Handling Hard Affine SDP Shape Constraints in RKHSs

Pierre-Cyril Aubin-Frankowski PIERRE-CYRIL.AUBIN@MINES-PARISTECH.FR
École des Ponts ParisTech and CAS
MINES ParisTech, PSL
France

Zoltán Szabó ZOLTAN.SZABO@POLYTECHNIQUE.EDU
Center of Applied Mathematics, CNRS
École Polytechnique, Institut Polytechnique de Paris
Route de Saclay, Palaiseau, 91128, France

Abstract

Shape constraints, such as non-negativity, monotonicity, convexity or supermodularity, play a key role in various applications of machine learning and statistics. However, incorporating this side information into predictive models in a hard way (for example at *all* points of an interval) for rich function classes is a notoriously challenging problem. We propose a unified and modular convex optimization framework, relying on second-order cone (SOC) tightening, to encode hard affine SDP constraints on function derivatives, for models belonging to vector-valued reproducing kernel Hilbert spaces (vRKHSs). The modular nature of the proposed approach allows to simultaneously handle multiple shape constraints, and to tighten an infinite number of constraints into finitely many. We prove the consistency of the proposed scheme and that of its adaptive variant, leveraging geometric properties of vRKHSs. The efficiency of the approach is illustrated in the context of shape optimization, safety-critical control and econometrics.

Keywords: vector-valued reproducing kernel Hilbert space, shape-constrained optimization, matrix-valued kernel, kernel derivatives

1. Introduction

The design of flexible predictive models is among the most fundamental problems of machine learning. However, in several applications one is faced with a limited number of samples due to the difficulty or the cost of data acquisition. One principled way to tackle this serious bottleneck and to improve sample-efficiency corresponds to incorporating qualitative priors on the shape of the model, such as non-negativity, monotonicity, convexity or supermodularity, collectively known as shape constraints (Guntuboyina and Sen, 2018). This side information can originate from both physical and theoretical constraints on the model such as “stay within boundaries“ in path-planning or “be nonnegative and integrate to one“ in density estimation.

Various scientific fields, including econometrics, statistics, biology, game theory or finance, impose shape constraints on their hypothesis classes. For instance, economic theory dictates increasing and concave utility functions, decreasing demand functions, or monotone link functions (Johnson and Jiang, 2018; Chetverikov et al., 2018). In statistics, applying a monotonicity assumption on the regression function (for instance in isotonic regression; Han et al. 2019) dates back at least to Brunk (1955). Density estimation entails non-negativity which can be paired with other constraints (Royset and Wets, 2015), whereas, in quantile regression, conditional quantile functions grow w.r.t. the quantile level (Koenker, 2005). In biology, monotone regression is particularly well-suited to dose-response studies (Hu et al., 2005) and to identification of genome interactions (Luss et al., 2012). Inventory problems, game theory and pricing models commonly rely on the assumption of supermodularity (Topkis, 1998; Simchi-Levi et al., 2014). In financial applications, call option prices should be increasing in volatility, monotone and convex in the underlying stock price (Aït-Sahalia and Duarte, 2003). In control theory, shape constraints are known as state constraints, and rank among the most difficult topics of the field (Hartl et al., 1995; Aubin-Frankowski, 2020).

A large and important class of these shape requirements takes the form of an affine SDP (positive semidefinite) inequality over the derivatives of $\mathbf{f} \in \mathcal{F}$ where $\mathcal{F}$ is a hypothesis class (a set of candidate predictive models). Particularly, these constraints are requested to hold *pointwise* at *all elements* of a set $\mathcal{K} \subseteq \mathbb{R}^d$:

$$\mathbf{0}_{P\times P} \preccurlyeq \operatorname{diag}(\mathbf{b}) + \mathbf{Df}(\mathbf{x}) \quad \forall\, \mathbf{x} \in \mathcal{K} \tag{1}$$

for some bias $\mathbf{b} \in \mathbb{R}^P$ and differential operator $\mathbf{D}$ (e.g., the Hessian). The fundamental challenge one faces when optimizing an objective $\mathcal{L}(\mathbf{f})$ over $\mathcal{F}$ is that in most relevant cases the set $\mathcal{K}$ has non-finite cardinality, and hence there is an infinite number of constraints to satisfy. For instance, in constrained path-planning, $\mathcal{K}$ corresponds to a time interval and the goal is to avoid collisions at all times.

In the statistics community, the main emphasis has been on designing consistent estimators and on studying their rates (Han and Wellner, 2016; Chen and Samworth, 2016; Freyberger and Reeves, 2018; Lim, 2020; Deng and Zhang, 2020; Kur et al., 2020). While these asymptotic results are of significant theoretical interest, imposing shape priors is generally beneficial in the small-sample regime. Since optimization with an infinite number of constraints (1) is *computationally intractable*, one has to either relax or tighten the problem. *Relaxing* corresponds to approaches for which the constraint (1) is not guaranteed to be satisfied. For instance, one can choose to enforce the constraint only at a finite number of points (Takeuchi et al., 2006; Blundell et al., 2012; Agrell, 2019) by replacing $\mathcal{K}$ with a discretization $\{\mathbf{x}_m\}_{m=1\ldots M} \subsetneq \mathcal{K}$ in (1). An alternative approach for relaxing is to add soft penalties to the objective $\mathcal{L}(\mathbf{f})$ (Sangnier et al., 2016; Koppel et al., 2019; Brault et al., 2019). *Tightening* on the contrary restricts the search space of functions to a smaller and more amenable subset $\mathcal{F}_0 \subsetneq \mathcal{F}$. This principle can be implemented by encoding the requirement (1) into $\mathcal{F}_0$ through algebraic techniques. The approach is feasible for restrictive finite-dimensional $\mathcal{F}_0$ such as subsets of polynomials (Hall, 2018) or polynomial splines (Turlach, 2005; Papp and Alizadeh, 2014; Pya and Wood, 2015; Wu and Sickles, 2018; Meyer, 2018). For infinite-dimensional sets $\mathcal{F}_0$, the idea has recently been extended elegantly (Marteau-Ferey et al., 2020) for a single non-negativity constraint over the whole space ($\mathcal{K} = \mathbb{R}^d$), forcing $\mathbf{f}$ to be an analogue of a sum-of-squares. These limitations motivate the design of novel shape-constrained optimization techniques which avoid (i) restricted function classes, (ii) limited out-of-sample guarantees and (iii) the lack of modularity in terms of the shape constraints imposed.

