Computation and verification of contraction metrics for periodic orbits

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Abstract

Exponentially stable periodic orbits of ordinary differential equations and their basins' of attraction are characterized by contraction metrics. The advantages of a contraction metric over a Lyapunov function include its insensitivity to small perturbations of the dynamics and the exact location of the periodic orbit. We present a novel algorithm to rigorously compute contraction metrics, that combines the numerical solving of a first order partial differential equation with rigorous verification of the conditions for a contraction metric for any ordinary differential equation possessing an exponentially stable periodic orbit. We demonstrate the applicability of our approach by computing contraction metrics for three systems from the literature.

Keywords: Contraction Metric, Lyapunov Stability, Periodic Orbits, Basin of Attraction, Numerical Method, Radial Basis Functions, Reproducing Kernel Hilbert Spaces, Continuous Piecewise Affine Interpolation, Verification

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1 Introduction

Consider an autonomous ordinary differential equation (ODE) of the form

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}), \quad \mathbf{x} \in \mathbb{R}^n$$
 (1.1)

with a C^s -vector field $\mathbf{f} : \mathbb{R}^n \to \mathbb{R}^n$. In this paper we study the existence and stability of periodic orbits and investigate their basins of attraction using a Riemannian contraction metric. A contraction metric is a local criterion that does not require knowledge of the precise

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location of the periodic orbit. Moreover, it is robust to small perturbations of the system, i.e. a contraction metric for (1.1) remains a contraction metric for a perturbed system, even with a perturbed periodic orbit.

In [5] a contraction metric for a periodic orbit was characterized as the solution of a linear matrix-valued PDE and an existence and uniqueness theorem was proved. Then in [4] a numerical method to compute such a contraction metric was presented, however, the method lacks a rigorous verification of the properties of a contraction metric. In this paper we will present such a verification and, in addition, show that the verification can be combined with the procedure from [4] to deliver a method that is able to compute a contraction metric for any system with an exponentially stable periodic orbit. The main idea is similar to [8], in which we have provided a computation and verification method for contraction metrics in case of exponentially stable equilibrium points. As in [8] we show that our novel method is successful in computing a metric if sufficiently many points are used in the collocation (as in [4]) and sufficiently small simplices in the verification. However, in contrast to the case of an equilibrium, the contraction condition involves the restriction to the (n-1)-dimensional subspace perpendicular to $f(\mathbf{x})$ at each point \mathbf{x} , which requires a more sophisticated argumentation. Contraction metrics for periodic orbits have been considered by Borg [2] with the Euclidean metric and Stenström [18] with a general Riemannian metric. They have also been studied in [13, 14, 15, 16].

Computational methods for contraction metrics have been proposed in [6] for periodic orbits in time-periodic systems, where the contraction metric was a continuous piecewise affine (CPA) function and the contraction conditions were transformed into constraints of a semidefinite optimization problem. In [17, Theorem 3] a contraction metric for periodic orbits was constructed using Linear Matrix Inequalities and SOS (sum of squares). While both of these methods also include a rigorous verification, similar to our approach, they are of higher computational complexity because they require solving a semidefinite optimization problem, whereas solving a system of linear equations is computationally the most demanding step in our approach.

Let us give an overview of the contents: we first review the characterization of a unique stable periodic orbit using a contraction metric in Section 2. In particular, we consider a contraction metric which satisfies a certain PDE. Then we approximate the contraction metric satisfying the PDE using mesh-free collocation with Radial Basis Functions (RBF) in Section 3. In order to verify the conditions of the contraction metric we make a Continuous Piecewise Affine (CPA) interpolation of the RBF approximation in Section 4. We show that if the CPA interpolation of the RBF approximation satisfies the constraints of Verification Problem 4.7, then it is a contraction metric. Further, we show that in the basin of attraction of an exponentially stable periodic orbit, the CPA-RBF construction method provides a function that satisfies the constraints of Verification Problem 4.7 whenever the collocation points of the RBF method are sufficiently dense and the triangulation of the CPA method is sufficiently fine. This is the main result of this paper: an algorithm that can rigourously compute a contraction metric for any system with an exponentially stable periodic orbit. In Section 5 we apply the method to three examples.

2 Riemannian Contraction Metric

In this section we review the definition of a Riemannian contraction metric and relax the conditions on its smoothness in order to consider CPA metrics later. In particular, we do not require the metric M to be a C^1 function.

2.1 Definition (Riemannian metric)

Let G be an open subset of \mathbb{R}^n . A Riemannian metric is a locally Lipschitz continuous matrixvalued function $M: G \to \mathbb{S}^{n \times n}$, such that $M(\mathbf{x})$ is positive definite for all $\mathbf{x} \in G$, where $\mathbb{S}^{n \times n}$ denotes the symmetric $n \times n$ matrices with real entries.

Then $\langle \mathbf{v}, \mathbf{w} \rangle_{M(\mathbf{x})} := \mathbf{v}^T M(\mathbf{x}) \mathbf{w}, \mathbf{v}, \mathbf{w} \in \mathbb{R}^n$, defines a (point-dependent) scalar product for each $\mathbf{x} \in G$.

The forward orbital derivative $M'_{+}(\mathbf{x})$ with respect to (1.1) at $\mathbf{x} \in G$ is defined by

$$M'_{+}(\mathbf{x}) := \limsup_{h \to 0^{+}} \frac{M(S_{h}\mathbf{x}) - M(\mathbf{x})}{h}$$
(2.1)

where $t \mapsto S_t \mathbf{x}$ is the solution to (1.1) passing through \mathbf{x} at time t = 0.

2.2 Remark Note that the forward orbital derivative (2.1) is formulated using a Dini derivative similar to [6, Definition 3.1] and always exists in $\mathbb{R} \cup \{\infty\}$. This assumption is less restrictive than [3, Definition 2.1], which is the existence and continuity of

$$M'(\mathbf{x}) = \left. \frac{d}{dt} M(S_t \mathbf{x}) \right|_{t=0}.$$

A sufficient condition for the existence and continuity of $M'_+(\mathbf{x})$ is that $M \in C^1(G; \mathbb{S}^{n \times n})$; then $(M'_+(\mathbf{x}))_{ij} = (M'(\mathbf{x}))_{ij} = (\nabla M_{ij}(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}))_{ij}$ for all $i, j \in \{1, 2, ..., n\}$. It is also worth mentioning that if $K \subset G$ is compact, then M in Definition 2.1 is uniformly

It is also worth mentioning that if $K \subset G$ is compact, then M in Definition 2.1 is uniformly positive definite on K, i.e. there exists an $\epsilon > 0$ such that $\mathbf{v}^T M(\mathbf{x})\mathbf{v} \ge \epsilon \|\mathbf{v}\|^2$ for all $\mathbf{v} \in \mathbb{R}^n$ and all $\mathbf{x} \in K$.

2.3 Remark It is useful to have a more accessible expression for the forward orbital derivative in terms of \mathbf{f} , see (1.1). In fact we have

$$M'_{+}(\mathbf{x}) := \limsup_{h \to 0^{+}} \frac{M(S_{h}\mathbf{x}) - M(\mathbf{x})}{h} = \limsup_{h \to 0^{+}} \frac{M(\mathbf{x} + h\mathbf{f}(\mathbf{x})) - M(\mathbf{x})}{h},$$

because by [6, Lemma 3.3] an analogous formula holds true for each entry M_{ij} of the matrix M.

The function $L_M(\mathbf{x}; \mathbf{v})$ in (2.3) below is negative for \mathbf{v} with $\mathbf{v}^T \mathbf{f}(\mathbf{x}) = 0$, if for small $\delta > 0$ the distance between solutions through \mathbf{x} and $\mathbf{x} + \delta \mathbf{v}$ decreases with respect to the metric $M(\mathbf{x})$. For a heuristic explanation of this fact, see, e.g. [4, Section 1].

2.4 Definition (Riemannian contraction metric)

A contraction metric for a periodic orbit is a Riemannian metric $M : G \to \mathbb{S}^{n \times n}$ fulfilling a contraction condition expressed by $L_M(\mathbf{x}) \leq -\nu < 0$ for all $\mathbf{x} \in K \subset G$, where L_M is defined

in (2.3) below and K is a compact subset of the open set $G \subset \mathbb{R}^n$ such that $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$ holds for all $\mathbf{x} \in K$.

For the definition of L_M we first define for all $\mathbf{x} \in \mathbb{R}^n$ with $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$

$$V(\mathbf{x}) = D\mathbf{f}(\mathbf{x}) - \frac{\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x})^T (D\mathbf{f}(\mathbf{x}) + D\mathbf{f}(\mathbf{x})^T)}{\|\mathbf{f}(\mathbf{x})\|_2^2}.$$
 (2.2)

For all $\mathbf{x} \in \mathbb{R}^n$ with $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$ we define

$$L_{M}(\mathbf{x}) = \max_{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T} M(\mathbf{x}) \mathbf{v} = 1, \mathbf{v}^{T} \mathbf{f}(\mathbf{x}) = 0} L_{M}(\mathbf{x}; \mathbf{v}) \text{ where}$$
(2.3)
$$L_{M}(\mathbf{x}; \mathbf{v}) = \frac{1}{2} \mathbf{v}^{T} \left(M'_{+}(\mathbf{x}) + V(\mathbf{x})^{T} M(\mathbf{x}) + M(\mathbf{x}) V(\mathbf{x}) \right) \mathbf{v}.$$

We refer to M as a (Riemannian) contraction metric on K or a metric contracting in K.

It turns out to be beneficial for the numerical computation to consider a particular Riemannian contraction metric, which is the solution to a (matrix-valued) PDE, see (2.7). We first define for all $\mathbf{x} \in \mathbb{R}^n$ with $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$ the linear differential operator L, acting on $N : \mathbb{R}^n \to \mathbb{S}^{n \times n}$ by

$$LN(\mathbf{x}) := N'_{+}(\mathbf{x}) + V(\mathbf{x})^{T}N(\mathbf{x}) + N(\mathbf{x})V(\mathbf{x}), \qquad (2.4)$$

where V was defined in (2.2). Moreover, we define the projection $P_{\mathbf{x}}$ for all $\mathbf{x} \in \mathbb{R}^n$ with $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$ onto the (n-1)-dimensional space perpendicular to $\mathbf{f}(\mathbf{x})$, i.e. $P_{\mathbf{x}}^2 = P_{\mathbf{x}}$, $P_{\mathbf{x}}\mathbf{f}(\mathbf{x}) = \mathbf{0}$ and $P_{\mathbf{x}}\mathbf{v} = \mathbf{v}$ if $\mathbf{v}^T\mathbf{f}(\mathbf{x}) = 0$, by

$$P_{\mathbf{x}} := I_{n \times n} - \frac{\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x})^T}{\|\mathbf{f}(\mathbf{x})\|_2^2}.$$
(2.5)

The next two theorems reveal the connection between periodic orbits and contraction metrics. Theorem 2.5 shows that the existence of a contraction metric on a compact, forward invariant set K asserts the existence of a unique exponentially stable periodic orbit $\Omega \subset K$ and that $K \subset \mathcal{A}(\Omega)$. Theorem 2.6 establishes the existence of a contraction metric for exponentially stable periodic orbits, which is the solution to a matrix-valued PDE.

2.5 Theorem (existence, uniqueness and stability of a periodic orbit) Let $K \subset \mathbb{R}^n$ be a compact, connected and positively invariant set that does not contain an equilibrium of (1.1), i.e. for all $\mathbf{x} \in K$ we have $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$. Assume $M : G \to \mathbb{S}^{n \times n}$, $G \supset K$ open, is a contraction metric fulfilling $L_M(\mathbf{x}) \leq -\nu < 0$ on K.

Then there exists a unique periodic orbit $\Omega \subset K$, Ω is exponentially stable and the largest real part of all non-trivial Floquet exponents is at most $-\nu$. Moreover, K is a subset of the basin of attraction $\mathcal{A}(\Omega)$ of Ω .

Proof: This theorem is identical to [5, Theorem 2.1], except that we have reduced the smoothness assumptions on M from C^1 to locally Lipschitz. Since similar multiplication and chain rules apply to the upper Dini derivative M'_+ as M', cf. e.g. [6, Lemma 3.2], the proof is essentially replacing M' by M'_+ in the proof of [5, Theorem 2.1].

The following theorem shows that a contraction metric can be characterized as the unique solution to a PDE. After fixing a positive definite matrix $B(\mathbf{x})$, the right-hand side $-C(\mathbf{x})$ of the PDE is the projection of $B(\mathbf{x})$ onto the (n-1)-dimensional subspace perpendicular to $\mathbf{f}(\mathbf{x})$. Hence, the solution $M(\mathbf{x})$ will be contracting in directions \mathbf{v} perpendicular to $\mathbf{f}(\mathbf{x})$, while staying constant in direction $\mathbf{f}(\mathbf{x})$. To guarantee that the solution $M(\mathbf{x})$ is positive definite in direction $\mathbf{f}(\mathbf{x})$, i.e. $\mathbf{f}(\mathbf{x})^T M(\mathbf{x}) \mathbf{f}(\mathbf{x}) > 0$, we need the condition (2.8) at an arbitrary point \mathbf{x}_0 in the basin of attraction.

2.6 Theorem (existence and uniqueness of the contraction metric) [5, Theorems 3.1, 4.2] Let Ω be an exponentially stable periodic orbit of $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$, $\mathbf{f} \in C^s(\mathbb{R}^n; \mathbb{R}^n)$, where $s \geq 2$, with basin of attraction $\mathcal{A}(\Omega)$. Fix $\mathbf{x}_0 \in \mathcal{A}(\Omega)$ and $c_0 \in \mathbb{R}^+$. Let $B \in C^{s-1}(\mathcal{A}(\Omega); \mathbb{S}^{n \times n})$ be such that $B(\mathbf{x})$ is positive definite for all $\mathbf{x} \in \mathcal{A}(\Omega)$ and define $C \in C^{s-1}(\mathcal{A}(\Omega); \mathbb{S}^{n \times n})$ by (see (2.5))

$$C(\mathbf{x}) = P_{\mathbf{x}}^T B(\mathbf{x}) P_{\mathbf{x}}.$$
(2.6)

Then there exists a unique solution $M \in C^{s-1}(\mathcal{A}(\Omega); \mathbb{S}^{n \times n})$ of the linear matrix-valued PDE (see (2.4))

$$LM(\mathbf{x}) = -C(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathcal{A}(\Omega)$$
 (2.7)

satisfying
$$\mathbf{f}(\mathbf{x}_0)^T M(\mathbf{x}_0) \mathbf{f}(\mathbf{x}_0) = c_0 \|\mathbf{f}(\mathbf{x}_0)\|_2^4.$$
 (2.8)

The solution $M(\mathbf{x})$ is positive definite for all $\mathbf{x} \in \mathcal{A}(\Omega)$ and it is of the form

$$M(\mathbf{x}) = \int_0^\infty \Phi(t, 0; \mathbf{x})^T C(S_t \mathbf{x}) \Phi(t, 0; \mathbf{x}) dt + c_0 \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^T$$

where $\Phi(t, 0; \mathbf{x})$ denotes the principal fundamental matrix solution of $\dot{\phi}(t) = D(S_t \mathbf{x})\phi(t)$ with $\Phi(0, 0; \mathbf{x}) = I_{n \times n}$.

Note that since $L_M(\mathbf{x}; \mathbf{v}) = \frac{1}{2} \mathbf{v}^T L M(\mathbf{x}) \mathbf{v}$, see (2.3), a function M satisfying (2.7) gives $L_M(\mathbf{x}; \mathbf{v}) = -\frac{1}{2} \mathbf{v}^T P_{\mathbf{x}}^T B(\mathbf{x}) P_{\mathbf{x}} \mathbf{v}$ and thus

$$L_M(\mathbf{x}) = -\frac{1}{2} \min_{\mathbf{v} \in \mathbb{R}^n, \mathbf{v}^T M(\mathbf{x}) \mathbf{v} = 1, \mathbf{v}^T \mathbf{f}(\mathbf{x}) = 0} \mathbf{v}^T B(\mathbf{x}) \mathbf{v},$$

which can be bounded above by a negative constant $-\nu$ for all **x** within a compact set $K \subset \mathcal{A}(\Omega)$. Moreover, M satisfying (2.7) and (2.8) is positive definite and therefore a contraction metric.

Although the previous theorem does not enable us to construct the contraction metric analytically in most cases, it provides a suitable way to approximate it by numerically solving the PDE (2.7), see Section 3.

We will now recall some norm-related definitions and inequalities that will be used throughout the paper. For an $A \in \mathbb{R}^{n \times n}$ define

$$\begin{split} \|A\|_{\max} &:= \max_{i,j=1,2,\dots,n} |a_{ij}|, \\ \|A\|_p &:= \max_{\|\mathbf{x}\|_p=1} \|A\mathbf{x}\|_p \text{ for } p = 1, 2, \infty, \\ \|A\|_F &:= \left(\sum_{i,j=1}^n a_{ij}^2\right)^{\frac{1}{2}}. \end{split}$$

The following well-known relations will be used later:

$$\|A\|_{1} = \max_{j=1,\dots,n} \sum_{i=1}^{n} |a_{ij}|, \quad \|A\|_{1} = \|A^{T}\|_{\infty},$$

$$\|A\|_{\max} \leq \|A\|_{2} \leq n \|A\|_{\max}, \quad \|A\|_{2} \leq \sqrt{n} \|A\|_{\infty},$$

$$\frac{1}{\sqrt{n}} \|A\|_{1} \leq \|A\|_{2} \leq \sqrt{n} \|A\|_{1},$$

$$\|A\|_{2} \leq \|A\|_{F} \leq \sqrt{n} \|A\|_{2}.$$

(2.9)

For a symmetric and positive definite A, the largest singular value λ_{\max} of A, which equals $||A||_2$ and is the largest of its eigenvalues, is the smallest number such that $\lambda_{\max}I_{n\times n} - A$ is positive semidefinite, written $A \leq \lambda_{\max}I_{n\times n}$.

We recall that $||M||_{L_{\infty}(K)} = \operatorname{ess\,sup}_{\mathbf{x}\in K} ||M(\mathbf{x})||_2$ for any measurable $K \subset \mathbb{R}^n$. Further, if M is continuous and $K \subset \mathbb{R}^n$ has the property, that every neighborhood (in K) of every $\mathbf{x} \in K$ has a strictly positive measure, then the essential supremum is identical to the supremum.

