{y} \end{pmatrix} = \begin{pmatrix} -x(x^2+y^2-1/4)(x^2+y^2-1)-y \\ -y(x^2+y^2-1/4)(x^2+y^2-1)+x \end{pmatrix}. \tag{35}$$

This system has an asymptotically stable equilibrium at the origin as well as two periodic orbits: an asymptotically stable periodic orbit at $\Omega_1 = \{(x, y) \in \mathbb{R}^2 \mid \sqrt{x^2+y^2} = 1\}$ and an unstable periodic orbit at $\Omega_2 = \{(x, y) \in \mathbb{R}^2 \mid \sqrt{x^2+y^2} = 1/2\}$.

For the quadratic programming problem we used the points of the hexagonal grid (34) with $\alpha_{\text{Hexa-basis}} = 0.0143$ in the area $[-1.5, 1.5]^2 \subseteq \mathbb{R}^2$. This results in a matrix A of size N^2 with $N = 50,820$. As kernel we used the Wendland function $\psi_{6,4}(r) = (1-r)_+^6(35r^2+18r+3)$, where $x_+ = x$ if $x > 0$ and $x_+ = 0$ otherwise.

Figure 1 displays the orbital derivative v' of the CLF candidate, which is approximately zero at the equilibrium and the two periodic orbits (circles with radii 0.5 and 1) and negative otherwise. Figure 2 shows the computed CLF candidate with a local minimum at the origin, which is an asymptotically stable equilibrium, a local maximum at the unstable periodic orbit (circle with radius 0.5) and a local minimum at the attracting periodic orbit (circle with radius 1). Figure 3 shows an approximation of the chain-recurrent set, namely the points (x, y), such that $v'(x, y) \geq 0$.

5.2. **Lorenz attractor.** We consider the classical Lorenz system

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} -\sigma x + \sigma x \\ rx - y - xz \\ xy - bz \end{pmatrix} =: f(x, y, z). \tag{36}$$

with the parameters $\sigma = 10$, $b = 8/3$ and $r = 28$, for which it has a global attractor.

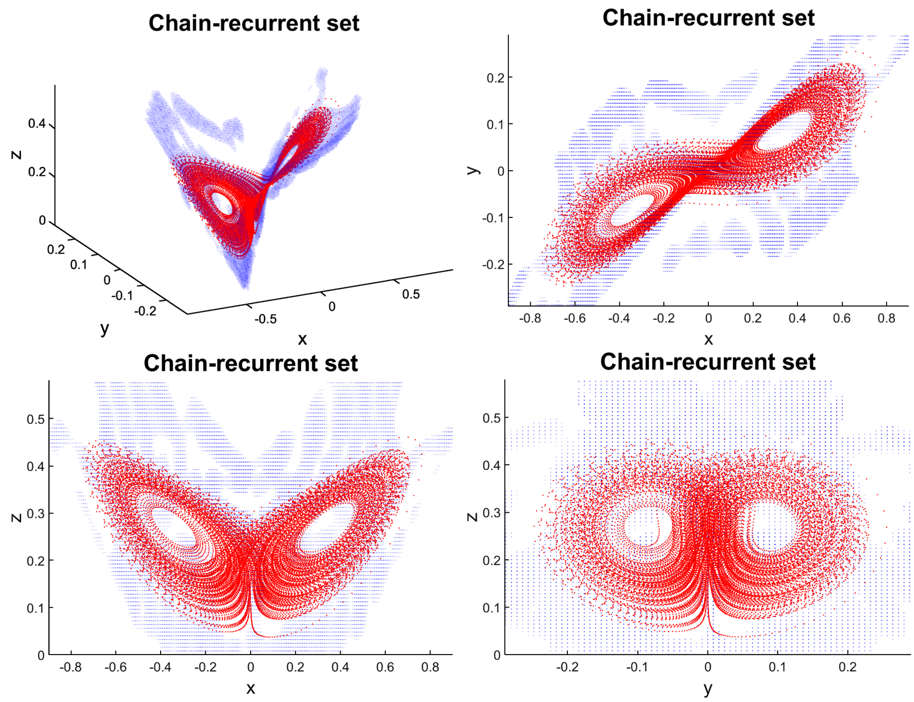

FIGURE 4. Approximation of the chain-recurrent set as the set $\{(x,y,z) \in \mathbb{R}^3 \mid v'(x,y,z) \geq 0\}$ for the Lorenz system (37) in blue. For comparison, the actual global attractor is shown in red and was computed using the computer software GAIO [15]. The proposed method characterizes the shape of the Lorenz attractor well, including the *butterfly*-like shape. The figures show the attractor in $\mathbb{R}^3$ (top left) as well its projections on the $xy-$, $xz-$ and $yz-$planes.