In this work the class of functions $\mathcal{F}$ is assumed to be a reproducing kernel Hilbert space $\mathcal{F} := \mathcal{F}_K$ (RKHS; Steinwart and Christmann 2008; Saitoh and Sawano 2016; also referred to as abstract splines; Wahba 1990; Berlinet and Thomas-Agnan 2004; Wang 2011). There are multiple advantages in selecting this family of functions. First, kernel methods rely inherently on pointwise evaluation (Aronszajn, 1950) which are well-suited to handle the pointwise constraints (1). In particular, the associated reproducing property (which also holds for derivatives; Zhou 2008) allows one to rephrase the inequality constraints (1) in $\mathcal{F}_K$ using a geometric perspective. Moreover, RKHSs can be rich enough to approximate various function classes (including the space of continuous bounded functions, a property known as universality; Steinwart 2001; Micchelli et al. 2006; Sriperumbudur et al. 2011; Simon-Gabriel and Schölkopf 2018). In addition, the models $\mathbf{f} \in \mathcal{F}_K$ obtained through kernel regression share the regularity of the underlying kernel (Steinwart and Christmann, 2008), allowing one to incorporate additional prior knowledge through the choice of K. Furthermore, vector-valued RKHSs (vRKHS; Micchelli and Pontil 2005; Brouard et al. 2011; Kadri et al. 2016) induced by operator-valued kernels can efficiently encode dependency between output coordinates. These vRKHSs have similar spectral decomposition (Vito et al., 2013) and universal approximation properties (Carmeli et al., 2010) as their real-valued counterpart. Finally, despite the infinite-dimensional nature of most vRKHSs of interest, kernel methods often remain computationally tractable thanks to representer theorems (Schölkopf et al., 2001; Zhou, 2008). However, classical representer theorems only hold for a finite number of evaluations both in the objective and in the constraints. This is one of the points we address through our approach based on finite compact coverings.

With a vRKHS choice for $\mathcal{F}$, our **contributions** can be summarized as follows.

1. We propose two principled ways to tighten the infinite number of SDP constraints (1) through compact coverings in vRKHSs and through an upper bound of the modulus of continuity of $\mathbf{Df}$. Specifically, we show that (1) can be tightened into a finite number of SDP inequalities with second-order cone (SOC) terms

$$\eta_m \|\mathbf{f}\|_K \, \mathbf{I}_P \preccurlyeq \operatorname{diag}(\mathbf{b}) + \mathbf{Df}(\tilde{\mathbf{x}}_m), \quad \forall\, m \in [M] \tag{2}$$

   for a suitable choice of $\eta_m > 0$ and $\tilde{\mathbf{x}}_m \in \mathcal{K}$.
2. When considering supervised learning over vRKHSs, we prove an existence result and a representer theorem for the strengthened problems; this approach allows handling several shape constraints in a modular way. In addition, we establish the convergence to the solution of the original problem with constraint (1).
3. We design adaptive variants of the previous schemes, in order to enforce the constraints only where it is necessary, and show their convergence.
4. We illustrate the efficiency of our approach in the context of shape optimization, safety-critical control and econometrics.

In this paper, we thus propose a unified and modular convex optimization framework for kernel machines relying on SOC tightening to encode hard affine SDP constraints on function derivatives. Our framework is suited for a large number of settings and applications owing to the ubiquity of shape constraints.

This article extends the results of Aubin-Frankowski and Szabó (2020) by (i) considering matrix-valued rather than real-valued kernels, (ii) generalizing the shape requirements studied from real-valued to affine SDP constraints, (iii) proposing an adaptive covering scheme and showing its convergence, and (iv) providing applications complementary to the previous focus on joint quantile regression. The present article also encompasses two prior domain-specific applications with $\mathcal{X} = [0, T]$: convoy trajectory reconstruction (Aubin-Frankowski et al., 2020) and linear quadratic optimal control (Aubin-Frankowski, 2020).

The paper is structured as follows. Our problem is introduced in Section 2. Section 3 is about the handling of hard affine SDP shape constraints. The constraints are then embedded into supervised learning in Section 4. In Section 5 we present the soap bubble algorithm which is an adaptive scheme combining the results of Section 3 and Section 4. Numerical illustrations are given in Section 6. Conclusions are drawn in Section 7. Proofs are collected in Section A.

Notations: Below we introduce the notations $\mathbb{N}$, $\mathbb{N}^*$, $\mathbb{R}_+$, $[\![n_1, n_2]\!]$, $[a, b]$, $[N]$, $\#S$, $A \backslash B$, $\prod_{i\in[I]} S_i$, S^I, χ_S, $\max(S)$, $\operatorname{diam}(\Omega)$, $\mathring{S}$, $\bar{S}$, $\langle \mathbf{a}, \mathbf{b} \rangle$, $\|\mathbf{a}\|_2$, $\mathbb{S}^{d-1}$, $\mathbf{a} \geq \mathbf{b}$, $\mathbf{a} > \mathbf{b}$, $\mathbf{u} \otimes \mathbf{v}$, $\operatorname{diag}(\mathbf{v})$, $\mathbf{M}^\top$, $\langle \mathbf{A}, \mathbf{B} \rangle_F$, $\mathbf{e}_i$, $\mathbf{0}_{d_1 \times d_2}$, $\mathbf{I}_d$, S_d^+, $[\mathbf{V}_1; \ldots; \mathbf{V}_N]$, $[\mathbf{H}_1, \ldots, \mathbf{H}_N]$, $\boldsymbol{\mathcal{K}}\mathbf{A}$, $|\mathbf{r}|$, $\partial^{\mathbf{r}}$, $\partial^{\mathbf{r},\mathbf{q}}$, $\mathcal{C}^s\left(\mathcal{X}, \mathbb{R}^d\right)$, $\mathcal{C}^{s,s}\left(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{d_1 \times d_2}\right)$, $O_{1,s}$, $O_{Q,s}$, $H^+_{\mathcal{F}}(f, \rho)$, $H^-_{\mathcal{F}}(f, \rho)$, $H_{\mathcal{F}}(f, \rho)$, $\mathbb{B}_{\mathcal{F}}(c, r)$, $\mathbb{B}_{\mathcal{X}}(\mathbf{c}, r)$, $V^\perp$. Depending on the reader's background, (s)he may skip these definitions, and return to them if necessary.

Sets: Let $\mathbb{N} = \{0, 1, \ldots\}$, $\mathbb{N}^* = \{1, 2, \ldots\}$ and $\mathbb{R}_+$ denote the set of natural numbers, positive integers and non-negative reals, respectively. We write $[\![n_1, n_2]\!]$ for the set of integers between $n_1, n_2 \in \mathbb{N}$ (not to be confused with the closed interval $[a, b]$) and use the shorthand $[N] := [\![1, N]\!]$ with $N \in \mathbb{N}$, with the convention that $[0]$ is the empty set. The cardinality of a set S is denoted by $\#S$, the difference of two sets A and B by $A \backslash B$. Given sets $(S_i)_{i\in[I]}$, let $\prod_{i\in[I]} S_i$ be their Cartesian product; we use the shorthand S^I if $S = S_1 = \ldots = S_I$. For a set S, its characteristic function is χ_S: $\chi_S(x) = 0$ if $x \in S$, $\chi_S(x) = \infty$ otherwise. The maximum of a set $S \subset \mathbb{R}$ with finite cardinality is denoted by $\max(S)$. Let the diameter of a set Ω contained in a normed space $(\mathcal{F}, \|\cdot\|_{\mathcal{F}})$ be denoted by $\operatorname{diam}(\Omega) = \sup_{\mathbf{x},\mathbf{y}\in\Omega} \|\mathbf{x} - \mathbf{y}\|_{\mathcal{F}}$; $\operatorname{diam}(\Omega) < \infty$ if Ω is bounded. The interior of a set $S \subseteq \mathcal{F}$ is denoted by $\mathring{S}$, its closure by $\bar{S}$. Throughout the paper $\mathcal{X} \subseteq \mathbb{R}^d$ denotes a set which is contained in the closure of its interior ($\mathcal{X} \subseteq \bar{\mathring{\mathcal{X}}}$).[1]