For a function $W \in C^k(\mathcal{D}; \mathcal{R})$, where $\mathcal{D} \subset \mathbb{R}^n$ is a non-empty open set and \mathcal{R} is $\mathbb{R}, \mathbb{R}^n, \mathbb{S}^{n \times n}$, or $\mathbb{R}^{n \times n}$, we define the C^k -norm as

$$\|W\|_{C^{k}(\mathcal{D};\mathcal{R})} := \sum_{|\boldsymbol{\alpha}| \le k} \sup_{\mathbf{x} \in \mathcal{D}} \|D^{\boldsymbol{\alpha}}W(\mathbf{x})\|_{2}, \qquad (2.10)$$

where $\boldsymbol{\alpha} \in \mathbb{N}_0^n$ is a multi-index and $|\boldsymbol{\alpha}| := \sum_{i=1}^n \alpha_i$. When all $D^{\boldsymbol{\alpha}} W$ can be continuously extended to $\overline{\mathcal{D}}$ for all $|\boldsymbol{\alpha}| \leq k$, the C^k -norm is also defined on $\overline{\mathcal{D}}$ with the same formula.

The final statement of this section is a powerful tool that describes the effect of perturbations on contraction metrics. It is an essential part of the error estimate statements that we provide later.

2.7 Theorem (Robustness of contraction metrics) [4, Theorem 3.1] Let the assumptions of Theorem 2.6 hold. Let $K \subset \mathcal{A}(\Omega)$ be a compact set with $\Omega \subset K^{\circ}$, denote $\gamma^+(K) = \bigcup_{t>0} S_t K$ and let $\mathbf{x}_0 \in K$ as well as $c_0 \in \mathbb{R}^+$.

Then there is an $\epsilon > 0$ such that for all $\widetilde{M}, \widetilde{C} \in C^1(\overline{\gamma^+(K)}; \mathbb{S}^{n \times n})$ satisfying

$$L\widetilde{M}(\mathbf{x}) = -\widetilde{C}(\mathbf{x}) \text{ for all } \mathbf{x} \in \overline{\gamma^+(K)}$$
 (2.11)

$$\mathbf{f}(\mathbf{x}_0)^T \overline{M}(\mathbf{x}_0) \mathbf{f}(\mathbf{x}_0) = c_0 \|\mathbf{f}(\mathbf{x}_0)\|_2^4$$
(2.12)

$$\|C(\mathbf{x}) - \tilde{C}(\mathbf{x})\|_2 \leq \epsilon \text{ for all } \mathbf{x} \in \overline{\gamma^+(K)}$$
(2.13)

$$\left\|\frac{d}{dx_i}\left(C(\mathbf{x}) - \widetilde{C}(\mathbf{x})\right)\right\|_2 \leq \epsilon \text{ for all } \mathbf{x} \in \overline{\gamma^+(K)} \text{ and } i = 1, \dots, n$$
(2.14)

we have that $\widetilde{M}(\mathbf{x})$ is positive definite for all $\mathbf{x} \in K$. Moreover, there is a constant $\tilde{\nu} > 0$ such that

$$L_{\widetilde{M}}(\mathbf{x}) \leq -\widetilde{\nu}$$

holds for all $\mathbf{x} \in \overline{\gamma^+(K)}$, where L_M was defined in (2.3).

3 Optimal Recovery by RBF

In this section we follow [5] and solve the PDE (2.7) numerically to obtain a contraction metric. We review the appropriate setting in which the contraction metric can be recovered or approximated knowing its values at finitely many points, hence called optimal recovery problem. For this we introduce reproducing kernel Hilbert spaces and show an error estimate for the approximated metric.

Let $\mathcal{O} \subset \mathbb{R}^n$ be a domain with Lipschitz boundary and $\sigma > n/2$ be given. Then, the matrixvalued Sobolev space $H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})$ consists of all symmetric matrix-valued functions M having each component M_{ij} in $H^{\sigma}(\mathcal{O})$ and it is a Hilbert space with inner product given by

$$\langle M, S \rangle_{H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})} := \sum_{i,j=1}^{n} \langle M_{ij}, S_{ij} \rangle_{H^{\sigma}(\mathcal{O})},$$

where $\langle \cdot, \cdot \rangle_{H^{\sigma}(\mathcal{O})}$ is the usual inner product on $H^{\sigma}(\mathcal{O})$. It is also a reproducing kernel Hilbert space, see below. On $\mathbb{S}^{n \times n}$ we define the inner product

$$\langle \boldsymbol{\alpha}, \boldsymbol{\beta} \rangle_{\mathbb{S}^{n \times n}} = \sum_{i,j=1}^{n} \alpha_{ij} \beta_{ij}, \quad \boldsymbol{\alpha} = (\alpha_{ij}), \quad \boldsymbol{\beta} = (\beta_{ij}),$$

which renders it a Hilbert space. We denote by $\mathcal{L}(\mathbb{S}^{n \times n})$ the linear space of all linear and bounded operators $\mathbb{S}^{n \times n} \to \mathbb{S}^{n \times n}$.

3.1 Definition (Reproducing Kernel Hilbert Space) A Hilbert space $\mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$ of functions $f : \mathcal{O} \to \mathbb{S}^{n \times n}$ is called reproducing kernel Hilbert space if there is a function $\Phi : \mathcal{O} \times \mathcal{O} \to \mathcal{L}(\mathbb{S}^{n \times n})$ with the following properties:

- 1. $\Phi(\cdot, \mathbf{x}) \alpha \in \mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$ for all $\mathbf{x} \in \mathcal{O}$ and all $\alpha \in \mathbb{S}^{n \times n}$.
- 2. $\langle f(\mathbf{x}), \alpha \rangle_{\mathbb{S}^{n \times n}} = \langle f, \Phi(\cdot, \mathbf{x}) \alpha \rangle_{\mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})}$ for all $f \in \mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$, $\mathbf{x} \in \mathcal{O}$ and $\alpha \in \mathbb{S}^{n \times n}$.

The function Φ is called reproducing kernel of $\mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$.

A kernel Φ is thus a mapping $\Phi : \mathcal{O} \times \mathcal{O} \to \mathcal{L}(\mathbb{S}^{n \times n})$ and can be represented by a tensor of order 4. We will write $\Phi = (\Phi_{ijk\ell})$ and define its action on $\alpha \in \mathbb{R}^{n \times n}$ by

$$(\Phi(\mathbf{x},\mathbf{y})\alpha)_{ij} = \sum_{k,\ell=1}^{n} \Phi(\mathbf{x},\mathbf{y})_{ijk\ell}\alpha_{k\ell}.$$

From [9, Lemma 3.2] we know that with $\phi : \mathcal{O} \times \mathcal{O} \to \mathbb{R}$ as the reproducing kernel of $H^{\sigma}(\mathcal{O})$, the reproducing kernel of $H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})$ is Φ defined by

$$\Phi(\mathbf{x}, \mathbf{y})_{ijk\ell} := \phi(\mathbf{x}, \mathbf{y}) \delta_{ik} \delta_{j\ell}$$
(3.1)

for $\mathbf{x}, \mathbf{y} \in \mathcal{O}$ and $1 \leq i, j, k, \ell \leq n$.

3.2 Definition (Optimal recovery of a function) Assume that we are given N linearly independent functionals $\lambda_1, \ldots, \lambda_N \in \mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})^*$ of a reproducing kernel Hilbert space $\mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$ and N values $r_1 = \lambda_1(M), \ldots, r_N = \lambda_N(M) \in \mathbb{R}$ generated by an element

 $M \in \mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$. The optimal recovery of M based on this information is defined to be the unique element $S \in \mathcal{H}(\mathcal{O}; \mathbb{S}^{n \times n})$ which solves

$$\min\left\{\|S\|_{\mathcal{H}(\mathcal{O};\mathbb{S}^{n\times n})}: S\in\mathcal{H}(\mathcal{O};\mathbb{S}^{n\times n}) \text{ with } \lambda_j(S)=r_j, 1\leq j\leq N\right\}.$$

We choose Wendland functions as the radial basis functions, which will define the reproducing kernel Φ needed for our optimal recovery problem. For more details on these functions and their properties, see [19]. Let $l \in \mathbb{N}$, $k \in \mathbb{N}_0$. Wendland functions are defined by recursion

$$\psi_{l,0}(r) = (1-r)_{+}^{l},$$

and $\psi_{l,k+1}(r) = \int_{r}^{1} t \psi_{l,k}(t) dt$

for $r \in \mathbb{R}_0^+$. Here we set $x_+ = x$ for $x \ge 0$, $x_+ = 0$ for x < 0, and $x_+^l := (x_+)^l$.

With $l := \lfloor \frac{n}{2} \rfloor + k + 1$ the function $\Phi(\mathbf{x}) := \psi_{l,k}(c \|\mathbf{x}\|_2)$ belongs to $C^{2k}(\mathbb{R}^n)$ for any c > 0and the reproducing kernel Hilbert space with reproducing kernel Φ given by a Wendland function is norm-equivalent to the Sobolev space $H^{\sigma}(\mathcal{O})$, where $\sigma = k + \frac{n+1}{2}$.

We will denote by $H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})$ the reproducing kernel Hilbert space with reproducing kernel $\Phi : \mathcal{O} \times \mathcal{O} \to \mathcal{L}(\mathbb{S}^{n \times n})$ as in (3.1), $\phi(\mathbf{x}, \mathbf{y}) = \psi_{l,k}(c \|\mathbf{x} - \mathbf{y}\|_2)$, where $\psi_{l,k}$ is a Wendland function with $l := \lfloor \frac{n}{2} \rfloor + k + 1$ and c > 0. We again have $\sigma = k + \frac{n+1}{2}$. Usually, this notation is used for the Sobolev space, which contains the same functions and is norm-equivalent to the reproducing kernel Hilbert space, but with a slight abuse of notation we denote both by the same symbol – note that all estimates still hold with a different constant.

We fix the pairwise distinct collocation points $X = {\mathbf{x}_1, \ldots, \mathbf{x}_N} \subset \mathcal{O}$ as well as the point $\mathbf{x}_0 \in \mathcal{O}$. Define the linear functionals $\lambda_k^{(i,j)}, \lambda_0 \colon H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n}) \to \mathbb{R}$ for $1 \leq i \leq j \leq n$, $1 \leq k \leq N$ by

$$\lambda_k^{(i,j)}(M) := \mathbf{e}_i^T L M(\mathbf{x}_k) \mathbf{e}_j, \qquad (3.2)$$

$$\lambda_0(M) := \mathbf{f}(\mathbf{x}_0)^T M(\mathbf{x}_0) \mathbf{f}(\mathbf{x}_0), \qquad (3.3)$$

where $\mathbf{e}_i \in \mathbb{R}^n$ denotes the vector $(0, \dots, 0, 1, 0, \dots, 0)$ with the 1 at position *i*.

3.3 Theorem (Existence and uniqueness of the optimal recovery) [4, Theorem 4.2] Let $\mathcal{O} \subset \mathcal{A}(\Omega)$ be a domain with Lipschitz boundary. Let $\sigma > n/2 + 1$, let $\Phi : \mathcal{O} \times \mathcal{O} \rightarrow \mathcal{L}(\mathbb{S}^{n \times n})$ be the reproducing kernel of $H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})$ and $\mathbf{f} \in C^{s}(\mathbb{R}^{n}; \mathbb{R}^{n})$ with $s = \sigma + 1$. Let $X = {\mathbf{x}_{1}, \ldots, \mathbf{x}_{N}} \subset \mathcal{O}$ be pairwise distinct points and $\mathbf{x}_{0} \in \mathcal{O}$ such that $\mathbf{f}(\mathbf{x}_{i}) \neq \mathbf{0}$ for all $i = 0, \ldots, N$. Let $c_{0} \in \mathbb{R}^{+}$, and let $\lambda_{k}^{(i,j)}, \lambda_{0} \in H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})^{*}, 1 \leq k \leq N$ and $1 \leq i \leq j \leq n$ be defined by (3.2) and (3.3).

Then these functionals are linearly independent and there is a unique function $S \in H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})$ solving

$$\min\left\{\|S\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}:\lambda_{k}^{(i,j)}(S)=-C_{ij}(\mathbf{x}_{k}), 1\leq i\leq j\leq n, 1\leq k\leq N\right.$$

and $\lambda_{0}(S)=c_{0}\|\mathbf{f}(\mathbf{x}_{0})\|_{2}^{4}$

where $C(\mathbf{x}) = P_{\mathbf{x}}^T B(\mathbf{x}) P_{\mathbf{x}}$ and $B(\mathbf{x}) = (B_{ij}(\mathbf{x}))_{i,j=1,\dots,n}$ is a symmetric, positive definite matrix for each $\mathbf{x} \in \mathcal{O}$.

The closed form formula for S and technical details for computations is given in Appendix B. One can measure the error of the optimal recovery in terms of the so-called *fill distance* or *mesh norm*

$$h_{X,\mathcal{O}} := \sup_{\mathbf{x}\in\mathcal{O}}\min_{\mathbf{x}_i\in X} \|\mathbf{x}-\mathbf{x}_i\|_2$$

3.4 Theorem (Error estimates for the RBF approximation) [4, Theorem 4.4] Let $\mathbf{f} \in C^s(\mathbb{R}^n; \mathbb{R}^n)$, $\mathbb{N} \ni s > n/2 + 3$ and set $\sigma = s - 1$. Let Ω be an exponentially stable periodic orbit of $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ with basin of attraction $A(\Omega)$.

Let $B \in C^{\sigma}(\mathbb{R}^n, \mathbb{S}^{n \times n})$ such that $B(\mathbf{x})$ is a positive definite matrix for all $\mathbf{x} \in \mathbb{R}^n$ and let $C(\mathbf{x}) = P_{\mathbf{x}}^T B(\mathbf{x}) P_{\mathbf{x}}$.

Let $M \in C^{\sigma}(\mathcal{A}(\Omega), \mathbb{S}^{n \times n})$ be the solution of (2.7) and (2.8). Let $\mathcal{O} \subset \mathcal{A}(\Omega)$ be a bounded domain with Lipschitz boundary. Finally, let S be the optimal recovery from Theorem 3.3. Then there exists a $\beta > 0$ such that we have the error estimates

$$\|LM - LS\|_{L_{\infty}(\mathcal{O};\mathbb{S}^{n\times n})} \leq \beta h_{X,\mathcal{O}}^{\sigma-1-n/2} \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})},$$

$$|\partial_{i}LM - \partial_{i}LS\|_{L_{\infty}(\mathcal{O};\mathbb{S}^{n\times n})} \leq \beta h_{X,\mathcal{O}}^{\sigma-2-n/2} \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})},$$
(3.4)

for i = 1, 2, ..., n and all $X \subset \mathcal{O}$ with sufficiently small fill distance $h_{X,\mathcal{O}}$.

By construction we have

$$\mathbf{f}(\mathbf{x}_0)^T S(\mathbf{x}_0) \mathbf{f}(\mathbf{x}_0) = c_0 \|\mathbf{f}(\mathbf{x}_0)\|_2^4.$$

Let $K \ni \mathbf{x}_0$ be a compact set such that $\overline{\gamma^+(K)} \subset \mathcal{O}$. Then S, provided $h_{X,\mathcal{O}}$ is sufficiently small, is a Riemannian metric contracting in $\overline{\gamma^+(K)}$, i.e. $S(\mathbf{x})$ is positive definite for all $\mathbf{x} \in \mathcal{O}$ and $L_S(\mathbf{x}) \leq -\tilde{\nu} < 0$ for all $\mathbf{x} \in \overline{\gamma^+(K)}$.

While this theorem provides a proof that S is a contraction metric if $h_{X,\mathcal{O}}$ is small enough, it does not quantify in a useful way how small $h_{X,\mathcal{O}}$ must be because $||M||_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}$ is in general unknown, cf. (3.4). This is why we need a verification method that allows us to check whether S is a contraction metric or whether we need to make $h_{X,\mathcal{O}}$ smaller. This is the topic of Section 4.

3.5 Remark It is worth mentioning another useful norm estimate for $S \in H^{\sigma}(\mathcal{O}; \mathbb{S}^{n \times n})$, the optimal recovery of M from Theorem 3.3. Assume $\mathcal{O} \subset \mathbb{R}^n$ is bounded and open with C^1 boundary. Let $k \geq 2$ if n is odd and $k \geq 3$ if n is even. Let S be the optimal recovery of M using the collocation points $X \subset \mathcal{O}$ and the Wendland function $\psi_{l,k}$ with $l = \lfloor \frac{n}{2} \rfloor + k + 1$. Note that with $\sigma = k + \frac{n+1}{2}$ and for a constant $\zeta > 0$ independent of the collocation points X we have

$$\|S\|_{C^2(\overline{\mathcal{O}};\mathbb{S}^{n\times n})} \le \zeta \,\|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})} \,. \tag{3.5}$$

This inequality is proved using that the optimal recovery S is norm-minimal, that is, $\|S\|_{H^{\sigma}(\mathcal{O}:\mathbb{S}^{n\times n})} \leq \|M\|_{H^{\sigma}(\mathcal{O}:\mathbb{S}^{n\times n})}$; for more details see [7, Lemma 3.8].

4 CPA Interpolation of the Solution

In this section we set the stage for a verification process, through which we will verify the conditions of a computed contraction metric P, in particular that $P(\mathbf{x})$ is positive definite

and $L_P(\mathbf{x})$ is negative definite for all \mathbf{x} (see Theorem 4.11). In order to do so, we introduce a continuous piecewise affine (CPA) approximation of the RBF approximation metric. We will provide error estimates and statements about the interpolation, and present criteria that assert that the interpolation is a contraction metric itself. These criteria can easily be verified numerically.