For computational purposes it is advantageous to scale the system so that the attractor fits into a smaller set. We follow [21] and consider the system

$$\begin{pmatrix} \dot{x} \\ \dot{y} \\ \dot{z} \end{pmatrix} = \begin{pmatrix} -\sigma x + \sigma(s_y/s_x)y \\ r(s_x/s_y)x - y - (s_x s_z/s_y)xz \\ -bz + (s_x s_y/s_z)xy \end{pmatrix} \tag{37}$$

and set $s_x = 24.5$ and $s_y = s_z = 100$. In system (37) the function $f(\cdot)$ in the classical Lorenz system has been replaced by $S^{-1}f(S\cdot)$, where $S = \mathrm{diag}(s_x, s_y, s_z)$. A solution trajectory $\mathbf{y}(t)$ to (37) corresponds to a solution trajectory $\mathbf{x}(t) = S\mathbf{y}(t)$ of (36). With this scaling one can use results from [12] to prove that the attractor of (37) must be in the cube $[-1,1] \times [-0.29, 0.29] \times [0, 0.57]$, cf. [21], which is the region shown in the figures.

For the quadratic programming problem we have used the points of the hexagonal grid (34) with $\alpha_{\text{Hexa-basis}} = 0.04$ in the area $[-1,1]^2 \times [-0.1, 0.6] \subseteq \mathbb{R}^3$. This results in a matrix A of size N^2 with $N = 61,092$. As kernel we have used the Wendland function $\psi_{6,4}(r) = (1-r)_+^6(35r^2 + 18r + 3)$, where $x_+ = x$ if $x > 0$ and $x_+ = 0$ otherwise.

Figure 4 displays the set of points with orbital derivative $v'(x, y, z) \geq 0$ in blue, characterizing the chain-recurrent set, i.e. the attractor. For comparison, we have plotted the actual attractor in red computed by the computer software GAIO [15]. The figures show that points with nonnegative orbital derivative of the computed CLF candidate include the attractor and the set displays the butterfly shape very well.

5.3. **Rate of convergence.** We have not developed a theory for determining the rate of convergence for our approach, i.e. how fast the solutions v_n of the discretized optimization problems (16) converge to the solution of the original problem (15) as a function of the diameter d_n of the areas Ω_n, cf. Theorem 3.5. We did, however, do some numerical experiments to estimate the rate of convergence. We used the system (35) and computed a CLF candidate with $\alpha_{\text{Hexa-basis}} = 0.0134$. Then we compared these results with those obtained using $\alpha_{\text{Hexa-basis}} = 0.02, 0.03, \ldots, 0.1$, where we defined the error as the root mean square (rms) of their difference on a uniform grid with $1,002,001$ points. Note that $\alpha_{\text{Hexa-basis}}$ is directly proportional to d_n. The results are quite clear as can be seen in Figure 5 and we get a good linear fit of the logarithm of the rms of the error vs. the logarithm of $\alpha_{\text{Hexa-basis}}$ with slope 1.0237, indicating that the v_n converge linearly in d_n in the $\|\cdot\|_\infty$ norm to v. These results were verified for the simple 1-dimensional system $\dot{x} = -1$ on $(-1, 1)$. We are optimistic that the rate of convergence can be improved, e.g. by including a higher-order approximations of the integral $\int_\Omega Lv(x)dx$. This will be investigated in future work.

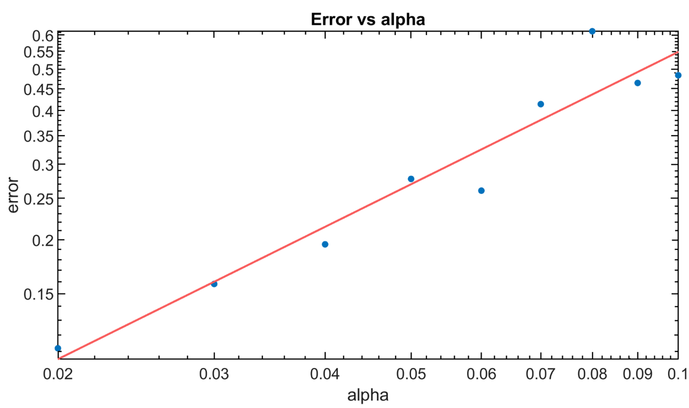

FIGURE 5. Numerical estimate of the rate of convergence: rms of the error as a function of $\alpha_{\text{Hexa-basis}}$ on a dense uniform grid. The convergence is clearly linear in $\alpha_{\text{Hexa-basis}} \propto d_n$.

6. SUMMARY

In this paper, we have considered a general quadratic minimization problem with linear differential inequality constraints and we have shown that it has a unique solution. Moreover, the unique minimizer is the (strong) limit of a sequence of solutions of corresponding discretized problems, which in turn can be determined by quadratic programming.

This general theory has been applied to the construction of a complete Lyapunov function candidate, which is a function with non-positive orbital derivative. So far, construction methods for complete Lyapunov functions have either needed information about the location of the chain-recurrent set or there has been no proof of convergence. Our new method, on the contrary, proves that a complete Lyapunov function can be constructed as the limit of solutions of quadratic programming problems, which do not require any knowledge about the chain-recurrent set at all.

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