Linear algebra: The inner product of vectors $\mathbf{a}, \mathbf{b} \in \mathbb{R}^d$ is denoted by $\langle \mathbf{a}, \mathbf{b} \rangle = \sum_{i\in[d]} a_i b_i$; the Euclidean norm is written as $\|\mathbf{a}\|_2 = \sqrt{\langle \mathbf{a}, \mathbf{a} \rangle}$. The d-dimensional sphere is denoted by $\mathbb{S}^{d-1} = \left\{\mathbf{x} \in \mathbb{R}^d : \|\mathbf{x}\|_2 = 1\right\}$. For vectors $\mathbf{a}$ and $\mathbf{b} \in \mathbb{R}^d$, $\mathbf{a} \geq \mathbf{b}$ means that $a_i \geq b_i$ for all $i \in [d]$. Similarly, $\mathbf{a} > \mathbf{b}$ is defined as $a_i > b_i$ for all $i \in [d]$. Let the tensor product of vector $\mathbf{u} \in \mathbb{R}^{d_1}$ and $\mathbf{v} \in \mathbb{R}^{d_2}$ be defined as $\mathbf{u} \otimes \mathbf{v} = [u_i v_j]_{i\in[d_1], j\in[d_2]} \in \mathbb{R}^{d_1 \times d_2}$. The $d \times d$ sized matrix with diagonal $\mathbf{v} \in \mathbb{R}^d$ is $\operatorname{diag}(\mathbf{v})$. The transpose of a matrix $\mathbf{M}$ is $\mathbf{M}^\top$. The Frobenius product of the matrices $\mathbf{A}, \mathbf{B} \in \mathbb{R}^{d_1 \times d_2}$ is $\langle \mathbf{A}, \mathbf{B} \rangle_F = \sum_{i\in[d_1], j\in[d_2]} A_{ij} B_{ij}$. The i-th canonical basis vector is $\mathbf{e}_i$; the zero matrix is $\mathbf{0}_{d_1 \times d_2} \in \mathbb{R}^{d_1 \times d_2}$; the identity matrix is denoted by $\mathbf{I}_d \in \mathbb{R}^{d \times d}$. The set of $d \times d$ symmetric positive semi-definite matrices is denoted by $S_d^+ = \left\{\mathbf{M} \in \mathbb{R}^{d \times d} : \mathbf{M} = \mathbf{M}^\top \text{ and } \mathbf{0}_{d \times d} \preccurlyeq \mathbf{M}\right\}$. The vertical concatenation of matrices $\mathbf{V}_1 \in \mathbb{R}^{d_1 \times d}, \ldots, \mathbf{V}_N \in \mathbb{R}^{d_N \times d}$ is $[\mathbf{V}_1; \ldots; \mathbf{V}_N] \in \mathbb{R}^{\left(\sum_{n\in[N]} d_n\right) \times d}$; similarly the horizontal concatenation of $\mathbf{H}_1 \in \mathbb{R}^{d \times d_1}, \ldots, \mathbf{H}_N \in \mathbb{R}^{d \times d_N}$ is $[\mathbf{H}_1, \ldots, \mathbf{H}_N] \in \mathbb{R}^{d \times \left(\sum_{n\in[N]} d_n\right)}$. A tensor $\boldsymbol{\mathcal{K}} \in \mathbb{R}^{d \times d \times d \times d}$ defines an $\mathbb{R}^{d \times d} \mapsto \mathbb{R}^{d \times d}$ bounded linear operator by acting on a matrix $\mathbf{A} \in \mathbb{R}^{d \times d}$ as $(\boldsymbol{\mathcal{K}}\mathbf{A})_{i,j} := \sum_{n,m\in[d]} a_{n,m} \boldsymbol{\mathcal{K}}_{i,j,n,m}$ with $i, j \in [d]$.

1. Examples of such sets include for instance open sets or half intervals $[a, b)$ where $a \in \mathbb{R}$, $b \in \mathbb{R} \cup \{\infty\}$.

Analysis: Given a multi-index $\mathbf{r} \in \mathbb{N}^d$ let $|\mathbf{r}| = \sum_{j\in[d]} r_j$ be its length, and let the $\mathbf{r}$-th order partial derivative of a function f be denoted by $\partial^{\mathbf{r}} f(\mathbf{x}) = \frac{\partial^{|\mathbf{r}|} f(\mathbf{x})}{\partial x_1^{r_1} \ldots \partial x_d^{r_d}}$. Similarly for multi-indices $\mathbf{r}, \mathbf{q} \in \mathbb{N}^d$, let $\partial^{\mathbf{r},\mathbf{q}} f(\mathbf{x}, \mathbf{y}) = \frac{\partial^{|\mathbf{r}|,|\mathbf{q}|} f(\mathbf{x},\mathbf{y})}{\partial x_1^{r_1} \ldots \partial x_d^{r_d} \partial y_1^{q_1} \ldots \partial y_d^{q_d}}$. For a fixed $s \in \mathbb{N}$, let the set of $\mathbb{R}^d$-valued functions on $\mathcal{X}$ with continuous derivatives up to order s be denoted by $\mathcal{C}^s\left(\mathcal{X}, \mathbb{R}^d\right)$. The set of $\mathbb{R}^{d_1\times d_2}$-valued functions on $\mathcal{X} \times \mathcal{X}$ for which $\partial^{\mathbf{r},\mathbf{r}} f$ exists and is continuous up to order $|\mathbf{r}| \le s \in \mathbb{N}$ is denoted by $\mathcal{C}^{s,s}\left(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{d_1\times d_2}\right)$. Let the set of linear differential operators of order at most $s \in \mathbb{N}$ on real-valued functions be denoted by $O_{1,s} = \left\{ D : D(f)(\mathbf{x}) = \sum_{j\in J} c_j \partial^{\mathbf{r}_j} f(\mathbf{x}), \#J < \infty, |\mathbf{r}_j| \le s, c_j \in \mathbb{R}\, (\forall j \in J) \right\}$. The set of linear differential operators of order at most $s \in \mathbb{N}$ on $\mathbb{R}^Q$-valued functions is $O_{Q,s} = \left\{ D : D(\mathbf{f})(\mathbf{x}) = \sum_{q\in[Q]} \beta_q D_q(f_q)(\mathbf{x}), \beta_q \in \mathbb{R}, D_q \in O_{1,s} \right\}$.