Let us review some basic preliminaries. Given vectors $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n \in \mathbb{R}^n$ that are affinely independent, i.e. the vectors $\mathbf{x}_1 - \mathbf{x}_0, \mathbf{x}_2 - \mathbf{x}_0, \ldots, \mathbf{x}_n - \mathbf{x}_0$ are linearly independent, the convex hull

$$\mathfrak{S} = \operatorname{co}(\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_n) := \left\{ \sum_{k=0}^n \lambda_k \mathbf{x}_k : \lambda_k \in [0, 1] \text{ and } \sum_{k=0}^n \lambda_k = 1 \right\}$$

is called an n-simplex or simply a simplex. A set

$$\operatorname{co}(\mathbf{x}_{k_0}, \mathbf{x}_{k_1}, \dots, \mathbf{x}_{k_j}) := \left\{ \sum_{i=0}^j \lambda_{k_i} \mathbf{x}_{k_i} : \lambda_{k_i} \in [0, 1] \text{ and } \sum_{i=0}^j \lambda_{k_i} = 1 \right\}$$

with $0 \le k_0 < k_1 < \ldots < k_j \le n$ and $0 \le j < n$ is called a *j*-face of the simplex \mathfrak{S} .

4.1 Definition (Triangulation) We call a set $\mathcal{T} = \{\mathfrak{S}_{\nu}\}_{\nu}$ of *n*-simplices \mathfrak{S}_{ν} a triangulation in \mathbb{R}^{n} , if two simplices $\mathfrak{S}_{\nu}, \mathfrak{S}_{\mu} \in \mathcal{T}, \ \mu \neq \nu$, intersect in a common face or not at all. For a triangulation \mathcal{T} we define its domain and vertex set as

$$\mathcal{D}_{\mathcal{T}} := \bigcup_{\mathfrak{S}_{\nu} \in \mathcal{T}} \mathfrak{S}_{\nu} \text{ and } \mathcal{V}_{\mathcal{T}} := \{ \mathbf{x} \in \mathbb{R}^n : \mathbf{x} \text{ is a vertex of a simplex in } \mathcal{T} \}.$$

We also say that \mathcal{T} is a triangulation of the set $\mathcal{D}_{\mathcal{T}}$ and we call the triangulation finite if the set \mathcal{T} is finite.

For a triangulation $\mathcal{T} = \{\mathfrak{S}_{\nu}\}_{\nu}$ and constants h, d > 0, we say that \mathcal{T} is (h, d)-bounded if it fulfills the following conditions:

(i) The diameter of every simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ is bounded by h, that is

$$h_{\nu} := diam(\mathfrak{S}_{\nu}) := \max_{\mathbf{x}, \mathbf{y} \in \mathfrak{S}_{\nu}} \|\mathbf{x} - \mathbf{y}\|_2 < h.$$

(ii) The degeneracy of every simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ is bounded by d in the sense that

$$h_{\nu} \| X_{\nu}^{-1} \|_{1} \le d,$$

where $X_{\nu} := (\mathbf{x}_1^{\nu} - \mathbf{x}_0^{\nu}, \mathbf{x}_2^{\nu} - \mathbf{x}_0^{\nu}, \cdots, \mathbf{x}_n^{\nu} - \mathbf{x}_0^{\nu})^T$ is the so-called shape matrix of the simplex \mathfrak{S}_{ν} .

Note that we defined a simplex as the convex hull of an ordered set of vectors and the constant d > 0 in the definition above depends on the order of the vertices of the simplices in \mathcal{T} .

Given a triangulation, we can now define a continuous piecewise affine function, which is affine on each simplex of the triangulation. In particular, we can interpolate a given function by a CPA function by fixing its values at the vertices. **4.2 Definition (CPA function, CPA interpolation)** Let \mathcal{T} be a triangulation in \mathbb{R}^n and assume some values $\widetilde{P}_{ij}(\mathbf{x}_k) \in \mathbb{R}$ are fixed for every $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$ and every i, j = 1, 2, ..., n. A CPA function $P : \mathcal{D}_{\mathcal{T}} \to \mathbb{R}^{n \times n}$, that is affine on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$, is uniquely defined by its values at the vertices $\widetilde{P}(\mathbf{x}_k)$ in the following way:

An $\mathbf{x} \in \mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \dots, \mathbf{x}_n)$ can be written uniquely as $\mathbf{x} = \sum_{k=0}^n \lambda_k \mathbf{x}_k$ with $\lambda_k \in [0, 1]$ and $\sum_{k=0}^n \lambda_k = 1$ and we define

$$P_{ij}(\mathbf{x}) := \sum_{k=0}^{n} \lambda_k \widetilde{P}_{ij}(\mathbf{x}_k)$$

and

$$P(\mathbf{x}) := \begin{pmatrix} P_{11}(\mathbf{x}) & P_{12}(\mathbf{x}) & \cdots & P_{1n}(\mathbf{x}) \\ P_{21}(\mathbf{x}) & P_{22}(\mathbf{x}) & \cdots & P_{2n}(\mathbf{x}) \\ \vdots & \vdots & \ddots & \vdots \\ P_{n1}(\mathbf{x}) & P_{n2}(\mathbf{x}) & \cdots & P_{nn}(\mathbf{x}) \end{pmatrix}.$$

We refer to the functions P_{ij} and P as the CPA interpolations of the values $\tilde{P}_{ij}(\mathbf{x}_k)$ and $\tilde{P}(\mathbf{x}_k) = (\tilde{P}_{ij}(\mathbf{x}_k))_{i,j=1,\dots,n}$, respectively. Note that the functions P_{ij} are affine on every simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$, i.e. there is a vector $\mathbf{w}_{ij}^{\nu} \in \mathbb{R}^n$ and a number $b_{ij}^{\nu} \in \mathbb{R}$, such that

$$P_{ij}(\mathbf{x}) = (\mathbf{w}_{ij}^{\nu})^T \mathbf{x} + b_{ij}^{\nu}$$

for all $\mathbf{x} \in \mathfrak{S}_{\nu}$. For every simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ we define $\nabla P_{ij}^{\nu} := \nabla P_{ij}|_{\mathfrak{S}_{\nu}^{\circ}} = \mathbf{w}_{ij}^{\nu}$. Assume W is a matrix-valued function defined on $\mathcal{D}_{\mathcal{T}}$, fix the values $\widetilde{P}(\mathbf{x}_k) = W(\mathbf{x}_k)$ for every vertex $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$, and continue the procedure mentioned above to create a continuous piecewise affine function P. Then we call P the CPA interpolation of the function W on \mathcal{T} . Note that if $\widetilde{P}(\mathbf{x}_k) \in \mathbb{S}^{n \times n}$ for all $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$, then $P(\mathbf{x}) \in \mathbb{S}^{n \times n}$ for all $\mathbf{x} \in \mathcal{D}_{\mathcal{T}}$.

The gradient ∇P_{ij}^{ν} can be computed directly from the values at the vertices, as explained in the following remark.

4.3 Remark The gradient ∇P_{ij}^{ν} of the affine function $P_{ij}|_{\mathfrak{S}_{\nu}^{\circ}}$ on the simplex $\mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \ldots, \mathbf{x}_n)$ is given by the expression

$$\nabla P_{ij}^{\nu} = X_{\nu}^{-1} \begin{pmatrix} P_{ij}(\mathbf{x}_1) - P_{ij}(\mathbf{x}_0) \\ \vdots \\ P_{ij}(\mathbf{x}_n) - P_{ij}(\mathbf{x}_0) \end{pmatrix} \in \mathbb{R}^n,$$
(4.1)

where $X_{\nu} = (\mathbf{x}_1 - \mathbf{x}_0, \mathbf{x}_2 - \mathbf{x}_0, \dots, \mathbf{x}_n - \mathbf{x}_0)^T \in \mathbb{R}^{n \times n}$ is the shape-matrix of the simplex \mathfrak{S}_{ν} .

4.4 Remark (Orbital derivative) Let $P(\mathbf{x})$ be as in Definition 4.2 and fix a point $\mathbf{x} \in \mathcal{D}^{\sim}_{\mathcal{T}}$. As shown in the proof of [6, Lemma 4.7], there exists a $\mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \ldots, \mathbf{x}_n) \in \mathcal{T}$ and a number $\theta^* > 0$ such that $\mathbf{x} + \theta \mathbf{f}(\mathbf{x}) \in \mathfrak{S}_{\nu}$ for all $\theta \in [0, \theta^*]$. Then the forward orbital derivative $(P_{ij})'_{+}(\mathbf{x})$ defined by formula (2.1) (see Remark 2.3), is given by

$$(P_{ij})'_{+}(\mathbf{x}) = \nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}),$$

where ∇P_{ij}^{ν} was defined in Definition 4.2.

Let us now review an error estimate for the CPA interpolation of a function.

4.5 Remark [8, Lemma 4.5] Let $\mathcal{T} = \{\mathfrak{S}_{\nu}\}$ be an (h, d)-bounded triangulation in \mathbb{R}^n and let $\mathcal{D} \supset \mathcal{D}_{\mathcal{T}}$ be an open set. Assume that $S \in C^2(\mathcal{D}; \mathbb{R}^{n \times n})$ with $\|S\|_{C^2(\mathcal{D}; \mathbb{R}^{n \times n})} < \infty$ and define

$$\gamma := 1 + \frac{dn^{3/2}}{2}.$$

Denote by S_C the CPA interpolation of S on \mathcal{T} . Then the following estimates hold true for all $1 \leq i, j \leq n$:

$$\|S_C(\mathbf{x}) - S(\mathbf{x})\|_2 \leq nh^2 \|S\|_{C^2(\mathcal{D}:\mathbb{R}^{n\times n})} \text{ for all } \mathbf{x} \in \mathcal{D}_{\mathcal{T}},$$

$$(4.2)$$

$$\|\nabla (S_C)_{ij}^{\nu} - \nabla S_{ij}(\mathbf{x})\|_1 \leq h\gamma \|S\|_{C^2(\mathcal{D};\mathbb{R}^{n\times n})} \text{ for all } \mathfrak{S}_{\nu} \in \mathcal{T} \text{ and all } \mathbf{x} \in \mathfrak{S}_{\nu}, \quad (4.3)$$

$$\|\nabla(S_C)_{ij}^{\nu}\|_1 \leq (1+h\gamma) \|S\|_{C^2(\mathcal{D}:\mathbb{R}^{n\times n})} \text{ for all } \mathfrak{S}_{\nu} \in \mathcal{T}.$$

$$(4.4)$$

The following lemma is essential to deal with the contraction condition, which involves the (n-1)-dimensional subspace of vectors **v** perpendicular to **f** (first statement). The lemma transforms the first statement, which is needed to show that the function $L_P(\mathbf{x})$ is negative, into a second statement, which is easier to handle, since it refers to the negative definiteness of a matrix.

4.6 Lemma (Evaluation method for contraction property) Let $n \ge 2$, $A \in \mathbb{S}^{n \times n}$ and $\mathbf{f} \in \mathbb{R}^n$, $\mathbf{f} \neq \mathbf{0}$. Then the two following statements are equivalent:

- 1. There exists a constant $\lambda > 0$ such that for every $\mathbf{v} \in \mathbb{R}^n$ with $\mathbf{v}^T \mathbf{f} = 0$ and $\|\mathbf{v}\|_2 = 1$ we have $\mathbf{v}^T A \mathbf{v} \leq -\lambda$.
- 2. There exists a constant $\kappa^* > 0$, such that for every $\kappa \ge \kappa^* > 0$ the matrix $A \kappa \mathbf{f} \mathbf{f}^T$ is negative definite.

Further, if $K \subset \mathbb{R}^n$ is compact, $\mathbf{f} : K \to \mathbb{R}^n$ and $A : K \to \mathbb{S}^{n \times n}$ are continuous, and there exists a constant $\lambda > 0$ such that for every $\mathbf{x} \in K$ and every $\mathbf{v} \in \mathbb{R}^n$, $\mathbf{v}^T \mathbf{f}(\mathbf{x}) = 0$, we have $\mathbf{v}^T A(\mathbf{x}) \mathbf{v} \leq -\lambda$, then there exists a constant $\kappa^* > 0$ such that for every $\kappa \geq \kappa^* > 0$ the matrix $A(\mathbf{x}) - \kappa \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^T$ is negative definite for every $\mathbf{x} \in K$.

Proof: Statement 1 follows immediately from Statement 2 with

$$\lambda = -\lambda_{\max}(A - \kappa^* \mathbf{f} \, \mathbf{f}^T) > 0. \tag{4.5}$$

Assume that statement 1 holds true; note that this implies $||A||_2 > 0$. Define $t^* \in [0, \pi/2)$ and κ^* by

$$t^* = \arccos\left(\min\left(1, \frac{\lambda}{4\|A\|_2}\right)\right), \tag{4.6}$$

$$\kappa^* = \frac{\frac{2 \|A\|_2}{\lambda} \sqrt{\max(0, 16 \|A\|_2^2 - \lambda^2) + \|A\|_2 + \lambda}}{\|\mathbf{f}\|_2^2}.$$
(4.7)

We have

$$\tan t^* = \sqrt{1/\cos^2 t^* - 1} = \sqrt{\max\left(1, \frac{16\|A\|_2^2}{\lambda^2}\right) - 1} = \frac{\kappa^* \|\mathbf{f}\|_2^2 - \|A\|_2 - \lambda}{2\|A\|_2}.$$
(4.8)

Let $\mathbf{u} \in \mathbb{R}^n$, $\|\mathbf{u}\|_2 = 1$, be arbitrary. Then, we can write $\mathbf{u} = \tilde{\mathbf{v}} + \tilde{\mathbf{f}}$ with $\tilde{\mathbf{f}} := (\mathbf{u}^T \mathbf{f} / \|\mathbf{f}\|_2^2) \mathbf{f}$ and $\tilde{\mathbf{v}} = \mathbf{u} - \tilde{\mathbf{f}}$. In particular, $\tilde{\mathbf{f}}$ is parallel to \mathbf{f} and $\tilde{\mathbf{v}}^T \mathbf{f} = 0$. Further, $\|\tilde{\mathbf{v}}\|_2^2 + \|\tilde{\mathbf{f}}\|_2^2 = 1$. Let $t \in [0, \pi/2]$ be such that $\|\tilde{\mathbf{v}}\|_2 = \sin t$ and $\|\tilde{\mathbf{f}}\|_2 = \cos t$. By Statement 1 it follows that

$$\mathbf{u}^{T}(A - \kappa^{*}\mathbf{f}\,\mathbf{f}^{T})\mathbf{u} = (\tilde{\mathbf{v}} + \tilde{\mathbf{f}})^{T}(A - \kappa^{*}\mathbf{f}\,\mathbf{f}^{T})(\tilde{\mathbf{v}} + \tilde{\mathbf{f}})
= \tilde{\mathbf{v}}^{T}A\tilde{\mathbf{v}} + 2\tilde{\mathbf{f}}^{T}A\tilde{\mathbf{v}} + \tilde{\mathbf{f}}^{T}A\tilde{\mathbf{f}} - \kappa^{*}(\mathbf{f}^{T}\tilde{\mathbf{f}})^{2}
\leq -\lambda\sin^{2}t + 2\|A\|_{2}\cos t\sin t + (\|A\|_{2} - \kappa^{*}\|\mathbf{f}\|_{2}^{2})\cos^{2}t \qquad (4.9)
= -\lambda + 2\|A\|_{2}\cos t\sin t + (\|A\|_{2} + \lambda - \kappa^{*}\|\mathbf{f}\|_{2}^{2})\cos^{2}t
= -\lambda + 2\|A\|_{2}\cos t\cdot \left(\sin t + \frac{\|A\|_{2} + \lambda - \kappa^{*}\|\mathbf{f}\|_{2}^{2}}{2\|A\|_{2}}\cos t\right)
= -\lambda + 2\|A\|_{2}\cos t\cdot (\sin t - \tan t^{*}\cos t) \ \text{by} \ (4.8) \qquad (4.10)
=: g(t).$$

From (4.9) one sees that g(t) only becomes smaller on $t \in [0, \pi/2]$ if κ^* is replaced by a larger number, hence, it suffices to show that g(t) < 0 for $t \in [0, \pi/2]$ to prove statement 2. First note that by (4.9) and (4.8)

$$g(0) = ||A||_2 - \kappa^* ||\mathbf{f}||_2^2 < ||A||_2 + \lambda - \kappa^* ||\mathbf{f}||_2^2 = -2||A||_2 \tan t^* \le 0$$

and $g(\pi/2) = -\lambda < 0$.

If $t^* > 0$, we have $g(t) \leq -\lambda$ for $t \in (0, t^*)$ by (4.10) because $\cos t > 0$ and $\tan t < \tan t^*$, i.e.

 $\sin t - \tan t^* \cos t = \cos t \left(\tan t - \tan t^* \right) < 0.$

For the case $t \in [t^*, \pi/2)$ note that

$$\sin t - \tan t^* \cos t < 1 - \tan t^* \cos t < 1$$

and we have by (4.10) and (4.6)

$$g(t) = -\lambda + 2 ||A||_2 \cos t \cdot (\sin t - \tan t^* \cos t) < -\lambda + 2 ||A||_2 \cos t \le -\lambda + 2 ||A||_2 \cos t^* \le -\lambda + 2 ||A||_2 \frac{\lambda}{4 ||A||_2} = -\frac{\lambda}{2}.$$

Since **u** was arbitrary $\lambda_{\max}(A - \kappa^* \mathbf{f} \mathbf{f}^T) < 0$ and Statement 2 follows.

For the last proposition just note that the right-hand side of (4.7) depends continuously on A and \mathbf{f} and that $\min_{\mathbf{x}\in K} \|\mathbf{f}(\mathbf{x})\|_2 > 0$. Hence

$$\kappa^* := \max_{\mathbf{x} \in K} \frac{\frac{2 \|A(\mathbf{x})\|_2}{\lambda} \sqrt{\max(0, 16 \|A(\mathbf{x})\|_2^2 - \lambda^2)} + \|A(\mathbf{x})\|_2 + \lambda}{\|\mathbf{f}(\mathbf{x})\|_2^2} > 0$$

is well defined and

$$\mathbf{u}^T (A(\mathbf{x}) - \kappa \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^T) \mathbf{u} < 0$$

for every $\mathbf{u} \in \mathbb{R}^n$, with $\|\mathbf{u}\|_2 = 1$, and $\kappa \ge \kappa^*$ can be proved analogously to above.

We have now provided the essential ingredients to state our verification process as a verification problem with constants, input data, and constraints described as follows.

4.1 Verification Problem

Our verification problem is a semidefinite feasibility problem and can in theory be solved as such. However, as we will assign values to the variables of the problem using the optimal recovery of the solution of (2.7) and (2.8) and then verify if the constraints of the feasibility problem are fulfilled, we will refer to this feasibility problem as *verification problem*. Note that it is much more efficient to verify the validity of a possible solution to a semidefinite problem than to solve it.