Hilbert spaces: Let $\mathcal{F}$ be a Hilbert space. For $f \in \mathcal{F}$ and $\rho \in \mathbb{R}$, let the closed half-spaces and the affine hyperplane associated to the pair (f, ρ) be defined as $H^+_{\mathcal{F}}(f, \rho) = \{g \in \mathcal{F} : \langle f, g\rangle_{\mathcal{F}} \ge \rho\}$, $H^-_{\mathcal{F}}(f, \rho) = \{g \in \mathcal{F} : \langle f, g\rangle_{\mathcal{F}} \le \rho\}$, $H_{\mathcal{F}}(f, \rho) = \{g \in \mathcal{F} : \langle f, g\rangle_{\mathcal{F}} = \rho\}$. The closed ball in $\mathcal{F}$ with center $c \in \mathcal{F}$ and radius $r > 0$ is $\mathbb{B}_{\mathcal{F}}(c, r) = \{f \in \mathcal{F} : \|c - f\|_{\mathcal{F}} \le r\}$. When $\mathcal{F} = \mathcal{X} \subseteq \mathbb{R}^d$ is endowed with a norm $\|\cdot\|_{\mathcal{X}}$, we write $\mathbb{B}_{\mathcal{X}}(\mathbf{c}, r)$ for balls. Let V be a closed subspace of a Hilbert space $\mathcal{F}$, the orthogonal complement of V in $\mathcal{F}$ is $V^{\perp} = \{f \in \mathcal{F} : \langle f, g\rangle_{\mathcal{F}} = 0 \ \ \forall g \in V\}$.

2. Problem Formulation

In this section we formulate our problem after recalling the definition of vector-valued reproducing kernel Hilbert spaces (vRKHS).

vRKHS: A function $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^{Q\times Q}$ is called a (positive definite) matrix-valued kernel on $\mathcal{X}$ if $K(\mathbf{x}, \mathbf{x}') = K(\mathbf{x}', \mathbf{x})^\top$ for all $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$ and $\sum_{i,j\in[N]} \mathbf{v}_i^\top K(\mathbf{x}_i, \mathbf{x}_j)\mathbf{v}_j \ge 0$ for all $N \in \mathbb{N}^*$, $\{\mathbf{x}_n\}_{n\in[N]} \subset \mathcal{X}$ and $\{\mathbf{v}_n\}_{n\in[N]} \subset \mathbb{R}^Q$. For $\mathbf{x} \in \mathcal{X}$, let $K(\cdot, \mathbf{x})$ be the mapping $\mathbf{x}' \in \mathcal{X} \mapsto K(\mathbf{x}', \mathbf{x}) \in \mathbb{R}^{Q\times Q}$. Let $\mathcal{F}_K$ denote the vRKHS associated to the kernel K; we use the shorthand $\|\cdot\|_K := \|\cdot\|_{\mathcal{F}_K}$ and $\langle\cdot,\cdot\rangle_K := \langle\cdot,\cdot\rangle_{\mathcal{F}_K}$ for the norm and the inner product on $\mathcal{F}_K$. The Hilbert space $\mathcal{F}_K$ consists of $\mathcal{X} \to \mathbb{R}^Q$ functions for which (i) $K(\cdot, \mathbf{x})\mathbf{c} \in \mathcal{F}_K$ for all $\mathbf{x} \in \mathcal{X}$ and $\mathbf{c} \in \mathbb{R}^Q$, and (ii) $\langle \mathbf{f}, K(\cdot, \mathbf{x})\mathbf{c}\rangle_K = \langle \mathbf{f}(\mathbf{x}), \mathbf{c}\rangle$ for all $\mathbf{f} \in \mathcal{F}_K$, $\mathbf{x} \in \mathcal{X}$ and $\mathbf{c} \in \mathbb{R}^Q$. The first property of vRKHSs describes the basic elements of $\mathcal{F}_K$, the second one is called the reproducing property. Constructively, $\mathcal{F}_K = \overline{\text{span}}\left\{K(\cdot, \mathbf{x})\mathbf{c} : \mathbf{x} \in \mathcal{X}, \mathbf{c} \in \mathbb{R}^Q\right\}$ where span denotes the linear hull of its argument and the bar stands for closure w.r.t. $\|\cdot\|_K$. Given a vRKHS $\mathcal{F}_K$, we use the shorthands $H^+_K(\mathbf{f}, \rho)$, $H^-_K(\mathbf{f}, \rho)$, $H_K(\mathbf{f}, \rho)$ and $\mathbb{B}_K(\mathbf{c}, r)$ for $H^+_{\mathcal{F}_K}(\mathbf{f}, \rho)$, $H^-_{\mathcal{F}_K}(\mathbf{f}, \rho)$, $H_{\mathcal{F}_K}(\mathbf{f}, \rho)$ and $\mathbb{B}_{\mathcal{F}_K}(\mathbf{c}, r)$. For differential operators $D, \tilde{D} \in O_{Q,s}$ defined as $D(\mathbf{f})(\mathbf{x}) = \sum_{q\in[Q]} \beta_q D_{q,\mathbf{x}}(f_q)(\mathbf{x})$ and $\tilde{D}(\mathbf{f})(\mathbf{x}') = \sum_{q\in[Q]} \tilde{\beta}_q \tilde{D}_{q,\mathbf{x}'}(f_q)(\mathbf{x}')$ and for a kernel $K \in \mathcal{C}^{s,s}\left(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{Q\times Q}\right)$, let

$$\tilde{D}^\top D K(\mathbf{x}', \mathbf{x}) = \sum_{q,q'\in[Q]} \tilde{\beta}_{q'} \beta_q \mathbf{e}_{q'}^\top \tilde{D}_{q',\mathbf{x}'} D_{q,\mathbf{x}} K(\mathbf{x}', \mathbf{x})\mathbf{e}_q \in \mathbb{R}.$$

In this paper we **focus** on optimization problems over vRKHSs with hard affine SDP shape constraints on derivatives. We formulate our problem in the empirical risk minimization framework. Assume that we have access to samples $S = ((\mathbf{x}_n, \mathbf{y}_n))_{n\in[N]} \subset \mathcal{X} \times \mathbb{R}^Q$

which are supposed to be fixed and $\mathcal{X} \subseteq \mathbb{R}^d$ is assumed to be contained in the closure of its interior. We are given a kernel $K : \mathcal{X} \times \mathcal{X} \to \mathbb{R}^{Q \times Q}$ with associated vRKHS $\mathcal{F}_K$; K is assumed to belong to $\mathcal{C}^{s,s}\left(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{Q \times Q}\right)$ with order $s \in \mathbb{N}$. The function family $\mathcal{F}_K$ is used to capture the relation between the random variables $\mathbf{x}$ and $\mathbf{y}$ via the samples S, with the optional usage of a bias term $\mathbf{b} \in \mathbb{R}^B$. The goodness of the estimated pair $(\mathbf{f}, \mathbf{b}) \in \mathcal{F}_K \times \mathbb{R}^B$ is measured through a loss function L (with the samples S kept fixed) which can take into account both function values and function derivatives at the input points $\mathbf{x}_n$; their number $\#J_n$ is allowed to differ for each n. The function values and derivatives of interest at each point $\mathbf{x}_n$ are represented by the linear differential operators $(D^0_{n,j})_{j \in J_n} \subset O_{Q,s}$. With these notations, our objective function to minimize is

$$\mathcal{L}(\mathbf{f}, \mathbf{b}) = L\left(\mathbf{b}, \left(\left(D^0_{n,j}(\mathbf{f})(\mathbf{x}_n)\right)_{j \in J_n}\right)_{n \in [N]}\right) + R\left(\|\mathbf{f}\|_K\right), \tag{3}$$

where $L : \mathbb{R}^B \times \mathbb{R}^{\sum_{n \in [N]} \#J_n} \to \mathbb{R} \cup \{\infty\}$, and $R : \mathbb{R}_+ \to \mathbb{R}$ is a regularizer. The pair $(\mathbf{f}, \mathbf{b})$ is constrained: the bias variable $\mathbf{b}$ has to belong to a closed convex set $\mathcal{B} \subseteq \mathbb{R}^B$, and more importantly $(\mathbf{f}, \mathbf{b})$ is required to satisfy $I \in \mathbb{N}^*$ *hard affine SDP shape constraints* on given sets $\mathcal{K}_i \subseteq \mathcal{X}$ which are assumed to be compact[2]:

$$C = \left\{(\mathbf{f}, \mathbf{b}) \,:\, \mathbf{0}_{P_i \times P_i} \preccurlyeq \mathbf{D}_i(\mathbf{f} - \mathbf{f}_{0,i})(\mathbf{x}) + \operatorname{diag}(\mathbf{\Gamma}_i \mathbf{b} - \mathbf{b}_{0,i}), \forall\, \mathbf{x} \in \mathcal{K}_i, \forall\, i \in [I]\right\}. \tag{$\mathcal{C}$}$$

In ($\mathcal{C}$) the operator $\mathbf{D}_i$ aggregates s-th order derivatives to the SDP constraints, i.e.

$$\mathbf{D}_i(\mathbf{f})(\mathbf{x}) = \left[D^i_{p_1,p_2}(\mathbf{f})(\mathbf{x})\right]_{p_1,p_2 \in [P_i]} \in S_{P_i} \tag{4}$$

with elements $D^i_{p_1,p_2} \in O_{Q,s}$. For instance, when $Q = 1$, $s = 2$, $I = 1$, $P_1 = d$, $\mathbf{0}_{d \times d} \preccurlyeq \mathbf{D}_1 := [\partial^{\mathbf{e}_i + \mathbf{e}_j}]_{i,j \in [d]}$ requires the estimated function to be convex when its domain is restricted to a (convex) compact set $\mathcal{K}_1$; requiring the function to be convex only in a subset of its arguments can be achieved by setting $P_i < d$. Possible shifts in ($\mathcal{C}$) are expressed by the terms $\mathbf{b}_{0,i} \in \mathbb{R}^{P_i}$ and $\mathbf{f}_{0,i} \in \mathcal{F}_K$. The matrices $\mathbf{\Gamma}_i \in \mathbb{R}^{P_i \times B}$ allow linear interaction between the bias coordinates. The bias $\mathbf{b} \in \mathbb{R}^B$ can be both variable (e.g. $f_q + b_q$) and constraint-related (such as $b_1 \le f(x)$, $b_2 \le f'(x)$); hence B can differ from Q. The geometric intuition of the $(\mathbf{f}, \mathbf{b})$ pair follows that of the classical support vector machines where $\mathbf{f}$ controls the direction, whereas $\mathbf{b}$ determines the bias of the optimal hyperplane. Thus our **problem of interest** combining the objective (3) and the hard affine SDP constraints ($\mathcal{C}$) can be written as

$$\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right) \in \underset{\substack{\mathbf{f} \in \mathcal{F}_K,\, \mathbf{b} \in \mathcal{B}, \\ (\mathbf{f}, \mathbf{b}) \in C}}{\arg\min}\ \mathcal{L}(\mathbf{f}, \mathbf{b}). \tag{$\mathcal{P}$}$$

Remarks:

- Rewriting SDP constraints as ($\mathcal{C}$): Using ($\mathcal{C}$) one can incorporate affine SDP constraints of the form

$$\{(\mathbf{f}, \mathbf{b}) \,|\, \mathbf{0}_{P \times P} \preccurlyeq \tilde{\mathbf{D}}(\mathbf{f} - \mathbf{f}_0)(\mathbf{x}) + \mathbf{M}, \forall\, \mathbf{x} \in \mathcal{K}\},$$

2. While in general we assume the $\mathcal{K}_i$-s to be compact in $\mathcal{X}$, this requirement can be relaxed to boundedness of their image in $\mathcal{F}_K$ under additional assumptions; see remark 'Non-compact $\mathcal{K}$' in Section 3.1.

where $\mathbf{M} \in S_P$. Indeed, by setting $\mathbf{\Gamma} = \mathbf{0}$ and $\mathbf{b}_0 = -\text{eig}(\mathbf{M})$ to be the negative of the eigenvalues of $\mathbf{M}$, and using the spectral theorem

$$\begin{aligned}
\mathbf{0}_{P\times P} \preccurlyeq \tilde{\mathbf{D}}(\mathbf{f}-\mathbf{f}_0)(\mathbf{x}) + \mathbf{M} &= \tilde{\mathbf{D}}(\mathbf{f}-\mathbf{f}_0)(\mathbf{x}) + \mathbf{U}^\top \text{eig}(\mathbf{M})\mathbf{U} \\
&= \tilde{\mathbf{D}}(\mathbf{f}-\mathbf{f}_0)(\mathbf{x}) + \mathbf{U}^\top \text{diag}(\mathbf{\Gamma}\mathbf{b}-\mathbf{b}_0)\mathbf{U} \Leftrightarrow \\
\mathbf{0}_{P\times P} \preccurlyeq \underbrace{\mathbf{U}\tilde{\mathbf{D}}(\mathbf{f}-\mathbf{f}_0)(\mathbf{x})\mathbf{U}^\top}_{=:\mathbf{D}(\mathbf{f}-\mathbf{f}_0)(\mathbf{x})} &+ \text{diag}(\mathbf{\Gamma}\mathbf{b}-\mathbf{b}_0).
\end{aligned}$$

- Further specific cases of $(\mathcal{C})$: Examples of $(\mathcal{C})$ beyond the more classical case of non-negativity, monotonicity or convexity include for instance n-monotonicity, monotonicity w.r.t. various partial orderings, n-alternating monotonicity, or supermodularity (Aubin-Frankowski and Szabó, 2020, Section C).
- Cases not covered in $(\mathcal{C})$: Examples *not* covered directly by $(\mathcal{C})$ include for instance the Slutzky shape constraint and the quasi-convexity formula which are alternative assumptions on demand or utility functions. These non-affine requirements write as $\frac{\partial f(x_1,x_2)}{\partial x_1} + f(x_1,x_2)\frac{\partial f(x_1,x_2)}{\partial x_2} \leq 0$ for $\forall x_1, x_2$ and $f(\alpha\mathbf{x} + (1-\alpha)\mathbf{x}') \leq \max(f(\mathbf{x}), f(\mathbf{x}'))$ for $\forall \alpha \in [0,1], \forall \mathbf{x}, \mathbf{x}'$, respectively.
- Equality constraints in $(\mathcal{P})$: In this article, our primary focus is on convex *inequality* constraints, handled through an interior approximation. Considering equalities, convex equalities are affine, so they would effectively restrict the hypothesis class to a closed affine subspace. A closed subspace of a vRKHS is also a vRKHS, possibly with a different kernel. Finitely many equality constraints can be handled in our framework without difficulty and without changing kernel; see our example on shape optimization in Section 6.1. On the other hand, an infinite number of equality requirements may require to determine explicitly the kernel of the subspace, which can be difficult. Nevertheless this is possible for instance in case of a linear control problem (see Section 6.2 and footnote 11).