4.7 Verification Problem Given is a system $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$, $\mathbf{f} \in C^3(\mathbb{R}^n; \mathbb{R}^n)$, and a finite triangulation \mathcal{T} of $\mathcal{D}_{\mathcal{T}} \subset \mathbb{R}^n$ such that $\mathbf{f}(\mathbf{x}) \neq \mathbf{0}$ for all $\mathbf{x} \in \mathcal{D}_{\mathcal{T}}$. The verification problem has the following constants, variables, and constraints.

Constants: The constants used in the problem are listed below. The first constant is a fixed, chosen parameter, the rest are computed from the input data.

- 1. $\kappa_{\nu}^* > 0$ quantities related to the matrices $A_{\nu}(\mathbf{x}_k)$ (as defined in (4.17) below) on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$.
- 2. The diameter h_{ν} of each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$h_{\nu} := \operatorname{diam}(\mathfrak{S}_{\nu}) = \max_{\mathbf{x}, \mathbf{y} \in \mathfrak{S}_{\nu}} \|\mathbf{x} - \mathbf{y}\|_{2}.$$

3. Upper bounds $B_{0,\nu}$ on the components f_l of \mathbf{f} on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$B_{0,\nu} \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}_{\nu}\\l=1,2,\dots,n}} |f_l(\mathbf{x})|.$$
(4.11)

4. Upper bounds $B_{1,\nu}$ on the first-order derivatives of the components f_l of \mathbf{f} on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$B_{1,\nu} \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}\nu\\i,l=1,2,\dots,n}} \left|\frac{\partial f_l}{\partial x_i}(\mathbf{x})\right|.$$
(4.12)

5. Upper bounds $B_{2,\nu}$ on the second-order derivatives of the components f_l of \mathbf{f} on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$B_{2,\nu} \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}_{\nu}\\i,j,l=1,2,\dots,n}} \left| \frac{\partial^2 f_l}{\partial x_i \partial x_j}(\mathbf{x}) \right|.$$
(4.13)

6. Upper bounds $B_{3,\nu}$ on the third-order derivatives of the components f_l of \mathbf{f} on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$B_{3,\nu} \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}\nu\\i,j,k,l=1,\dots,n}} \left| \frac{\partial^3 f_l}{\partial x_i \partial x_j \partial x_k}(\mathbf{x}) \right|.$$
(4.14)

7. Upper bounds $B_{V_{1,\nu}}$ on the first-order derivatives of the components V_{lj} of V defined in (2.2) on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$B_{V_{1,\nu}} \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}_{\nu}\\r,l,j=1,2,\dots,n}} \left|\frac{\partial V_{lj}}{\partial x_r}(\mathbf{x})\right|.$$
(4.15)

8. Upper bounds $B_{V_{2,\nu}}$ on the second-order derivatives of the components V_{lj} of V defined in (2.2) on each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$:

$$B_{V_{2,\nu}} \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}_{\nu}\\r,s,j,l=1,2,\dots,n}} \left| \frac{\partial^2 V_{lj}}{\partial x_r \partial x_s}(\mathbf{x}) \right|.$$
(4.16)

Input data: The input data of the problem are

1. $P_{ij}(\mathbf{x}_k) \in \mathbb{R}$ for all $1 \le i \le j \le n$ and all vertices $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$. For $1 \le i \le j \le n$ the value $P_{ij}(\mathbf{x}_k)$ is the (i, j)-th entry of the $(n \times n)$ matrix $P(\mathbf{x}_k)$. The matrix $P(\mathbf{x}_k)$ is assumed to be symmetric and therefore these components determine it.

Constraints:

(VP1) Positive definiteness of P

For each $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$:

$$P(\mathbf{x}_k) \succ 0_{n,n}$$

(VP2) Negative definiteness of $A_{\nu} - \kappa_{\nu}^* \mathbf{f} \mathbf{f}^T$

For each simplex $\mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \dots, \mathbf{x}_n) \in \mathcal{T}$ and each vertex \mathbf{x}_k of \mathfrak{S}_{ν} :

$$A_{\nu}(\mathbf{x}_k) - \kappa_{\nu}^* \mathbf{f}(\mathbf{x}_k) \mathbf{f}^T(\mathbf{x}_k) + h_{\nu}^2 E_{\nu} I_{n \times n} \prec \mathbf{0}_{n,n}$$

Here

$$A_{\nu}(\mathbf{x}_k) := P(\mathbf{x}_k)V(\mathbf{x}_k) + V(\mathbf{x}_k)^T P(\mathbf{x}_k) + \left(\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}_k)\right)_{i,j=1,2,\dots,n},$$
(4.17)

where V is the function defined in (2.2), $(\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}_k))_{i,j=1,2,...,n}$ denotes the symmetric $(n \times n)$ -matrix with entries $\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}_k)$ and ∇P_{ij}^{ν} is defined as in (4.1), and

$$E_{\nu} := n^2 \cdot \left((4\sqrt{n}B_{V_{1,\nu}} + B_{2,\nu}) \|\nabla P_{ij}^{\nu}\|_1 + 2nB_{V_{2,\nu}}P_{\nu} + 2\kappa_{\nu}^* B_{0,\nu}B_{2,\nu} + 2\kappa_{\nu}^* B_{1,\nu}^2 \right),$$

where

$$P_{\nu} := \max_{\mathbf{x} \in \mathfrak{S}_{\nu}} \|P(\mathbf{x})\|_2 = \max_{k=0,1,\dots,n} \|P(\mathbf{x}_k)\|_2.$$

4.8 Remark In order to implement the Verification Problem, one can formulate an equivalent semidefinite feasibility problem: fix a small constant $\epsilon_0 > 0$ and replace $\succ 0_{n,n}$ by $\succeq \epsilon_0 I_{n \times n}$ in (VP1) and $\prec 0_{n,n}$ by $\preceq \epsilon_0 I_{n \times n}$ in (VP2). Further, introduce auxiliary variables $C_{\nu}, D_{\nu}^k, D_{\nu} \in \mathbb{R}_0^+$, with $1 \le k \le n$, for all simplices $\mathfrak{S}_{\nu} \in \mathcal{T}$, that serve as upper bounds on the eigenvalues of P and on the derivative of all P_{ij} in \mathfrak{S}_{ν} , respectively. The upper bounds can then be implemented through the following constraints:

1. For each simplex $\mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \dots, \mathbf{x}_n) \in \mathcal{T}$ and each vertex \mathbf{x}_k of \mathfrak{S}_{ν} we must have:

 $P(\mathbf{x}_k) \preceq C_{\nu} I_{n \times n}.$

This makes sure that $P_{\nu} = \max_{k=0,1,\dots,n} \|P(\mathbf{x}_k)\|_2 \le C_{\nu}.$

2. For each simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ and all $1 \leq i \leq j \leq n$ and $1 \leq k \leq n$ we must have:

$$-D_{\nu}^{k} \leq \left[\nabla P_{ij}^{\nu}\right]_{k} \leq D_{\nu}^{k},$$

where $\left[\nabla P_{ij}^{\nu}\right]_{k}$ is the *k*th component of the gradient ∇P_{ij}^{ν} . This ensures that $\|\nabla P_{ij}^{\nu}\|_{1} \leq D_{\nu} := \sum_{k=1}^{n} D_{\nu}^{k}$.

3. Finally, the constant E_{ν} for each simplex in (VP2) is replaced by

$$E_{\nu} := n^2 \cdot \left((4\sqrt{n}B_{V_{1,\nu}} + B_{2,\nu})D_{\nu} + 2nB_{V_{2,\nu}}C_{\nu} + 2\kappa_{\nu}^* B_{0,\nu}B_{2,\nu} + 2\kappa_{\nu}^* B_{1,\nu}^2 \right).$$
(4.18)

Clearly a feasible solution to this semidefinite feasibility problem also fulfills the constraints of the Verification Problem 4.7. Further, it is not difficult to see that if a CPA function $P: \mathcal{D}_{\mathcal{T}} \to \mathbb{S}^{n \times n}$ fulfills the constraints of Verification Problem 4.7, then αP is a feasible solution to the semidefinite feasibility problem if $\alpha > 0$ is large enough; just note that C_{ν} , D_{ν} , and A_{ν} scale linearly with α and thus the conditions are satisfied if we replace κ_{ν}^* by $\alpha \kappa_{\nu}^*$.

We seek to show that a CPA function satisfying the Verification Problem 4.7 is a contraction metric in Theorem 4.11. This is based on estimates between a function and its CPA interpolation.

4.9 Remark (Function estimates over a triangulation) Let $\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_k \in \mathbb{R}^n$ be affinely independent vectors, define $\mathfrak{S} := \operatorname{co}(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_k)$, $h := \operatorname{diam}(\mathfrak{S})$ and consider a convex combination $\sum_{i=0}^k \lambda_i \mathbf{x}_i \in \mathfrak{S}$. If $g \in C^2(\mathcal{U}, \mathbb{R})$ with $\mathfrak{S} \subset \mathcal{U} \subset \mathbb{R}^n$, \mathcal{U} open, then

$$\left| g\left(\sum_{i=0}^{k} \lambda_i \mathbf{x}_i\right) - \sum_{i=0}^{k} \lambda_i g(\mathbf{x}_i) \right| \le B_H h^2, \tag{4.19}$$

where $B_H := \max_{\mathbf{z} \in \mathfrak{S}} ||H(\mathbf{z})||_2$ and $H(\mathbf{z})$ is the Hessian of g at \mathbf{z} , see [1, Proposition 4.1]. A similar result holds for a function $\mathbf{h} \in C^2(\mathbb{R}^n; \mathbb{R}^n)$, cf. [11, Lemma 4.8],

$$\left\| \mathbf{h}(\mathbf{x}) - \sum_{k=0}^{n} \lambda_k \mathbf{h}(\mathbf{x}_k) \right\|_{\infty} \le n B_2 h^2,$$

where B_2 is an upper bound on the second order derivatives of the components of **h**,

$$B_2 \ge \max_{\substack{\mathbf{x}\in\mathfrak{S}\\i,j,l=1,2,\dots,n}} \left| \frac{\partial^2 h_l}{\partial x_i \partial x_j}(\mathbf{x}) \right|$$

The following lemma will provide an estimate on the difference between the true value of the mapping A of Verification Problem 4.7 (VP2) and the value approximated by a convex combination of its values at vertices.

4.10 Lemma (Operator estimate over a triangulation) Assume P is defined as in Definition 4.2 from a feasible solution $P_{ij}(\mathbf{x}_k)$ to the Verification Problem 4.7. Fix a point $\mathbf{x} \in \mathcal{D}^{\circ}_{\mathcal{T}}$ and a corresponding simplex $\mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \mathbf{x}_1, \ldots, \mathbf{x}_n) \in \mathcal{T}$ with $\mathbf{x} \in \mathfrak{S}_{\nu}$. Set

$$A_{\nu}(\mathbf{y}) := P(\mathbf{y})V(\mathbf{y}) + V(\mathbf{y})^{T}P(\mathbf{y}) + \left(\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{y})\right)_{i,j=1,2,\dots,n}$$

for all $\mathbf{y} \in \mathfrak{S}_{\nu}$.

Then we have the following estimate with fixed $\kappa_{\nu}^* > 0$, for any $\mathbf{x} = \sum_{k=0}^n \lambda_k \mathbf{x}_k \in \mathfrak{S}_{\nu}, \lambda_k \ge 0$ and $\sum_{k=0}^n \lambda_k = 1$:

$$\left\| \left[A_{\nu}(\mathbf{x}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^{T} \right] - \sum_{k=0}^{n} \lambda_{k} \left[A_{\nu}(\mathbf{x}_{k}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}_{k}) \mathbf{f}(\mathbf{x}_{k})^{T} \right] \right\|_{2} \le h_{\nu}^{2} E_{\nu},$$
(4.20)

in particular

$$A_{\nu}(\mathbf{x}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^{T} \leq \sum_{k=0}^{n} \lambda_{k} \left[A_{\nu}(\mathbf{x}_{k}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}_{k}) \mathbf{f}(\mathbf{x}_{k})^{T} \right] + h_{\nu}^{2} E_{\nu} I_{n \times n},$$

where $E_{\nu} = n^2 \cdot \left(4\sqrt{n}B_{V_{1,\nu}} \|\nabla P_{ij}^{\nu}\|_1 + 2nB_{V_{2,\nu}}P_{\nu} + B_{2,\nu} \|\nabla P_{ij}^{\nu}\|_1 + 2\kappa_{\nu}^* B_{0,\nu}B_{2,\nu} + 2\kappa_{\nu}^* B_{1,\nu}^2 \right)$ is defined as in (VP2).

Proof: We show this in several steps:

Step 1: Entry-wise bounds on $\mathbf{P}'_+(\mathbf{x})$ The estimate

$$\left|\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}) - \sum_{k=0}^{n} \lambda_k \nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}_k)\right| \le n B_{2,\nu} \|\nabla P_{ij}^{\nu}\|_1 h_{\nu}^2 \tag{4.21}$$

follows by Hölder's inequality and Remark 4.9:

$$\left|\nabla P_{ij}^{\nu} \cdot \left(\mathbf{f}(\mathbf{x}) - \sum_{k=0}^{n} \lambda_k \mathbf{f}(\mathbf{x}_k)\right)\right| \le \|\nabla P_{ij}^{\nu}\|_1 \left\|\mathbf{f}(\mathbf{x}) - \sum_{k=0}^{n} \lambda_k \mathbf{f}(\mathbf{x}_k)\right\|_{\infty} \le \|\nabla P_{ij}^{\nu}\|_1 n B_{2,\nu} h_{\nu}^2.$$

Step 2: Entry-wise bounds on $\mathbf{P}(\mathbf{x})\mathbf{V}(\mathbf{x})$ and $\mathbf{V}(\mathbf{x})^{T}\mathbf{P}(\mathbf{x})$ We show that

$$\left| [P(\mathbf{x})V(\mathbf{x})]_{ij} - \sum_{k=0}^{n} \lambda_k \left[P(\mathbf{x}_k)V(\mathbf{x}_k) \right]_{ij} \right| \le nh_{\nu}^2 (2\sqrt{n}B_{V_{1,\nu}} \|\nabla P_{ij}^{\nu}\|_1 + nB_{V_{2,\nu}}P_{\nu}).$$
(4.22)

Consider two scalar-valued functions $g, h \in C^2(\mathfrak{S}_{\nu}; \mathbb{R})$. We apply Remark 4.9 to gh, yielding

$$\left| g(\mathbf{x})h(\mathbf{x}) - \sum_{k=0}^{n} \lambda_k g(\mathbf{x}_k)h(\mathbf{x}_k) \right| \le \max_{\mathbf{y}\in\mathfrak{S}_{\nu}} \|H(\mathbf{y})\|_2 h_{\nu}^2, \tag{4.23}$$

where the matrix $H(\mathbf{y})$ is defined by $[H(\mathbf{y})]_{rs} := \frac{\partial^2(gh)}{\partial x_r \partial x_s}(\mathbf{y})$. Set $g(\mathbf{y}) := P_{il}(\mathbf{y})$. Since $P_{il}(\mathbf{y}) = \nabla P_{il}^{\nu} \cdot \mathbf{y} + b_{il}^{\nu}$, we obtain $\frac{\partial g}{\partial x_s}(\mathbf{y}) = [\nabla P_{il}^{\nu}]_s$ and $\frac{\partial^2 g}{\partial x_r \partial x_s}(\mathbf{y}) = 0$ for all $\mathbf{y} \in \mathfrak{S}_{\nu}$. Hence,

$$\frac{\partial}{\partial x_s}(gh)(\mathbf{y}) = \frac{\partial g}{\partial x_s}(\mathbf{y})h(\mathbf{y}) + g(\mathbf{y})\frac{\partial h}{\partial x_s}(\mathbf{y}) = [\nabla P_{il}^{\nu}]_sh(\mathbf{y}) + g(\mathbf{y})\frac{\partial h}{\partial x_s}(\mathbf{y})$$

and then

$$\frac{\partial^2}{\partial x_r \partial x_s} (gh)(\mathbf{y}) = [\nabla P_{il}^{\nu}]_s \frac{\partial h}{\partial x_r}(\mathbf{y}) + \frac{\partial g}{\partial x_r}(\mathbf{y}) \frac{\partial h}{\partial x_s}(\mathbf{y}) + g(\mathbf{y}) \frac{\partial^2 h}{\partial x_r \partial x_s}(\mathbf{y})$$
$$= [\nabla P_{il}^{\nu}]_s \frac{\partial h}{\partial x_r}(\mathbf{y}) + [\nabla P_{il}^{\nu}]_r \frac{\partial h}{\partial x_s}(\mathbf{y}) + P_{il}(\mathbf{y}) \frac{\partial^2 h}{\partial x_r \partial x_s}(\mathbf{y}).$$

Now set $h(\mathbf{y}) := V_{lj}(\mathbf{y})$, then $\left|\frac{\partial h}{\partial x_s}(\mathbf{y})\right| \le B_{V_{1,\nu}}$, and $\left|\frac{\partial^2 h}{\partial x_r \partial x_s}(\mathbf{y})\right| \le B_{V_{2,\nu}}$. Thus

$$|[H(\mathbf{y})]_{rs}| = \left|\frac{\partial^2(gh)}{\partial x_r \partial x_s}(\mathbf{y})\right| \le |[\nabla P_{il}^{\nu}]_s|B_{V_{1,\nu}} + |[\nabla P_{il}^{\nu}]_r|B_{V_{1,\nu}} + |P_{il}(\mathbf{y})|B_{V_{2,\nu}}.$$