Examples: It is instructive to consider a few examples for the problem family $(\mathcal{P})$.

- Joint quantile regression (JQR; as for instance defined by Sangnier et al. (2016)): Assume that we are given samples $((\mathbf{x}_n, y_n))_{n\in[N]}$ from the random variable (X, Y) with values in $\mathcal{X} \times \mathbb{R} \subseteq \mathbb{R}^{d+1}$, as well as Q levels $0 < \tau_1 < \ldots < \tau_Q < 1$. Our goal is to estimate *jointly* the τ_q-quantiles of the conditional distributions $\mathbb{P}(Y|X = \mathbf{x})$ for $q \in [Q]$. In the JQR problem the estimated τ_q-quantile functions $(f_q + b_q)_{q\in[Q]}$ (modulo the biases $b_q \in \mathbb{R}$) belong to a real-valued RKHS $\mathcal{F}_k$ associated to a kernel $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$, and they have to satisfy jointly a monotonically increasing property w.r.t. the quantile level τ. It is natural to require this non-crossing property on the smallest rectangle containing the input points $(\mathbf{x}_n)_{n\in[N]}$, in other words on $\mathcal{K} = \prod_{j\in[d]} \left[\min\{(\mathbf{x}_n)_j\}_{n\in[N]}, \max\{(\mathbf{x}_n)_j\}_{n\in[N]}\right]$. Hence, the optimization problem in JQR takes the form

$$\begin{aligned}
\min_{\substack{\mathbf{f}\in(\mathcal{F}_k)^Q,\\ \mathbf{b}\in\mathbb{R}^Q}} \quad & \mathcal{L}(\mathbf{f},\mathbf{b}) := \frac{1}{N}\sum_{q\in[Q]}\sum_{n\in[N]} \ell_{\tau_q}(y_n - [f_q(\mathbf{x}_n) + b_q]) + \lambda_{\mathbf{b}}\|\mathbf{b}\|_2^2 + \lambda_f \sum_{q\in[Q]} \|f_q\|_{\mathcal{F}_k}^2 \\
\text{s.t.} \quad & f_q(\mathbf{x}) + b_q \leq f_{q+1}(\mathbf{x}) + b_{q+1},\ \forall q \in [Q-1],\ \forall \mathbf{x} \in \mathcal{K}
\end{aligned}$$

where $\lambda_{\mathbf{b}} > 0$, $\lambda_f > 0$,[3] and the pinball loss is defined as $\ell_\tau(e) = \max(\tau e, (\tau-1)e)$ with $\tau \in (0,1)$. This problem can be obtained as a specific case of ($\mathcal{P}$) by choosing $B = Q$, $s = 0$, $I = Q-1$, $P_i = 1$, $\mathbf{D}_i(\mathbf{f}) = f_{i+1} - f_i$, $\mathbf{\Gamma}_i(\mathbf{b}) = b_{i+1} - b_i$ ($\forall i \in [I]$), $K(\mathbf{x},\mathbf{x}') = k(\mathbf{x},\mathbf{x}')\mathbf{I}_Q$, $\mathbf{f}_{0,i} = \mathbf{0}$, $\mathbf{b}_0 = \mathbf{0}$, $\mathcal{B} = \mathbb{R}^B$. Further details and numerical illustration on the JQR problem are provided by Aubin-Frankowski and Szabó (2020).

- Convoy trajectory reconstruction (CTR): Here, the goal is to estimate vehicle trajectories based on noisy observations. This is a typical situation with GPS measurements, where the imprecision can be compensated through side information, not using only the position of every vehicle but also that of its neighbors. Assume that there are Q vehicles forming a convoy (i.e. they do not overtake and keep a minimum inter-vehicular distance between each other) with speed limit on the vehicles. For each vehicle q we have N_q noisy position measurements $(y_{q,n})_{n\in[N_q]} \subset \mathbb{R}$, each associated with vehicle-specific time points $(x_{q,n})_{n\in[N_q]} \subset \mathcal{X} := [0,T]$. Without loss of generality, let the vehicles be ordered in the lane according to their indices ($q = 1$ is the first, $q = Q$ is the last one). Let $d_{\min} \geq 0$ be the minimum inter-vehicular distance, and $v_{\min}$ be the minimal speed to keep.[4] By modelling the location of the q^{th} vehicle at time x as $b_q + f_q(x)$ where $b_q \in \mathbb{R}$, $f_q \in \mathcal{F}_k$ and $k : \mathcal{X} \times \mathcal{X} \to \mathbb{R}$ is a real-valued kernel, the CTR task can be formulated as

$$\begin{aligned} \min_{\substack{\mathbf{f}=[f_q]_{q\in[Q]}\in(\mathcal{F}_k)^Q,\\ \mathbf{b}\in\mathbb{R}^Q}} \quad & \mathcal{L}(\mathbf{f},\mathbf{b}) := \frac{1}{Q}\sum_{q=1}^{Q}\left[\left(\frac{1}{N_q}\sum_{n=1}^{N_q}|y_{q,n} - (b_q + f_q(x_{q,n}))\,|^2\right) + \lambda\|f_q\|^2_{\mathcal{F}_k}\right] \\ \text{s.t.} \quad & d_{\min} + b_{q+1} + f_{q+1}(x) \leq b_q + f_q(x), \quad \forall q \in [Q-1], \forall x \in \mathcal{X}, \\ & v_{\min} \leq f_q'(x) \quad \forall q \in [Q], \forall x \in \mathcal{X}. \end{aligned}$$

  This problem can be obtained as a specific case of ($\mathcal{P}$) by choosing $B = Q$, $s = 1$, $I = 2Q-1$, $P_i = 1$ ($i \in [I]$), $K(\mathbf{x},\mathbf{x}') = k(\mathbf{x},\mathbf{x}')\mathbf{I}_Q$, $\mathbf{D}_i(\mathbf{f}) = f_i - f_{i+1}$ ($i \in [Q-1]$), $\mathbf{\Gamma}_i\mathbf{b} = b_i - b_{i+1}$ ($i \in [Q-1]$), $b_{0,i} = d_{\min}$ ($i \in [Q-1]$), $\mathbf{D}_i(\mathbf{f}) = f'_{i-(Q-1)}$ ($i \in \{Q, Q+1, \ldots, 2Q-1\}$), $\mathbf{\Gamma}_i = \mathbf{0}_{1,Q}$ ($i \in \{Q, Q+1, \ldots, 2Q-1\}$), $b_{0,i} = v_{\min}$ ($i \in \{Q, Q+1, \ldots, 2Q-1\}$), $\mathcal{B} = \mathbb{R}^B$. This application was investigated by Aubin-Frankowski et al. (2020).

- Further examples: In Section 6 we consider three complementary problems with numerical illustration. The examples cover a shape optimization task (minimizing the deformation of a catenary under its weight, with a stand underneath), safety-critical control (piloting an underwater vehicle while avoiding obstacles), and econometrics (learning production functions).