Using in succession for any $H_1, H_2, H_3 \in \mathbb{R}^{n \times n}$ that

$$||H_1 + H_2 + H_3||_2 \le ||H_1||_2 + ||H_2||_2 + ||H_3||_2$$

and

$$||H_2||_2 \le \sqrt{n} ||H_2||_1, ||H_1||_2 \le \sqrt{n} ||H_1||_{\infty}, \text{ and } ||H_3||_2 \le n ||H_3||_{\max}$$

this delivers

$$\begin{aligned} \|H(\mathbf{y})\|_{2} &\leq \sqrt{n} \|\nabla P_{il}^{\nu}\|_{1} B_{V_{1,\nu}} + \sqrt{n} \|\nabla P_{il}^{\nu}\|_{1} B_{V_{1,\nu}} + n B_{V_{2,\nu}} \max_{\mathbf{x} \in \mathfrak{S}_{\nu}} \max_{1 \leq i \leq l \leq n} |P_{il}(\mathbf{x})| \\ &\leq 2\sqrt{n} B_{V_{1,\nu}} \|\nabla P_{ij}^{\nu}\|_{1} + n B_{V_{2,\nu}} P_{\nu}, \end{aligned}$$

$$(4.24)$$

for all $\mathbf{y} \in \mathfrak{S}_{\nu}$, because we have $|P_{il}(\mathbf{y})| \leq ||P(\mathbf{y})||_2 \leq P_{\nu}$. Hence, (4.23) and (4.24) establish

$$\begin{aligned} \left| [P(\mathbf{x})V(\mathbf{x})]_{ij} - \sum_{k=0}^{n} \lambda_k [P(\mathbf{x}_k)V(\mathbf{x}_k)]_{ij} \right| \\ &= \left| \sum_{l=1}^{n} P_{il}(\mathbf{x})V_{lj}(\mathbf{x}) - \sum_{l=1}^{n} \sum_{k=0}^{n} \lambda_k P_{il}(\mathbf{x}_k)V_{lj}(\mathbf{x}) \right| \\ &\leq \sum_{l=1}^{n} \left| P_{il}(\mathbf{x})V_{lj}(\mathbf{x}) - \sum_{k=0}^{n} \lambda_k P_{il}(\mathbf{x}_k)V_{lj}(\mathbf{x}) \right| \\ &\leq n \cdot (2\sqrt{n}B_{V_{1,\nu}} \|\nabla P_{ij}^{\nu}\|_1 + nB_{V_{2,\nu}}P_{\nu}) \cdot h_{\nu}^2. \end{aligned}$$

Step 3: Bounds on $f(x)f(x)^T$

Similarly to the previous steps, we obtain

$$\left| \left[\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x})^T - \sum_{k=0}^n \lambda_k \mathbf{f}(\mathbf{x}_k)\mathbf{f}(\mathbf{x}_k)^T \right]_{ij} \right| \le 2n \left(B_{0,\nu} B_{2,\nu} + B_{1,\nu}^2 \right) h_{\nu}^2.$$
(4.25)

In detail, consider the following

$$\left| \left[\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x})^T - \sum_{k=0}^n \lambda_k \mathbf{f}(\mathbf{x}_k)\mathbf{f}(\mathbf{x}_k)^T \right]_{ij} \right| = \left| f_i(\mathbf{x})f_j(\mathbf{x}) - \sum_{k=0}^n \lambda_k f_i(\mathbf{x}_k)f_j(\mathbf{x}_k) \right|.$$

Let $g(\mathbf{x}) = f_i(\mathbf{x})f_j(\mathbf{x})$, and apply Remark 4.9 to g to get

$$\begin{aligned} \frac{\partial g}{\partial x_s}(\mathbf{y}) &= \frac{\partial f_i(\mathbf{y})}{\partial x_s} f_j(\mathbf{y}) + f_i(\mathbf{y}) \frac{\partial f_j(\mathbf{y})}{\partial x_s}, \\ \frac{\partial^2 g}{\partial x_r \partial x_s}(\mathbf{y}) &= \frac{\partial^2 f_i}{\partial x_r \partial x_s}(\mathbf{y}) f_j(\mathbf{y}) + \frac{\partial f_i}{\partial x_s}(\mathbf{y}) \frac{\partial f_j}{\partial x_r}(\mathbf{y}) + \frac{\partial f_i}{\partial x_r}(\mathbf{y}) \frac{\partial f_j}{\partial x_s}(\mathbf{y}) + f_i(\mathbf{y}) \frac{\partial^2 f_j}{\partial x_r \partial x_s}(\mathbf{y}). \end{aligned}$$

Thus, we get $\left|\frac{\partial^2 g}{\partial x_r \partial x_s}(\mathbf{y})\right| \leq 2B_{0,\nu}B_{2,\nu} + 2B_{1,\nu}^2$.

Step 4: Bounds on matrices

From the definition of $A_{\nu}(\mathbf{y})$ we get

$$\begin{aligned} \left\| A_{\nu}(\mathbf{x}) - \sum_{k=0}^{n} \lambda_{k} A_{\nu}(\mathbf{x}_{k}) \right\|_{2} &\leq \left\| P(\mathbf{x}) V(\mathbf{x}) - \sum_{k=0}^{n} \lambda_{k} P(\mathbf{x}_{k}) V(\mathbf{x}_{k}) \right\|_{2} \\ &+ \left\| V(\mathbf{x})^{T} P(\mathbf{x}) - \sum_{k=0}^{n} \lambda_{k} V(\mathbf{x}_{k})^{T} P(\mathbf{x}_{k}) \right\|_{2} \\ &+ \left\| (\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}))_{i,j=1,\dots,n} - \sum_{k=0}^{n} \lambda_{k} (\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}_{k}))_{i,j=1,\dots,n} \right\|_{2}. \end{aligned}$$

The first two norms on the right-hand side are equal because P is symmetric and therefore the matrices in the norms are conjugate and $||B||_2 = ||B^T||_2$ for any matrix $B \in \mathbb{R}^{n \times n}$.

The entry-wise bounds (4.21), (4.22) and (4.25) together with $||H||_2 \leq n ||H||_{\text{max}}$ for any $H \in \mathbb{R}^{n \times n}$ now deliver (4.20).

Note that upper bounds on the auxiliary function V, cf. (2.2), can be obtained directly form the data of the problem, i.e. from **f**. The formulas are derived in Appendix A. However, these bounds are in general more conservative than when working directly with V.

We are now ready to prove the first main result, which shows that a CPA matrix-valued function which fulfills the constraints of Verification Problem 4.7 is a contraction metric.

4.11 Theorem (CPA contraction metric)

Let $\mathbf{f} \in C^3(\mathbb{R}^n, \mathbb{R}^n)$. Assume that the constraints of Verification Problem 4.7 are satisfied for some values $P_{ij}(\mathbf{x}_k)$. Then the matrix-valued function P, where $P(\mathbf{x})$ is interpolated from the values $P_{ij}(\mathbf{x}_k)$ as in Definition 4.2, is a Riemannian metric, contracting in any compact set $\widetilde{K} \subset \mathcal{D}^{\circ}_{\mathcal{T}}$. **Proof:** Let $\mathbf{x} \in \mathcal{D}_{\mathcal{T}}$ be an arbitrary point. Then there exists a $\mathfrak{S}_{\nu} = \operatorname{co}(\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_n) \in \mathcal{T}$ with $\mathbf{x} = \sum_{k=0}^n \lambda_k \mathbf{x}_k, \ \lambda_k \ge 0$ and $\sum_{k=0}^n \lambda_k = 1$. The symmetry of $P(\mathbf{x})$ follows directly from $P_{ij}(\mathbf{x}_k) = P_{ji}(\mathbf{x}_k)$ assumed in *Input Data 1*. of Verification Problem 4.7:

$$P_{ij}(\mathbf{x}) = P_{ij}\left(\sum_{k=0}^{n} \lambda_k \mathbf{x}_k\right) = \sum_{k=0}^{n} \lambda_k P_{ij}(\mathbf{x}_k) = \sum_{k=0}^{n} \lambda_k P_{ji}(\mathbf{x}_k) = P_{ji}(\mathbf{x}).$$

For positive definiteness, we have $P(\mathbf{x}_k) \succ 0_{n \times n}$ for each $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$ by (VP1), so

$$P(\mathbf{x}) = \sum_{k=0}^{n} \lambda_k P(\mathbf{x}_k) \succ \sum_{k=0}^{n} \lambda_k \, \mathbf{0}_{n,n} = \mathbf{0}_{n,n}.$$

Now let $\mathbf{x} \in \widetilde{K} \subset \mathcal{D}^{\circ}_{\mathcal{T}}$. Then there is a simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ with $\mathbf{x} \in \mathfrak{S}_{\nu}$ as well as $\mathbf{x} + \theta \mathbf{f}(\mathbf{x}) \in \mathfrak{S}_{\nu}$ for all $\theta \in [0, \theta^*]$ with $\theta^* > 0$. Then we have $(P'_+)_{ij}(\mathbf{x}) = \nabla P^{\nu}_{ij} \cdot \mathbf{f}(\mathbf{x})$, see Remark 4.4. Since (VP2) consists of finitely many constraints, there exists $\epsilon_0 > 0$ such that

$$A_{\nu}(\mathbf{x}_k) - \kappa_{\nu}^* \mathbf{f}(\mathbf{x}_k) \mathbf{f}(\mathbf{x}_k)^T + h_{\nu}^2 E_{\nu} I_{n \times n} \preceq -\epsilon_0 I_{n \times n}$$

for all $\mathfrak{S}_{\nu} \in \mathcal{T}$ and all \mathbf{x}_k of \mathfrak{S}_{ν} . Hence, for an arbitrary $\mathbf{z} \in \mathbb{R}^n$ we get from Lemma 4.10 that

$$\begin{aligned} \mathbf{z}^{T} \left(A_{\nu}(\mathbf{x}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^{T} \right) \mathbf{z} &\leq \mathbf{z}^{T} \left(\sum_{k=0}^{n} \lambda_{k} [A_{\nu}(\mathbf{x}_{k}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}_{k}) \mathbf{f}(\mathbf{x}_{k})^{T} + h_{\nu}^{2} E_{\nu} I_{n \times n}] \right) \mathbf{z} \\ &\leq -\epsilon_{0} \sum_{k=0}^{n} \lambda_{k} \| \mathbf{z} \|_{2}^{2} \\ &= -\epsilon_{0} \| \mathbf{z} \|_{2}^{2}, \end{aligned}$$

that is,

$$\lambda_{\max} \left(A_{\nu}(\mathbf{x}) - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^{T} \right) \leq -\epsilon_{0}.$$
(4.26)

Moreover, we have

$$\mathbf{v}^{T} P(\mathbf{x}) \mathbf{v} = \sum_{k=1}^{n} \lambda_{k} \mathbf{v}^{T} P(\mathbf{x}_{k}) \mathbf{v} \le \sum_{k=1}^{n} \lambda_{k} \|P(\mathbf{x}_{k})\|_{2} \|\mathbf{v}\|_{2}^{2} \le \sum_{k=1}^{n} \lambda_{k} P_{\nu} \|\mathbf{v}\|_{2}^{2} = P_{\nu} \|\mathbf{v}\|_{2}^{2}$$

Hence, if $\mathbf{v}^T P(\mathbf{x})\mathbf{v} = 1$, then

$$\frac{1}{P_{\nu}} \leq \|\mathbf{v}\|_{2}^{2}.$$
(4.27)

Now we have with (4.26)

$$L_{P}(\mathbf{x}) = \max_{\substack{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T}P(\mathbf{x})\mathbf{v}=1, \\ \mathbf{v}^{T}\mathbf{f}(\mathbf{x})=0}} L_{P}(\mathbf{x}; \mathbf{v})$$

$$= \max_{\substack{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T}P(\mathbf{x})\mathbf{v}=1, \\ \mathbf{v}^{T}\mathbf{f}(\mathbf{x})=0}} \frac{1}{2} \mathbf{v}^{T}[P(\mathbf{x})V(\mathbf{x}) + V(\mathbf{x})^{T}P(\mathbf{x}) + P'_{+}(\mathbf{x})]\mathbf{v}}$$

$$= \max_{\substack{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T}P(\mathbf{x})\mathbf{v}=1, \\ \mathbf{v}^{T}\mathbf{f}(\mathbf{x})=0}} \frac{1}{2} \mathbf{v}^{T}A_{\nu}(\mathbf{x})\mathbf{v}$$

$$= \max_{\substack{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T}P(\mathbf{x})\mathbf{v}=1, \\ \mathbf{v}^{T}\mathbf{f}(\mathbf{x})=0}} \frac{1}{2} \|\mathbf{v}\|_{2}^{2} \frac{\mathbf{v}^{T}}{\|\mathbf{v}\|_{2}} [A_{\nu}(\mathbf{x}) - \kappa_{\nu}^{*}\mathbf{f}(\mathbf{x}_{k})\mathbf{f}(\mathbf{x}_{k})^{T}] \frac{\mathbf{v}}{\|\mathbf{v}\|_{2}}$$

$$\leq \max_{\substack{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T}P(\mathbf{x})\mathbf{v}=1}} \frac{1}{2} \|\mathbf{v}\|_{2}^{2} \lambda_{\max} \left(A_{\nu}(\mathbf{x}) - \kappa_{\nu}^{*}\mathbf{f}(\mathbf{x})\mathbf{f}(\mathbf{x})^{T}\right)$$

$$\leq -\frac{\epsilon_{0}}{2} \min_{\substack{\mathbf{v} \in \mathbb{R}^{n}, \mathbf{v}^{T}P(\mathbf{x})\mathbf{v}=1}} \|\mathbf{v}\|_{2}^{2}$$

$$\leq -\frac{\epsilon_{0}}{2P_{\nu}}$$

$$< 0,$$

using (4.27).

4.12 Remark The following observation is useful for the application of the next theorem with $\mathcal{D} = K^{\circ}$: Given an open set \mathcal{D} , a compact set $\widetilde{K} \subset \mathcal{D}$, and $d = 2\sqrt{n}$, one can always construct an (h, d)-bounded triangulation \mathcal{T} such that $\widetilde{K} \subset D^{\circ}_{\mathcal{T}} \subset D_{\mathcal{T}} \subset \mathcal{D}$. Indeed, [12, Remark 2] shows that the so-called scaled standard triangulation $\mathcal{T}^{\text{std}}_{\rho}$ is $(h, 2\sqrt{n})$ -bounded for any $h > \rho/\sqrt{n}$. By setting $3\epsilon := \text{dist}(\widetilde{K}, \mathbb{R}^n \setminus \mathcal{D}) = \min\{\|\mathbf{x} - \mathbf{y}\|_2 : \mathbf{x} \in \widetilde{K}, \mathbf{y} \in \mathbb{R}^n \setminus \mathcal{D}\}$ and $K_{\epsilon} := \{\mathbf{x} \in \mathbb{R}^n : \text{dist}(\mathbf{x}, \widetilde{K}) < \epsilon\}$, it is easy to see that with $0 < \rho \leq \epsilon/\sqrt{n}$ the triangulation $\mathfrak{S} := \{\mathfrak{S}_{\nu} \in \mathcal{T}^{\text{std}}_{\rho} : \mathfrak{S}_{\nu} \cap K_{\epsilon} \neq \emptyset\}$ fulfills $\widetilde{K} \subset D^{\circ}_{\mathcal{T}} \subset D_{\mathcal{T}} \subset \mathcal{D}$.

So, fixing the sets \mathcal{D} and K as above, we can choose (h, d)-bounded triangulations with $d = 2\sqrt{n}$ and arbitrarily small h > 0 that satisfy $\widetilde{K} \subset D^{\circ}_{\mathcal{T}} \subset D_{\mathcal{T}} \subset \mathcal{D}$.

Next, we prove that a CPA interpolation of a contraction metric satisfies the constraints of Verification Problem 4.7.

4.13 Theorem (RBF-CPA contraction metric) Let $k \in \mathbb{N}$ with $k \geq 2$ if n is odd and $k \geq 3$ if n is even. Define $\sigma = k + \lceil \frac{n+1}{2} \rceil$ and assume that Ω is an exponentially stable periodic orbit of $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ where $\mathbf{f} \in C^{\sigma+1}(\mathbb{R}^n; \mathbb{R}^n)$. Let $B \in C^{\sigma}(\mathbb{R}^n; \mathbb{S}^{n \times n})$, such that $B(\mathbf{x})$ is positive definite for all $\mathbf{x} \in \mathbb{R}^n$, define $C(\mathbf{x})$ as in (2.6); assume $M \in C^{\sigma}(\mathcal{A}(\Omega); \mathbb{S}^{n \times n})$ is the solution of PDE (2.7) from Theorem 2.6, and S is the optimal recovery of M from Theorem 3.3 with kernel given by the Wendland function $\psi_{l,k}$ with $l = \lfloor \frac{n}{2} \rfloor + k + 1$ and the collocation points X. Let $\mathcal{O} \subset \mathbb{R}^n$ be a bounded domain with C^1 boundary and $\overline{\mathcal{O}} \subset \mathcal{A}(\Omega)$. Let $K \subset \mathcal{O}$ be a positively invariant compact set, such that $\Omega \subset K^{\circ}$.

Fix constants

$$\begin{split} d &\geq 2\sqrt{n}, \quad B_0^* \geq \max_{\substack{\mathbf{x} \in K \\ l=1,2,\dots,n}} \left| f_l(\mathbf{x}) \right|, \quad B_1^* \geq \max_{\substack{\mathbf{x} \in K \\ i,l=1,2,\dots,n}} \left| \frac{\partial f_l}{\partial x_i}(\mathbf{x}) \right|, \\ B_2^* &\geq \max_{\substack{\mathbf{x} \in K \\ i,j,l=1,2,\dots,n}} \left| \frac{\partial^2 f_l}{\partial x_i \partial x_j}(\mathbf{x}) \right|, \quad B_3^* \geq \max_{\substack{\mathbf{x} \in K \\ i,j,k,l=1,\dots,n}} \left| \frac{\partial^3 f_l}{\partial x_i \partial x_j \partial x_k}(\mathbf{x}) \right| \\ B_{V_1}^* &\geq \max_{\substack{\mathbf{x} \in K \\ r,l,j=1,2,\dots,n}} \left| \frac{\partial V_{lj}}{\partial x_r}(\mathbf{x}) \right|, \quad B_{V_2}^* \geq \max_{\substack{\mathbf{x} \in K \\ r,s,j,l=1,2,\dots,n}} \left| \frac{\partial^2 V_{lj}}{\partial x_r \partial x_s}(\mathbf{x}) \right|. \end{split}$$

Then there exist constants $h_{X,\mathcal{O}}^*$, h^* , $\kappa^* > 0$, such that for any set of collocation points $X \subset \mathcal{O}$ with fill distance $h_{X,\mathcal{O}} \leq h_{X,\mathcal{O}}^*$ and any (h,d)-bounded triangulation \mathcal{T} with $D_{\mathcal{T}} \subset K^\circ$ and $h < h^*$ the following holds:

Fix the constants and variables of Verification Problem 4.7 as follows for all $\mathfrak{S}_{\nu} \in \mathcal{T}$, $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$, and $1 \leq i \leq j \leq n$:

$$\begin{split} P_{ij}(\mathbf{x}_{k}) &= S_{ij}(\mathbf{x}_{k}), \quad \frac{1}{h} \geq \kappa_{\nu}^{*} \geq \kappa^{*}, \quad B_{0}^{*} \geq B_{0,\nu} \geq \max_{\substack{\mathbf{x} \in \mathfrak{S}_{\nu} \\ l=1,2,\dots,n}} \left| f_{l}(\mathbf{x}) \right|, \\ B_{1}^{*} \geq B_{1,\nu} \geq \max_{\substack{\mathbf{x} \in \mathfrak{S}_{\nu} \\ i,l=1,2,\dots,n}} \left| \frac{\partial f_{l}}{\partial x_{i}}(\mathbf{x}) \right|, \quad B_{2}^{*} \geq B_{2,\nu} \geq \max_{\substack{\mathbf{x} \in \mathfrak{S}_{\nu} \\ i,j,l=1,2,\dots,n}} \left| \frac{\partial^{2} f_{l}}{\partial x_{i} \partial x_{j}}(\mathbf{x}) \right|, \\ B_{3}^{*} \geq B_{3,\nu} \geq \max_{\substack{\mathbf{x} \in \mathfrak{S}_{\nu} \\ i,j,k,l=1,\dots,n}} \left| \frac{\partial^{3} f_{l}}{\partial x_{i} \partial x_{j} \partial x_{k}}(\mathbf{x}) \right|, \\ B_{V_{1}}^{*} \geq B_{V_{1,\nu}} \geq \max_{\substack{\mathbf{x} \in \mathfrak{S}_{\nu} \\ r,l,j=1,2,\dots,n}} \left| \frac{\partial V_{lj}}{\partial x_{r}}(\mathbf{x}) \right|, \quad B_{V_{2}}^{*} \geq B_{V_{2,\nu}} \geq \max_{\substack{\mathbf{x} \in \mathfrak{S}_{\nu} \\ r,s,j,l=1,2,\dots,n}} \left| \frac{\partial^{2} V_{lj}}{\partial x_{r} \partial x_{s}}(\mathbf{x}) \right|. \end{split}$$

Then the constraints of Verification Problem 4.7 are fulfilled by these values. In particular, we can assert that the CPA interpolation P of S on \mathcal{T} is a contraction metric on any compact set \widetilde{K} with $\widetilde{K} \subset D^{\circ}_{\mathcal{T}} \subset D_{\mathcal{T}} \subset K^{\circ}$.

Proof: First note that by the construction method of Theorem 3.3, we know that the $S(\mathbf{x}_k)$ and hence the $P(\mathbf{x}_k)$ are symmetric matrices. Since $\overline{\mathcal{O}}$ is compact and M is positive definite by Theorem 2.6, there are constants $\lambda_0, \Lambda_0 > 0$ such that for all $\mathbf{x} \in \overline{\mathcal{O}}$ we have

$$\lambda_0 I_{n \times n} \preceq M(\mathbf{x}) \preceq \Lambda_0 I_{n \times n}. \tag{4.28}$$

Moreover, since $B(\mathbf{x})$ is also positive definite for all $\mathbf{x} \in \mathcal{A}(\Omega)$, there is a constant $\lambda_1 > 0$ such that for all $\mathbf{x} \in \overline{\mathcal{O}}$ and $\mathbf{v} \in \mathbb{R}^n$ with $\|\mathbf{v}\|_2 = 1$, and $\mathbf{v}^T \mathbf{f}(\mathbf{x}) = 0$ we have

$$4\lambda_1 \le \mathbf{v}^T B(\mathbf{x})\mathbf{v} = \mathbf{v}^T C(\mathbf{x})\mathbf{v}.$$
(4.29)

Since $\mathbf{v}^T (-C(\mathbf{x}) + 3\lambda_1 I_{n \times n}) \mathbf{v} \leq -\lambda_1 < 0$ for all $\mathbf{x} \in \overline{\mathcal{O}}$, by Lemma 4.6 there exists a $\kappa^* > 0$ such that

$$-C(\mathbf{x}) + 3\lambda_1 I_{n \times n} - \kappa \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^T \prec \mathbf{0}_{n,n}$$
(4.30)

for every $\mathbf{x} \in K$ and every $\kappa \geq \kappa^*$. Define

$$C^* := \Lambda_0 + \frac{1}{2}\lambda_0,$$

$$D^* := (1+\gamma)\zeta \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})},$$

$$E^* := n^2 \cdot \left(4\sqrt{n}B^*_{V_1}D^* + 2nB^*_{V_2}C^* + B^*_2D^* + 2B^*_0B^*_2 + 2(B^*_1)^2\right).$$

Now set

$$h^* := \min\left(1, \frac{\lambda_1}{n\gamma\zeta \|\mathbf{f}\|_{C^0(\mathcal{O};\mathbb{R}^n)} \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})} + E^*}\right),$$

$$h^*_{X,O} := \min\left(\frac{\lambda_0}{2\beta \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}}, \frac{\lambda_1}{\beta \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}}\right)^{1/(\sigma-1-n/2)}$$

Error estimates

Note that the assumptions of Theorem 3.4 hold true with $\sigma = s - 1$ and thus so does the error estimate (3.4). Following the idea of [10, Theorem 2.4], we derive upper bounds on the approximation error $||M(\mathbf{x}) - S(\mathbf{x})||_2$ for all $\mathbf{x} \in K$. The starting point is that for $C_1, C_2 \in C^{s-1}(\mathcal{A}(\Omega), \mathbb{S}^{n \times n})$ the unique solutions $M_i \in C^{s-1}(\mathcal{A}(\Omega), \mathbb{S}^{n \times n})$, i = 1, 2 to the linear matrix-valued PDEs

$$LM_i(\mathbf{x}) = -C_i(\mathbf{x}) \text{ for all } \mathbf{x} \in \mathcal{A}(\Omega)$$

satisfying $\mathbf{f}(\mathbf{x}_0)^T M_i(\mathbf{x}_0) \mathbf{f}(\mathbf{x}_0) = c_0 \|\mathbf{f}(\mathbf{x}_0)\|_2^4$,

exist by Theorem 2.6 and are of the form

$$M_i(\mathbf{x}) = \int_0^\infty \Phi(t,0;\mathbf{x})^T C_i(S_t \mathbf{x}) \Phi(t,0;\mathbf{x}) dt + c_0 \mathbf{f}(\mathbf{x}) \mathbf{f}(\mathbf{x})^T.$$

Thus, we obtain

$$\begin{split} \|M_{1}(\mathbf{x}) - M_{2}(\mathbf{x})\|_{2} &= \left\| \int_{0}^{\infty} \Phi(t,0;\mathbf{x})^{T} \left[C_{1}(S_{t}\mathbf{x}) - C_{2}(S_{t}\mathbf{x}) \right] \Phi(t,0;\mathbf{x}) \, dt \right\|_{2} \\ &\leq \int_{0}^{\infty} \|\Phi(t,0;\mathbf{x})\|_{2}^{2} \|C_{1}(S_{t}\mathbf{x}) - C_{2}(S_{t}\mathbf{x})\|_{2} \, dt \\ &\leq \|C_{1} - C_{2}\|_{L_{\infty}(K;\mathbb{S}^{n\times n})} \int_{0}^{\infty} \|\Phi(t,0;\mathbf{x})\|_{2}^{2} \, dt. \end{split}$$

Using [10, Theorem 2.4] one can show that there are constants ρ and c_1 such that $\|\Phi(t, 0; \mathbf{x})\|_2 \leq c_1 e^{-\rho t}$ for all $\mathbf{x} \in K$ and all $t \geq 0$. And by Theorem 3.4 we get

$$\sup_{\mathbf{x}\in K} \|M(\mathbf{x}) - S(\mathbf{x})\|_2 \le \beta h_{X,\mathcal{O}}^{\sigma-1-n/2} \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}.$$
(4.31)

(VP1) We have for all $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$ with (4.31) that

$$P(\mathbf{x}_{k}) = M(\mathbf{x}_{k}) - M(\mathbf{x}_{k}) + P(\mathbf{x}_{k})$$

$$\succeq \lambda_{0}I_{n \times n} - M(\mathbf{x}_{k}) + S(\mathbf{x}_{k})$$

$$\succeq \left(\lambda_{0} - \left(\beta h_{X,\Omega}^{\sigma-1-n/2}\right) \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n \times n})}\right) I_{n \times n} \succeq \frac{\lambda_{0}}{2} I_{n \times n} \succ 0_{n,n}.$$

(VP2) We have for all $\mathbf{x}_k \in \mathcal{V}_{\mathcal{T}}$, similarly to above, that

J

$$P(\mathbf{x}_{k}) = M(\mathbf{x}_{k}) - M(\mathbf{x}_{k}) + S(\mathbf{x}_{k})$$

$$\leq \left(\Lambda_{0} + \beta h_{X,\Omega}^{\sigma-1-n/2} \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}\right) I_{n\times n}$$

$$\leq \left(\Lambda_{0} + \frac{\lambda_{0}}{2}\right) I_{n\times n} = C^{*} I_{n\times n}.$$

This shows for all simplices $\mathfrak{S}_{\nu} \in \mathcal{T}$ that

$$P_{\nu} := \max_{\mathbf{x} \in \mathfrak{S}_{\nu}} \|P(\mathbf{x})\|_2 \le C^*.$$

Consider a simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ and let $1 \leq i \leq j \leq n$. We show that $\|\nabla P_{ij}^{\nu}\|_1 \leq D^*$.

$$\begin{aligned} \|\nabla P_{ij}^{\nu}\|_{1} &\leq (1+h\gamma)\|S\|_{C^{2}(\mathcal{O};\mathbb{S}^{n\times n})} \\ &\leq (1+\gamma)\zeta\|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})} = D^{*}. \end{aligned}$$

where we used inequalities (4.4), (3.5), $h \leq h^* \leq 1$, and the definition of D^* . Thus, we have, using $h_{\nu} \leq h \leq h^* \leq 1$ and $\kappa_{\nu}^* \leq \frac{1}{h} \leq \frac{1}{h_{\nu}}$, that

$$\begin{aligned}
h_{\nu}^{2}E_{\nu} &\leq h_{\nu} n^{2} \cdot \left(4\sqrt{n}B_{V_{1,\nu}} \|\nabla P_{ij}^{\nu}\|_{1} + 2nB_{V_{2,\nu}}P_{\nu} + B_{2,\nu}\|\nabla P_{ij}^{\nu}\|_{1} \\
&+ 2h_{\nu} \kappa_{\nu}^{*} B_{0,\nu}B_{2,\nu} + 2h_{\nu} \kappa_{\nu}^{*} B_{1,\nu}^{2}\right) \\
&\leq h^{*} n^{2} \cdot \left(4\sqrt{n}B_{V_{1,\nu}}D^{*} + 2nB_{V_{2,\nu}}C^{*} + B_{2,\nu}D^{*} + 2B_{0,\nu}B_{2,\nu} + 2B_{1,\nu}^{2}\right) \\
&\leq h^{*} n^{2} \cdot \left(4\sqrt{n}B_{V_{1}}^{*}D^{*} + 2nB_{V_{2}}^{*}C^{*} + B_{2}^{*}D^{*} + 2B_{0}^{*}B_{2}^{*} + 2(B_{1}^{*})^{2}\right) \\
&= h^{*} E^{*}.
\end{aligned}$$
(4.32)

Fix a simplex $\mathfrak{S}_{\nu} \in \mathcal{T}$ and let \mathbf{x}_k be one of its vertices. Then $\mathbf{x}_k \in D_{\mathcal{T}} \subset K$. Since $P(\mathbf{x}_k) = S(\mathbf{x}_k)$ we get by (4.3)

$$\begin{aligned} A_{\nu}(\mathbf{x}_{k}) &= P(\mathbf{x}_{k})V(\mathbf{x}_{k}) + V(\mathbf{x}_{k})^{T}P(\mathbf{x}_{k}) + (\nabla P_{ij}^{\nu} \cdot \mathbf{f}(\mathbf{x}_{k}))_{i,j=1,2,...,n} \\ &= S(\mathbf{x}_{k})V(\mathbf{x}_{k}) + V(\mathbf{x}_{k})^{T}S(\mathbf{x}_{k}) + (\nabla S_{ij}(\mathbf{x}_{k}) \cdot \mathbf{f}(\mathbf{x}_{k}))_{i,j=1,2,...,n} \\ &+ ((\nabla P_{ij}^{\nu} - \nabla S_{ij}(\mathbf{x}_{k})) \cdot \mathbf{f}(\mathbf{x}_{k}))_{i,j=1,2,...,n} \\ &\preceq LS(\mathbf{x}_{k}) + n \cdot \max_{i,j=1,...,n} \|\nabla P_{ij}^{\nu} - \nabla S_{ij}(\mathbf{x}_{k})\|_{1} \sup_{\mathbf{x}\in\mathcal{O}} \|\mathbf{f}(\mathbf{x})\|_{\infty}I_{n\times n} \\ &\preceq LM(\mathbf{x}_{k}) + LS(\mathbf{x}_{k}) - LM(\mathbf{x}_{k}) + nh\gamma\|S\|_{C^{2}(K;\mathbb{S}^{n\times n})}\|\mathbf{f}\|_{C^{0}(\mathcal{O};\mathbb{R}^{n})}I_{n\times n} \\ &\preceq -C(\mathbf{x}_{k}) + \left(\beta h_{X,\mathcal{O}}^{\sigma-1-n/2} + nh\gamma\zeta\|\mathbf{f}\|_{C^{0}(\mathcal{O};\mathbb{R}^{n})}\right) \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n\times n})}I_{n\times n}, \end{aligned}$$

where the last inequality follows by (3.4) and (3.5). Using $h_{X,\mathcal{O}} \leq h_{X,\mathcal{O}}^*$, $h_{\nu} \leq h \leq h^*$, (4.32), we have with the definitions of h^* and $h_{X,O}^*$

$$\begin{aligned} A_{\nu}(\mathbf{x}_{k}) + h_{\nu}^{2} E_{\nu} I_{n \times n} - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}_{k}) \mathbf{f}(\mathbf{x}_{k})^{T} &\preceq -C(\mathbf{x}_{k}) + \beta \, h_{X,\mathcal{O}}^{*\sigma^{-1-n/2}} \, \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n \times n})} \, I_{n \times n} \\ &+ nh^{*} \gamma \zeta \|\mathbf{f}\|_{C^{0}(\mathcal{O};\mathbb{R}^{n})} \, \|M\|_{H^{\sigma}(\mathcal{O};\mathbb{S}^{n \times n})} \, I_{n \times n} \\ &+ h^{*} E^{*} I_{n \times n} - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}_{k}) \mathbf{f}(\mathbf{x}_{k})^{T} \\ &\preceq -C(\mathbf{x}_{k}) + 2\lambda_{1} I_{n \times n} - \kappa_{\nu}^{*} \mathbf{f}(\mathbf{x}_{k}) \mathbf{f}(\mathbf{x}_{k})^{T} \\ &\preceq -\lambda_{1} I_{n \times n} \prec 0_{n \times n} \end{aligned}$$

by (4.30) and the definition of $\kappa^* > 0$, since $\kappa^*_{\nu} \ge \kappa^*$. This completes the proof.

In the next section we demonstrate the applicability of our theoretical results to three examples. Note that the periodic orbit is displayed in the figures through a numerical approximation for comparison in orange, but the methods verify rigorously that it exists, is exponentially stable and they determine a subset of its basin of attraction.

5 Examples

We implemented our methods in C++ and ran the examples on an AMD Ryzen 2700X processor with 8 cores at 3.7 GHz and with 64GB RAM. Appendix B details how we numerically solve the generalized interpolation problem from Theorem 3.4 to compute the approximation S to the contraction metric M from Theorem 2.6 using RBF.

In order to compute a positively invariant set K for the dynamical systems $\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x})$ we use a procedure motivated by [7]. First we solve numerically the PDE

$$\sum_{i=1}^{n} \frac{\partial V}{\partial x_i}(\mathbf{x}) f_i(\mathbf{x}) = \nabla V(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) = -\sqrt{\delta^2 + \|\mathbf{f}(\mathbf{x})\|_2^2}, \quad \delta = 10^{-8}, \tag{5.1}$$

using RBF. Then we use CPA interpolation V_P of the numerical solution and verify where $\nabla V_P(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) < 0$ holds true. In this area the function V_P is decreasing along solution trajectories and a sublevel set $\{\mathbf{x} \in \mathbb{R}^n : V_P(\mathbf{x}) \leq c\}$ is necessarily forward invariant, if its boundary is wholly contained in this area. Note that we only need $\nabla V_P(\mathbf{x}) \cdot \mathbf{f}(\mathbf{x}) < 0$ in a neighbourhood of the boundary; not on the whole sublevel set. We refer to V_P as Lyapunov-like function.

The failing points of the Lyapunov-like function (see for example Figure 2) are the points where the function V_P is not decreasing along solution trajectories. In order to obtain a positively invariant set, we need to find a sublevel set of V_P with boundary (level set) that does not pass through these points.

In the following we apply our method to find a periodic orbit and its basin of attraction to three examples. The parameters c for the Wendland function and the density of the collocation grids X and the verification grids were determined by trial and error.

5.1 Unit Circle Periodic

As a first example, we consider the following system

$$\begin{cases} \dot{x} = x(1-x^2-y^2) - y\\ \dot{y} = y(1-x^2-y^2) + x \end{cases}$$
(5.2)

of which the unit circle is an exponentially stable periodic orbit and the origin is an unstable equilibrium.