3. Constraints

In this section we propose two approaches to handle a single hard affine SDP shape constraint ($I = 1$) appearing in ($\mathcal{C}$) over a (non-finite) compact[2] set $\mathcal{K}$

$$C_P = \{(\mathbf{f},\mathbf{b}) \,:\, \mathbf{0}_{P\times P} \preccurlyeq \mathbf{D}(\mathbf{f}-\mathbf{f}_0)(\mathbf{x}) + \operatorname{diag}(\mathbf{\Gamma}\mathbf{b} - \mathbf{b}_0), \forall \mathbf{x} \in \mathcal{K}\}. \qquad (\mathcal{C}_P)$$

3. Sangnier et al. (2016) used the same loss function but a soft non-crossing inducing regularizer inspired by matrix-valued kernels, and also set $\lambda_{\mathbf{b}} = 0$.
4. The requirement $v_{\min} = 0$ means that the vehicles go forward. A maximum speed constraint can be imposed similarly.

Multiple shape constraints ($I > 1$) can be addressed by stacking the presented results.

There are two main challenges to tackle: (i) C_P cannot be directly implemented since $\mathcal{K}$ is non-finite, (ii) deriving a representer theorem is also problematic as the number of evaluations of $\mathbf{f}$ is non-finite. To address these challenges, we propose two complementary approaches (depending on the value of P) to tighten C_P through finite coverings[5]:

1. **Compact covering in $\mathcal{F}_K$ with balls and half-spaces,** $P = 1$: This first approach focuses on the real-valued case of $P = 1$, i.e.

$$C_1 = \{(\mathbf{f}, \mathbf{b}) \,:\, 0 \le D(\mathbf{f} - \mathbf{f}_0)(\mathbf{x}) + \mathbf{\Gamma b} - b_0, \forall\, \mathbf{x} \in \mathcal{K}\}\,. \tag{$\mathcal{C}_1$}$$

   We show that ($\mathcal{C}_1$) can be written as the inclusion in the vRKHS $\mathcal{F}_K$ of a compact set in a half-space. We then tighten this inclusion by taking a finite covering of the compact set through balls and half-spaces in $\mathcal{F}_K$, and present a general theorem which enables one to translate such inclusions into convex equations.

2. **Upper bounding the modulus of continuity,** $P \ge 1$: Our second approach tackles the general case of $P \ge 1$, i.e. ($\mathcal{C}_P$), through an upper bound on the modulus of continuity of $\mathbf{D}(\mathbf{f} - \mathbf{f}_0)$ defined on a finite covering of $\mathcal{K}$. The upper bound has the form $\eta_{m,P}\|\mathbf{f} - \mathbf{f}_0\|_K$ which leads to second-order cone (SOC) constraints instead of affine inequalities. We will see that the two methods coincide when $P = 1$ and when only ball coverings are considered.

We start with a lemma stating the reproducing property for derivatives of matrix-valued kernels.

Lemma 1 (Reproducing property for derivatives with matrix-valued kernels) *Let $s \in \mathbb{N}$, $\mathcal{X} \subseteq \mathbb{R}^d$ be a set which is contained in the closure of its interior, K be a matrix-valued kernel such that $K \in \mathcal{C}^{s,s}\left(\mathcal{X} \times \mathcal{X}, \mathbb{R}^{Q\times Q}\right)$, and $D \in O_{Q,s}$ be a differential operator such that $D(\mathbf{f})(\mathbf{x}) = \sum_{q\in[Q]} \beta_q D_q f_q(\mathbf{x})$. Let*

$$DK(\mathbf{x}', \mathbf{x}) := \sum_{q\in[Q]} \beta_q [D_{q,\mathbf{x}} K(\mathbf{x}', \mathbf{x})]\mathbf{e}_q \in \mathbb{R}^Q, \tag{5}$$

where $D_{q,\mathbf{x}}K(\mathbf{x}', \mathbf{x}) := D_q[\mathbf{x}'' \mapsto K(\mathbf{x}', \mathbf{x}'')](\mathbf{x}) \in \mathbb{R}^{Q\times Q}$ and $\mathbf{e}_q \in \mathbb{R}^Q$ is the q-th canonical basis vector. Then

$$\mathbf{f} \in \mathcal{C}^s\left(\mathcal{X}, \mathbb{R}^Q\right), \qquad DK(\cdot, \mathbf{x}) \in \mathcal{F}_K, \qquad D(\mathbf{f})(\mathbf{x}) = \langle \mathbf{f}, DK(\cdot, \mathbf{x})\rangle_K \tag{6}$$

for all $\mathbf{f} \in \mathcal{F}_K$ and $\mathbf{x} \in \mathcal{X}$.

Remark: Specifically for $s = 0$, one has that $D(\mathbf{f})(\mathbf{x}) = \sum_{q\in[Q]} \beta_q f_q(\mathbf{x}) = \boldsymbol{\beta}^\top \mathbf{f}(\mathbf{x})$ and (6) reduces to the classical reproducing property in vRKHSs, i.e. $\boldsymbol{\beta}^\top \mathbf{f}(\mathbf{x}) = \langle \mathbf{f}, K(\cdot, \mathbf{x})\boldsymbol{\beta}\rangle_K$. The reproducing property for kernel derivatives has been studied over open sets $\mathcal{X}$, for real-valued (Saitoh and Sawano, 2016) and matrix-valued (Micheli and Glaunés, 2014) kernels, and over compact sets which are the closure of their interior for real-valued kernels (Zhou, 2008). In Lemma 1 we generalize these results to matrix-valued kernels and to sets $\mathcal{X}$ which are contained in the closure of their interior.

5. By considering finite coverings, we make the problem amenable to optimization. This computational aspect is elaborated in Section 4.

3.1 Constraints by Compact Covering in $\mathcal{F}_K$

In our **first approach**, applying Lemma 1, we rephrase constraint $(\mathcal{C}_1)$ as an inclusion of sets using the non-linear embedding $\mathbf{\Phi}_D : \mathbf{x} \in \mathcal{K} \mapsto DK(\cdot, \mathbf{x}) \in \mathcal{F}_K$

$$\begin{aligned}(\mathbf{f}, \mathbf{b}) \in C_1 &\Leftrightarrow b_0 - \mathbf{\Gamma b} \leq D(\mathbf{f} - \mathbf{f}_0)(\mathbf{x}) = \langle \mathbf{f} - \mathbf{f}_0, DK(\cdot, \mathbf{x})\rangle_K \; \forall \mathbf{x} \in \mathcal{K} \\ &\Leftrightarrow \mathbf{\Phi}_D(\mathcal{K}) := \{DK(\cdot, \mathbf{x}) \,:\, \mathbf{x} \in \mathcal{K}\} \subseteq H_K^+(\mathbf{f} - \mathbf{f}_0, b_0 - \mathbf{\Gamma b}). \end{aligned} \tag{7}$$

The set $\mathbf{\Phi}_D(\mathcal{K})$ is compact in $\mathcal{F}_K$ since $\mathcal{K}$ is compact in $\mathcal{X}$ and $\mathbf{\Phi}_D$ is continuous. However it is intractable to directly ensure the inclusion described in (7) whenever $\mathcal{K}$ is not finite. We thus consider an approximation with a “simpler“ set $\bar{\Omega}$ containing $\mathbf{\Phi}_D(\mathcal{K})$, and require the inclusion

$$\mathbf{\Phi}_D(\mathcal{K}) \subseteq \bar{\Omega} \subseteq H_K^+(\mathbf{f} - \mathbf{f}_0, b_0 - \mathbf{\Gamma b}) \tag{8}$$

which implies (7).[6] Since $\mathbf{\Phi}_D(\mathcal{K})$ is compact, drawing upon compact coverings, we assume that

$$\bar{\Omega} = \cup_{m \in [M]} \bar{\Omega}_m, \tag{9}$$

where each $\bar{\Omega}_m$ is the closure of a non-empty finite intersection ($J_{B,m}, J_{H,m} \in \mathbb{N}$) of non-trivial ($r_{m,j} > 0$, $\mathbf{v}_{m,j} \neq \mathbf{0}$) open balls and open half-spaces.