We choose $B(\mathbf{x}) = I_{2\times 2}$ and the collocation points $X = \frac{1.6}{15}\mathbb{Z}^2 \cap \{(x, y) \in \mathbb{R}^2 : 0.25 < \sqrt{x^2 + y^2} < 1.5\}$ as well as the point $\mathbf{x}_0 = (1, 0)$ with $c_0 = 1$. We use a kernel as in (3.1), where $\phi(\mathbf{x}, \mathbf{y}) = \psi_{6,4}(||\mathbf{x} - \mathbf{y}||_2)$ is given by the Wendland function $\psi_{6,4}(r) = (1 - r)^{10}_+[25 + 250r + 1,050r^2 + 2,250r^3 + 2,145r^4]$ and $x_+ = x$ for $x \ge 0$ and $x_+ = 0$ for x < 0. The

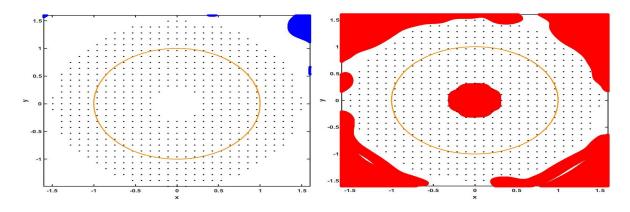


Figure 1: Example (5.1). The black dots show the collocation points and the orange curve is the periodic orbit. We plot the area where the constraints of Verification Problem 4.7 fail to be fulfilled; in blue if (VP1) is violated and in red if (VP2) is violated. Where neither is violated the CPA interpolation P fulfills the properties of a contraction metric.

corresponding Sobolev space is $H^{5.5}(\mathcal{O}; \mathbb{S}^{2\times 2})$. The grid X has N = 600 collocation points, black dots in Figure 1. We mark the area where the constraints of Verification Problem 4.7 fail to be fulfilled; in blue if (VP1) is violated and in red if (VP2) is violated. We used the scaled down standard triangulation, cf. [7], of the area $[-1.6, 1.6] \times [-1.6, 1.6]$ with 1500^2 vertices for the CPA interpolation.

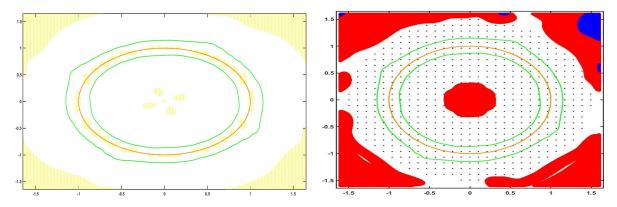


Figure 2: Example (5.1). The orange curve indicates the periodic orbit. The yellow areas (left) denote the simplices, where the Lyapunov-like function is not decreasing along solution trajectories. The green curves are the level set of the Lyapunov-like function, which thus indicate the boundary of a positively invariant set. The right figure shows the positively invariant set (green), the collocation points (black dots) as well as the blue area, where (VP1), is not fulfilled and the red area, where (VP2) is not satisfied. The positively invariant set (bounded by the green curves) is thus a subset of the basin of attraction of a unique periodic orbit within it.

In order to obtain a positively invariant set, we computed a Lyapunov-like function solving numerically (5.1) and interpolating the solution. We used the same collocation grid X but another Wendland function $\psi_{5,3}(cr)$ with parameter c = 0.9 and a triangulation of $[-1.65, 1.65]^2$ with 1000^2 vertices. In the left-hand side plot of Figure 2, the failing points for the Lyapunovlike function are marked as yellow dots, and the level set is the curve in green. The periodic orbit is the curve in orange. In the right-hand side figure, the level set of the Lyapunov-like function and the area suggested by our method suitable for the contraction metric are put together. Then by Theorem 2.5, the sublevel set is a subset of the basin of attraction of a unique periodic orbit.

5.2 Van der Pol Oscillator

We consider the van der Pol system, given by

$$\begin{cases} \dot{x} = y \\ \dot{y} = -x + (1 - x^2)y \end{cases}$$
(5.3)

which has an exponentially stable periodic orbit; the origin is an unstable equilibrium.

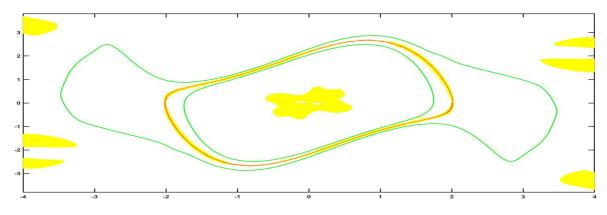


Figure 3: Example (5.2). The yellow areas denote the simplices, where the Lyapunov-like function is not decreasing along solution trajectories. The green curves are the level set of the Lyapunov-like function, which thus indicate the boundary of a positively invariant set.

In this example, we first compute a Lyapunov-like function using the collocation points $X_L = \left(\frac{2.3}{35}\mathbb{Z} \times \frac{3.1}{45}\mathbb{Z}\right) \cap \left(\left[-2.3, 2.3\right] \times \left[-3.1, 3.1\right]\right) \cap \left\{(x, y) \in \mathbb{R}^2 : 0.8 < \sqrt{x^2 + y^2}\right\}$, and the kernel given by the Wendland function $\psi_{5,3}$, with parameter c = 0.7. This results in N = 6,022 collocation points. Similar to the other example, in Figure 3, the failing points of the Lyapunov-like function are marked as yellow dots, and an appropriate level set is given in green. The periodic orbit is presented in orange.

In the next step we use another sublevel set of the Lyapunov-like function to create an appropriate set of collocation points, namely a hexagonal grid which lies in a slightly larger sublevel set than the one shown in Figure 3 intersected within the area $[-4, 4] \times [-4, 4]$, see black dots in Figure 4. This results in N = 14,922 collocation points for the calculation of the contraction metric. Then we use a triangulation of the area $[-4, 4] \times [-3.9, 3.9]$ with 4001^2 vertices for the CPA interpolation. We choose $B(\mathbf{x}) = I_{2\times 2}$ as well as the point $\mathbf{x}_0 = (2, 0)$, and $c_0 = 1$. We use the kernel given by the Wendland function $\psi_{6,4}$ with parameter c = 0.55.

In Figure 4, the left-hand side figure illustrates in blue the vertices at which Constraints (VP1) are not fulfilled, while the right-hand side figure shows in red the vertices of any simplex at which Constraints (VP2) are not satisfied. In both figures, the black dots represent the set of collocation points and the periodic orbit is displayed in orange.

In Figure 5 we present all results together, showing that inside the compact, connected, and positively invariant set, bounded by the green curves, the constraints of the verification

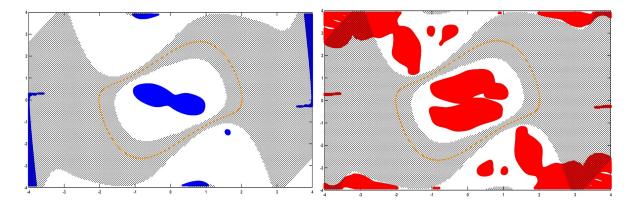


Figure 4: Example (5.2). The black dots show the collocation points. The blue (left) indicate the area where (VP1) is not satisfied, and the red (right) indicate the area where (VP2) is not satisfied. The triangulation is over the area $[-4, 4] \times [-3.9, 3.9]$ with 4001² vertices. The orange curve indicates the periodic orbit.

problem are satisfied. Hence, it is a subset of the basin of attraction of a unique periodic orbit within it.

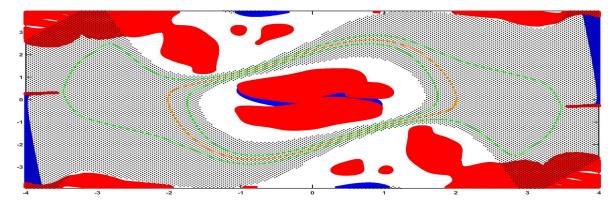


Figure 5: Example (5.2). The figure shows the collocation points (black dots) as well as the areas where (VP1) and (VP2) are not fulfilled in blue and red, respectively. The orange curve indicates the periodic orbit. The positively invariant set (bounded by the green curves) is thus a subset of the basin of attraction of a unique periodic orbit within it.

5.3 A Three-dimensional example

We consider the following three-dimensional system from [4, Section 5.3]

$$\begin{cases} \dot{x} = x(1-x^2-y^2) - y + 0.1yz \\ \dot{y} = y(1-x^2-y^2) + x \\ \dot{z} = -z + xy \end{cases}$$
(5.4)

which has an exponentially stable periodic orbit.

We choose the parameters of the method in the following way: $B(\mathbf{x}) = I_{3\times3}$ and the collocation points $X = \left(\frac{13.98}{100}\mathbb{Z}^2 \times 0.09\mathbb{Z}\right) \cap \{(x, y, z) \in \mathbb{R}^3 : 0.75 < \sqrt{x^2 + y^2} < 1.55, |z| < 0.45\}$ as well

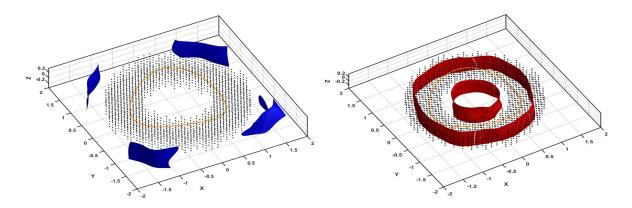


Figure 6: Example (5.3). The black dots show the collocation points. The blue area (left) indicates the boundary of simplices where (VP1) is not fulfilled. The red area (right) indicates the boundary of simplices where (VP2) is not satisfied. The orange curve indicates the periodic orbit.

as the point $\mathbf{x}_0 = (1, 0, 0)$ with $c_0 = 1$. We use again the kernel given by the Wendland function $\psi_{6,4}$ with parameter c = 0.55, the corresponding Sobolev space is $H^6(\mathcal{O}; \mathbb{S}^{3\times3})$. This results in N = 3,256 collocation points. In Figure 6, the black dots are the set of collocation points, the orange curve is the periodic orbit, the blue area in the left hand-side represents the boundary of area where (VP1) is not satisfied and the red surface on the right handside is the boundary of area where (VP2) is not fulfilled. We have triangulated the area $[-1.67, 1.67] \times [-1.67, 1.67] \times [-0.67, 0.67]$ with 601^3 vertices.

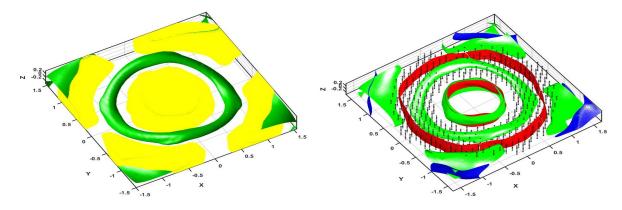


Figure 7: Example (5.3). The yellow area (left) denotes the boundary of the area where the Lyapunov-like function is not decreasing along solution trajectories. The green surface is the level set of the Lyapunov-like function, which thus indicates the boundary of a positively invariant set. The right figure shows the collocation points (black dots) as well as the boundary of the area where (VP1) is not fulfilled (blue) and the boundary of the area where (VP2) is not satisfied (red). The positively invariant set (bounded by the green surface in the middle) is thus a subset of the basin of attraction of a unique periodic orbit within it.

For the Lyapunov-like function we use $X = \left(\frac{1.3}{9}\mathbb{Z}^2 \times 0.1\mathbb{Z}\right) \cap \{(x, y, z) \in \mathbb{R}^3 : 0.75 < \sqrt{x^2 + y^2} < 1.25, |z| < 0.45\}$ as the set of collocation points, and the kernel given by the Wendland function $\psi_{5,3}$ with parameter c = 0.6. In Figure 7, a suitable level set of the Lyapunov function is presented in green, while its failing points are in yellow (left), and the last figure (right) combines all the calculations, showing that the conditions of the verification

problem are satisfied within a compact and positively invariant set.

6 Conclusion

In this paper we presented a method to compute and rigorously verify a contraction metric for exponentially stable periodic orbits. Having a PDE characterization of the contraction metric, we first used Radial Basis Functions to approximate the solution of the PDE and then used Continuous Piecewise Affine functions to interpolate that approximation. The conditions for a contraction metric are then rigorously verified for the interpolation by checking some constraints at a finite number of points.

Vice versa, we proved that using this method the conditions of the verification problem are fulfilled, whenever the collocation points are sufficiently dense and the triangulation is sufficiently fine. Thus, our method is able to compute a contraction metric for any system with an exponentially stable periodic orbit. We demonstrated the applicability of our method by computing contraction metrics for three examples showing different aspects of the computation and verification process.

References

- R. Baier, L. Grüne, and S. Hafstein, *Linear programming based Lyapunov function computation for differential inclusions*, Discrete Contin. Dyn. Syst. Ser. B **17** (2012), no. 1, 33–56.
- G. Borg, A condition for the existence of orbitally stable solutions of dynamical systems, vol. 153, Elander, 1960.
- [3] P. Giesl, Converse theorems on contraction metrics for an equilibrium, J. Math. Anal. Appl. (2015), no. 424, 1380–1403.
- [4] P. Giesl, Computation of a contraction metric for a periodic orbit using meshfree collocation, SIAM J. Appl. Dyn. Syst. 18 (2019), no. 3, 1536–1564.
- [5] P. Giesl, On a matrix-valued PDE characterizing a contraction metric for a periodic orbit, Discrete Contin. Dyn. Syst. Ser. B (2020).
- [6] P. Giesl and S. Hafstein, Construction of a CPA contraction metric for periodic orbits using semidefinite optimization, Nonlinear Anal. 86 (2013), 114–134.
- [7] P. Giesl and S. Hafstein, Computation and verification of Lyapunov functions, SIAM J. Appl. Dyn. Syst. 14 (2015), no. 4, 1663–1698.
- [8] P. Giesl, S. Hafstein, and I. Mehrabinezhad, Computation and verification of contraction metrics for exponentially stable equilibria, J. Comput. Appl. Math. to appear (2021).
- [9] P. Giesl and H. Wendland, Kernel-based discretization for solving matrix-valued PDEs, SIAM J. Numer. Anal. 56 (2018), no. 6, 3386–3406.
- [10] P. Giesl and H. Wendland, Construction of a contraction metric by meshless collocation, Discrete Contin. Dyn. Syst. Ser. B 24 (2019), no. 8, 3843–3863.
- [11] S. Hafstein and C. Kawan, Numerical approximation of the data-rate limit for state estimation under communication constraints, J. Math. Anal. Appl. 473 (2019), no. 2, 1280–1304.

- [12] S Hafstein and A Valfells, Study of dynamical systems by fast numerical computation of Lyapunov functions, Proceedings of the 14th International Conference on Dynamical Systems: Theory and Applications (DSTA), Mathematical and Numerical Aspects of Dynamical System Analysis, vol. Mathematical and Numerical Aspects of Dynamical System Analysis Lodz, Poland, 2017, pp. 229– 240.
- [13] P. Hartman, Ordinary differential equations, Wiley, New York, 1964.
- [14] P. Hartman and C. Olech, On global asymptotic stability of solutions of differential equations, Trans. Amer. Math. Soc. 104 (1962), 154–178.
- [15] A. Yu. Kravchuk, G. A. Leonov, and D. V. Ponomarenko, Criteria for strong orbital stability of trajectories of dynamical systems. I, Differentsialnye Uravneniya 28 (1992), no. 9, 1507–1520, 1652. MR 1207684
- [16] G. A. Leonov, I. M. Burkin, and A. I. Shepelyavyi, Frequency methods in oscillation theory, Ser. Math. and its Appl.: Vol. 357, Kluwer, 1996.
- [17] I. R. Manchester and J.-J. E. Slotine, Transverse contraction criteria for existence, stability, and robustness of a limit cycle, Systems Control Lett. 63 (2014), 32–38. MR 3144669
- [18] B. Stenström, Dynamical systems with a certain local contraction property, Math. Scand. 11 (1962), 151–155.
- [19] H. Wendland, Error estimates for interpolation by compactly supported Radial Basis Functions of minimal degree, J. Approx. Theory 93 (1998), 258–272.

Appendices

A Upper bounds on V

We derive upper bounds on the components of V in Verification Problem 4.7, Constants 7 and 8, in terms of **f**. The constants $B_{i,\nu}$, i = 0, 1, 2, 3, are upper bounds on the *i*th order derivatives of the components of **f** defined in Verification Problem 4.7. Further we need the lower bounds

$$0 < b_{0,\nu} \leq \min_{\mathbf{x} \in \mathfrak{S}_{\nu}} \|\mathbf{f}(\mathbf{x})\|_2.$$

We set $h(\mathbf{y}) := V_{lj}(\mathbf{y}) = \frac{\partial f_l}{\partial x_j}(\mathbf{y}) - \frac{h_2}{h_1}(\mathbf{y})$, with functions $h_1(\mathbf{y}) := \|\mathbf{f}(\mathbf{y})\|_2^2 = \mathbf{f}(\mathbf{y})^T \mathbf{f}(\mathbf{y})$, and $h_2(\mathbf{y}) := \sum_{m=1}^n f_l(\mathbf{y}) f_m(\mathbf{y}) \left(\frac{\partial f_m}{\partial x_j}(\mathbf{y}) + \frac{\partial f_j}{\partial x_m}(\mathbf{y}) \right)$. Then

$$\begin{split} \frac{\partial h}{\partial x_s} &= \frac{\partial^2 f_l}{\partial x_s \partial x_j} - \frac{\frac{\partial h_2}{\partial x_s} h_1 - \frac{\partial h_1}{\partial x_s} h_2}{h_1^2}, \\ \frac{\partial^2 h}{\partial x_r \partial x_s} &= \frac{\partial^3 f_l}{\partial x_r \partial x_s \partial x_j} - \frac{1}{h_1} \frac{\partial^2 h_2}{\partial x_r \partial x_s} + \frac{h_2}{h_1^2} \frac{\partial^2 h_1}{\partial x_r \partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_r \partial x_s} \frac{\partial h_1}{\partial x_r} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_r} \frac{\partial h_1}{\partial x_r} - \frac{2h_2}{h_1^3} \frac{\partial h_1}{\partial x_r} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_r} \frac{\partial h_1}{\partial x_s} - \frac{2h_2}{h_1^3} \frac{\partial h_1}{\partial x_r} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} - \frac{1}{h_1^3} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^2} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} - \frac{1}{h_1^3} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^3} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^3} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^3} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^3} \frac{\partial h_2}{\partial x_s} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial x_s} + \frac{1}{h_1^3} \frac{\partial h_1}{\partial x_s} \frac{\partial h_1}{\partial$$

The detailed calculations and estimates for h_1 are

$$\begin{aligned} \frac{\partial h_1}{\partial x_s}(\mathbf{y}) &= 2\mathbf{f}^T(\mathbf{y}) \frac{\partial \mathbf{f}}{\partial x_s}(\mathbf{y}), \quad \left| \frac{\partial h_1}{\partial x_s}(\mathbf{y}) \right| \le 2nB_{0,\nu}B_{1,\nu}, \\ \frac{\partial^2 h_1}{\partial x_r \partial x_s}(\mathbf{y}) &= 2\mathbf{f}^T(\mathbf{y}) \frac{\partial^2 \mathbf{f}}{\partial x_r \partial x_s}(\mathbf{y}) + 2\left(\frac{\partial \mathbf{f}}{\partial x_r}(\mathbf{y})\right)^T \frac{\partial \mathbf{f}}{\partial x_s}(\mathbf{y}), \\ \left| \frac{\partial^2 h_1}{\partial x_r \partial x_s}(\mathbf{y}) \right| \le 2n\left(B_{0,\nu}B_{2,\nu} + B_{1,\nu}^2\right) \end{aligned}$$

and the detailed calculations and estimates for h_2 are (where we skip the sum over m for brevity)

$$\begin{split} \frac{\partial h_2}{\partial x_s} &= \frac{\partial f_l}{\partial x_s} f_m \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_m} \right) + f_l \frac{\partial f_m}{\partial x_s} \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_m} \right) + f_l f_m \left(\frac{\partial^2 f_m}{\partial x_s \partial x_j} + \frac{\partial^2 f_j}{\partial x_s \partial x_m} \right) \\ \frac{\partial^2 h_2}{\partial x_r \partial x_s} &= \frac{\partial^2 f_l}{\partial x_r \partial x_s} f_m \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_m} \right) + \frac{\partial f_l}{\partial x_s} \frac{\partial f_m}{\partial x_r} \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_m} \right) + \frac{\partial f_l}{\partial x_s} f_m \left(\frac{\partial^2 f_m}{\partial x_r \partial x_j} + \frac{\partial^2 f_j}{\partial x_r \partial x_m} \right) \\ &+ \frac{\partial f_l}{\partial x_r} \frac{\partial f_m}{\partial x_s} \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_m} \right) + f_l \frac{\partial^2 f_m}{\partial x_r \partial x_s} \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_m} \right) + f_l \frac{\partial f_m}{\partial x_r \partial x_s} \left(\frac{\partial f_m}{\partial x_j} + \frac{\partial f_j}{\partial x_r \partial x_m} \right) \\ &+ \frac{\partial f_l}{\partial x_r} f_m \left(\frac{\partial^2 f_m}{\partial x_s \partial x_j} + \frac{\partial^2 f_j}{\partial x_s \partial x_m} \right) + f_l \frac{\partial f_m}{\partial x_r} \left(\frac{\partial^2 f_m}{\partial x_r} + \frac{\partial^2 f_j}{\partial x_s \partial x_j} \right) \\ &+ f_l f_m \left(\frac{\partial^3 f_m}{\partial x_r \partial x_s \partial x_j} + \frac{\partial^3 f_j}{\partial x_r \partial x_s \partial x_m} \right) \end{split}$$

Thus,

$$\left| \frac{\partial h_2}{\partial x_s}(\mathbf{y}) \right| \le 2n \left(2B_{0,\nu} B_{1,\nu}^2 + B_{0,\nu}^2 B_{2,\nu} \right) \quad \text{and} \\ \left| \frac{\partial^2 h_2}{\partial x_r \partial x_s}(\mathbf{y}) \right| \le 2n \left(6B_{0,\nu} B_{1,\nu} B_{2,\nu} + 2B_{1,\nu}^3 + B_{0,\nu}^2 B_{3,\nu} \right).$$

Finally,

$$\left| \frac{\partial h}{\partial x_{s}}(\mathbf{y}) \right| \leq B_{2,\nu} + \frac{4nB_{0,\nu}B_{1,\nu}^{2} + 2nB_{0,\nu}^{2}B_{2,\nu}}{b_{0,\nu}^{2}} + \frac{4n^{2}B_{0,\nu}^{3}B_{1,\nu}^{2}}{b_{0,\nu}^{4}} \tag{A.1}$$

$$\left| \frac{\partial^{2}h}{\partial x_{r}\partial x_{s}}(\mathbf{y}) \right| \leq B_{3,\nu} + \frac{12nB_{0,\nu}B_{1,\nu}B_{2,\nu} + 4nB_{1,\nu}^{3} + 2nB_{0,\nu}^{2}B_{3,\nu}}{b_{0,\nu}^{2}} + \frac{4n^{2}B_{0,\nu}^{2}B_{1,\nu}(5B_{1,\nu}^{2} + 3B_{0,\nu}B_{2,\nu})}{b_{0,\nu}^{4}} + \frac{16n^{3}B_{0,\nu}^{4}B_{1,\nu}^{3}}{b_{0,\nu}^{6}} \tag{A.1}$$

Therefore, we should have $B_{V_{1,\nu}}$ and $B_{V_{2,\nu}}$ greater than the right-hand side of (A.1), and (A.2), respectively.

B Computation of *S* using mesh-free collocation

In this section, we provide some details about the algorithm, following [4]. To derive explicit formulas, let us choose a radially symmetric kernel of the form $\phi(\mathbf{x}, \mathbf{y}) = \psi_0(\|\mathbf{x} - \mathbf{y}\|_2)$

and denote $\psi_{i+1}(r) = \frac{1}{r} \frac{d\psi_i}{dr}(r)$ for i = 0, 1 and r > 0. We assume that ψ_1 and ψ_2 can be continuously extended to r = 0; this is, e.g. the case for sufficiently smooth Wendland functions. We use the kernel Φ of the form (3.1), hence

$$\Phi(\cdot, \mathbf{x})_{ij\mu\nu} = \psi_0(\|\cdot - \mathbf{x}\|_2)\delta_{i\mu}\delta_{j\nu}.$$
(B.1)

We define $E_{\mu\mu}^s$ to be the matrix with value 1 at position (μ, μ) and value zero everywhere else. For $\mu < \nu$, we define $E_{\mu\nu}^s$ to be the matrix with value $1/\sqrt{2}$ at positions (μ, ν) and (ν, μ) and value zero everywhere else. It is easy to see that $\{E_{\mu\nu}^s: 1 \leq \mu \leq \nu \leq n\}$ is an orthonormal basis of $\mathbb{S}^{n \times n}$. We also define $E_{\mu\nu} \in \mathbb{R}^{n \times n}$ to be the matrix with value 1 at position (μ, ν) and value zero everywhere else. With the operator L defined as in (2.4) we define $L_k M := LM(\mathbf{x})|_{\mathbf{x}=\mathbf{x}_k}$.

From Theorem 3.3 or [4, Theorem 4.2], we obtain that S has the form

$$S(\mathbf{x}) = \sum_{k=1}^{N} \sum_{\substack{1 \le i \le j \le n}} \gamma_{k}^{(i,j)} \left[\sum_{\mu=1}^{n} L_{k}(\Phi(\cdot, \mathbf{x})_{\cdot, \cdot, \mu, \mu})_{ij} E_{\mu\mu\mu} + \frac{1}{2} \sum_{\substack{\mu,\nu=1\\\mu \ne \nu}}^{n} [L_{k}(\Phi(\cdot, \mathbf{x})_{\cdot, \cdot, \mu, \nu})_{ij} + L_{k}(\Phi(\cdot, \mathbf{x})_{\cdot, \cdot, \nu, \mu})_{ij}] E_{\mu\nu} \right] + \gamma_{0} \sum_{\substack{i,j=1\\i,j=1}}^{n} f_{i}(\mathbf{x}_{0}) f_{j}(\mathbf{x}_{0}) \left[\sum_{\mu=1}^{n} \Phi(\mathbf{x}_{0}, \mathbf{x})_{i,j,\mu,\mu} E_{\mu\mu\mu} + \frac{1}{2} \sum_{\substack{\mu,\nu=1\\\mu \ne \nu}}^{n} [\Phi(\mathbf{x}_{0}, \mathbf{x})_{i,j,\mu,\nu} + \Phi(\mathbf{x}_{0}, \mathbf{x})_{i,j,\nu,\mu}] E_{\mu\nu} \right].$$
(B.2)

where the coefficients $\gamma_k = (\gamma_k^{(i,j)})_{1 \le i \le j \le n}$ and $\gamma_0 \in \mathbb{R}$ are determined by $\lambda_\ell^{(i,j)}(S) = -C_{ij}(\mathbf{x}_\ell)$ for $1 \le i \le j \le n, 1 \le \ell \le N$ and $\lambda_0(S) = c_0 \|\mathbf{f}(\mathbf{x}_0)\|_2^4$.

If the kernel Φ is given by (3.1), then S is given by

$$S(\mathbf{x}) = \sum_{k=1}^{N} \sum_{i,j=1}^{n} \beta_{k}^{(i,j)} \sum_{\mu,\nu=1}^{n} L_{k}(\Phi(\cdot, x)_{\cdot,\cdot,\mu,\nu})_{ij} E_{\mu\nu} + \beta_{0}\phi(\mathbf{x}_{0}, \mathbf{x}) \mathbf{f}(\mathbf{x}_{0}) \mathbf{f}(\mathbf{x}_{0})^{T}$$
(B.3)

where the coefficients $\beta_k = (\beta_k^{(i,j)})_{1 \le i,j \le n} \in \mathbb{S}^{n \times n}$ and $\beta_0 \in \mathbb{R}$ are given by $\beta_0 = \gamma_0$, $\beta_k^{(i,i)} = \gamma_k^{(i,i)}$ and $\beta_k^{(i,j)} = \beta_k^{(j,i)} = \frac{1}{2} \gamma_k^{(i,j)}$ for i < j.

Using (B.3), we can compute $S(\mathbf{x})$ with

$$S(\mathbf{x}) = \sum_{k=1}^{N} \left[\psi_0(\|\mathbf{x}_k - \mathbf{x}\|_2) \left[V(\mathbf{x}_k) \beta_k + \beta_k V(\mathbf{x}_k)^T \right] + \psi_1(\|\mathbf{x}_k - \mathbf{x}\|_2) \langle \mathbf{x}_k - \mathbf{x}, \mathbf{f}(\mathbf{x}_k) \rangle \beta_k \right] + \beta_0 \psi_0(\|\mathbf{x}_0 - \mathbf{x}\|_2) \mathbf{f}(\mathbf{x}_0) \mathbf{f}(\mathbf{x}_0)^T.$$
(B.4)

In order to compute the coefficients β_k , let us first calculate the coefficients $b_{(\ell,i,j),(k,\mu,\nu)}$, $b_{0,(k,\mu,\nu)}$, $b_{(\ell,i,j),0}$ and $b_{0,0}$ for $1 \le k, \ell \le N$, $1 \le i, j, \mu, \nu \le n$

$$b_{0,(k,\mu,\nu)} = \psi_0(\|\mathbf{x}_k - \mathbf{x}_0\|_2) \left[\sum_{p=1}^n V_{p\mu}(\mathbf{x}_k) f_p(\mathbf{x}_0) f_\nu(\mathbf{x}_0) + \sum_{p=1}^n V_{p\nu}(\mathbf{x}_k) f_p(\mathbf{x}_0) f_\mu(\mathbf{x}_0) \right] \\ + \psi_1(\|\mathbf{x}_k - \mathbf{x}_0\|_2) \langle \mathbf{x}_k - \mathbf{x}_0, \mathbf{f}(\mathbf{x}_k) \rangle f_\mu(\mathbf{x}_0) f_\nu(\mathbf{x}_0)$$
(B.5)

$$b_{0,0} = \psi_0(0) \| \mathbf{f}(\mathbf{x}_0) \|_2^4.$$
(B.6)

$$b_{(\ell,i,j),(k,\mu,\nu)} = \psi_0(\|\mathbf{x}_k - \mathbf{x}_\ell\|_2) \left[\sum_{p=1}^{n} V_{pi}(\mathbf{x}_\ell) V_{p\mu}(\mathbf{x}_k) \delta_{\nu j} + V_{\mu i}(\mathbf{x}_\ell) V_{j\nu}(\mathbf{x}_k) \right. \\ \left. + V_{i\mu}(\mathbf{x}_k) V_{\nu j}(\mathbf{x}_\ell) + \delta_{i\mu} \sum_{p=1}^{n} V_{p\nu}(\mathbf{x}_k) V_{pj}(\mathbf{x}_\ell) \right] \\ \left. + \psi_1(\|\mathbf{x}_k - \mathbf{x}_\ell\|_2) \langle \mathbf{x}_k - \mathbf{x}_\ell, \mathbf{f}(\mathbf{x}_k) \rangle \left[V_{\mu i}(\mathbf{x}_\ell) \delta_{\nu j} + \delta_{i\mu} V_{\nu j}(\mathbf{x}_\ell) \right] \\ \left. + \psi_1(\|\mathbf{x}_k - \mathbf{x}_\ell\|_2) \langle \mathbf{x}_\ell - \mathbf{x}_k, \mathbf{f}(\mathbf{x}_\ell) \rangle \left[V_{i\mu}(\mathbf{x}_k) \delta_{\nu j} + \delta_{i\mu} V_{j\nu}(\mathbf{x}_k) \right] \\ \left. - \psi_1(\|\mathbf{x}_k - \mathbf{x}_\ell\|_2) \langle \mathbf{f}(\mathbf{x}_\ell), \mathbf{f}(\mathbf{x}_k) \rangle \delta_{i\mu} \delta_{j\nu} \\ \left. + \psi_2(\|\mathbf{x}_k - \mathbf{x}_\ell\|_2) \langle \mathbf{x}_k - \mathbf{x}_\ell, \mathbf{f}(\mathbf{x}_k) \rangle \langle \mathbf{x}_\ell - \mathbf{x}_k, \mathbf{f}(\mathbf{x}_\ell) \rangle \delta_{i\mu} \delta_{j\nu} \right] \right] \\ \text{and } b_{(\ell,i,j),0} = \psi_0(\|\mathbf{x}_0 - \mathbf{x}_\ell\|_2) \left[\sum_{p=1}^{n} V_{pi}(\mathbf{x}_\ell) f_p(\mathbf{x}_0) f_j(\mathbf{x}_0) + \sum_{p=1}^{n} V_{pj}(\mathbf{x}_\ell) f_p(\mathbf{x}_0) f_i(\mathbf{x}_0) \right] \right]$$

$$f b_{(\ell,i,j),0} = \psi_0(\|\mathbf{x}_0 - \mathbf{x}_\ell\|_2) \Big[\sum_{p=1}^{\infty} V_{pi}(\mathbf{x}_\ell) f_p(\mathbf{x}_0) f_j(\mathbf{x}_0) + \sum_{p=1}^{\infty} V_{pj}(\mathbf{x}_\ell) f_p(\mathbf{x}_0) f_i(\mathbf{x}_0) \Big]
 + \psi_1(\|\mathbf{x}_0 - \mathbf{x}_\ell\|_2) \langle \mathbf{x}_\ell - \mathbf{x}_0, \mathbf{f}(\mathbf{x}_\ell) \rangle f_i(\mathbf{x}_0) f_j(\mathbf{x}_0).$$
(B.8)

It is now easy to see that

$$b_{(\ell,i,j),(k,\mu,\nu)} = b_{(\ell,j,i),(k,\nu,\mu)},$$
 (B.9)

$$b_{(\ell,i,j),(k,\mu,\nu)} = b_{(k,\mu,\nu),(\ell,i,j)},$$
 (B.10)

$$b_{0,(\ell,i,j)} = b_{0,(\ell,j,i)},$$
 (B.11)

$$b_{(\ell,i,j),0} = b_{0,(\ell,i,j)}.$$
 (B.12)

We now compute the $\gamma_k^{(\mu,\nu)},$ which solve the (smaller) linear system

$$\sum_{k=1}^{N} \sum_{1 \le \mu \le \nu \le n} c_{(\ell,i,j),(k,\mu,\nu)} \gamma_{k}^{(\mu,\nu)} + c_{(\ell,i,j),0} \gamma_{0} = LS(\mathbf{x}_{\ell})_{i,j}$$
$$= \lambda_{\ell}^{(i,j)}(S)$$
$$= -C_{ij}(\mathbf{x}_{\ell})$$
(B.13)

$$\sum_{k=1}^{N} \sum_{1 \le \mu \le \nu \le n} c_{0,(k,\mu,\nu)} \gamma_k^{(\mu,\nu)} + c_{0,0} \gamma_0 = c_0 \|\mathbf{f}(\mathbf{x}_0)\|_2^4$$
(B.14)

for $1 \leq \ell \leq N, 1 \leq i \leq j \leq n$. The coefficients $c_{\cdot,\cdot}$ form a symmetric (see below) matrix of size $N\frac{n(n+1)}{2} + 1$. Let us express the $c_{(\ell,i,j),(k,\mu,\nu)}$ in terms of the previously calculated $b_{(\ell,i,j),(k,\mu,\nu)}$. we have from the first equation for all (ℓ, i, j)

$$c_{(\ell,i,j),0} = b_{(\ell,i,j),0},$$
 (B.15)

$$c_{(\ell,i,j),(k,\mu,\nu)} = \frac{1}{4} \left(b_{(\ell,i,j),(k,\mu,\nu)} + b_{(\ell,j,i),(k,\nu,\mu)} + b_{(\ell,i,j),(k,\nu,\mu)} + b_{(\ell,j,i),(k,\mu,\nu)} \right)$$
(B.16)

where we assume $\mu < \nu$ and i < j.

$$c_{0,0} = b_{0,0} \tag{B.17}$$

$$c_{0,(k,\mu,\nu)} = \frac{1}{2} \left(b_{0,(k,\mu,\nu)} + b_{0,(k,\nu,\mu)} \right) = b_{0,(k,\mu,\nu)}, \quad (B.18)$$

where we assume $\mu < \nu$. The matrix $c_{\cdot,\cdot}$ is symmetric due to (B.10) and (B.12).

Then we determine $\gamma_k^{(\mu,\nu)}$ and γ_0 by solving (B.13) and (B.14) and compute $\beta_k \in \mathbb{S}^{n \times n}$ from γ_k ; recall that $\beta_k^{(j,i)} = \beta_k^{(i,j)} = \frac{1}{2} \gamma_k^{(i,j)}$ if i < j and $\beta_k^{(i,i)} = \gamma_k^{(i,i)}$ as well as $\beta_0 = \gamma_0$. $S(\mathbf{x})$ is then given by (B.4).