$$\Omega_m = \left(\bigcap_{j \in [J_{B,m}]} \mathring{\mathbb{B}}_K(\mathbf{c}_{m,j}, r_{m,j}) \right) \cap \left(\bigcap_{j \in [J_{H,m}]} \mathring{H}_K^-(\mathbf{v}_{m,j}, \rho_{m,j}) \right). \tag{10}$$

Remarks:

- Form of (10): The motivation for considering $\bar{\Omega}$ and $\bar{\Omega}_m$ of the form (9) and (10) is several-fold. Having a finite description enables one to derive a representer theorem. However, only a few sets (mainly points, balls and half-spaces) enjoy explicit convex separation formulas (which arise naturally when considering inclusions, see footnote 8). Focusing on *points* leads to a discretization of $\mathbf{\Phi}_D(\mathcal{K})$ and greedy strategies (such as the Frank-Wolfe algorithm), but without guarantees outside of the points considered. A finite union of *balls* can approximate any compact set, but balls result in enforcing “buffers“ in every direction of $\mathcal{F}_K$. A finite intersection of *half-spaces* can approximate any convex set,[7] but this finite intersection is always unbounded for infinite-dimensional $\mathcal{F}_K$ resulting in a poor approximation of compact sets. Motivated by obtaining guarantees, we thus consider combinations of balls and half-spaces as in (9)-(10).

---

6. A simple example for translation-invariant kernels $K(\mathbf{x}, \mathbf{y}) = K_0(\mathbf{x} - \mathbf{y})$ is the (coarse) approximation $\mathbf{\Phi}_D(\mathcal{K}) \subseteq \mathbb{B}_K\left(\mathbf{0}, \sqrt{D^\top D K_0(\mathbf{0})}\right)$. Indeed, $\|DK(\cdot, \mathbf{x})\|_K = \sqrt{\langle DK(\cdot, \mathbf{x}), DK(\cdot, \mathbf{x})\rangle_K} = \sqrt{D^\top D K(\mathbf{x}, \mathbf{x})} = \sqrt{D^\top D K_0(\mathbf{0})}$ for any $\mathbf{x} \in \mathcal{X}$ by Lemma 1.
7. To motivate the use of half-spaces in (10): notice that since the half-space on the r.h.s. of (7) is closed and convex, (7) is equivalent to showing that the closed convex hull $\overline{\mathrm{co}}(\Phi_D(\mathcal{K}))$ is a subset of $H_K^+(\mathbf{f} - \mathbf{f}_0, b_0 - \mathbf{\Gamma b})$. Using the support function characterization of closed convex sets, we have that $\overline{\mathrm{co}}(\Phi_D(\mathcal{K})) = \bigcap_{\mathbf{g} \in \mathcal{F}_K} H_K^-(\mathbf{g}, \sigma_{\mathcal{K}}(\mathbf{g}))$ where $\sigma_{\mathcal{K}}(\mathbf{g}) := \sup_{x \in \mathcal{K}} D(\mathbf{g})(x)$ has to be computed. Considering any finite collection of $g \in \mathcal{F}_K$ provides an over-approximation of $\overline{\mathrm{co}}(\Phi_D(\mathcal{K}))$ with finite description.

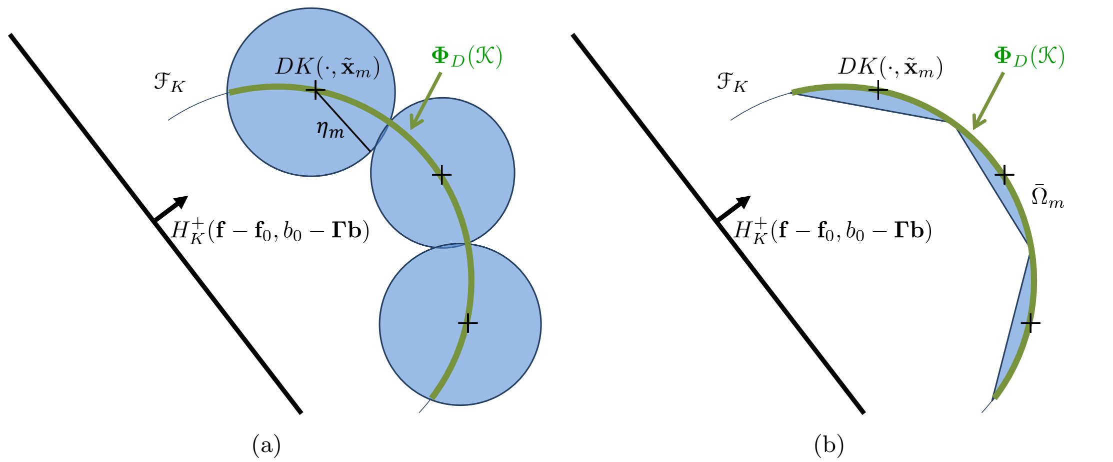


Figure 1: Two examples of coverings in $\mathcal{F}_K$ of $\mathbf{\Phi}_D(\mathcal{K})$ by a set $\bar{\Omega} = \cup_{m\in[M]}\bar{\Omega}_m$ contained in the halfspace $H_K^+(\mathbf{f}-\mathbf{f}_0, b_0-\mathbf{\Gamma b})$. (a): covering through balls $\Omega_m = \mathring{\mathbb{B}}_K\left(DK(\cdot,\tilde{\mathbf{x}}_m),\eta_m\right)$. (b): covering through a ball intersected with halfspaces ($J_{B,m} = J_{H,m} = 1$).

- Non-compact $\mathcal{K}$: Coverings of the form (9) and (10) exist for any bounded $\mathbf{\Phi}_D(\mathcal{K})$. In particular, if the kernel $D^\top DK(\cdot,\cdot)$ is bounded, then for any set $\mathcal{K}\subseteq\mathcal{X}$, $\mathbf{\Phi}_D(\mathcal{K})\subset\mathcal{F}_K$ is bounded as well. Consequently the proposed method can be applied to non-compact $\mathcal{K}$ provided that the derivatives of the chosen kernel are bounded.

Theorem 2 below provides an explicit convex formula to be satisfied that is equivalent to the tightened inclusion (8) under the choice (9)-(10). Since $\bar{\Omega}_m$ is the closure of the non-empty open set Ω_m, and the half-spaces H_K^+ are closed,

$$\begin{aligned}\bar{\Omega} = \cup_{m\in[M]}\bar{\Omega}_m \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0-\mathbf{\Gamma b}) &\Leftrightarrow \bar{\Omega}_m \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0-\mathbf{\Gamma b})\,\forall\, m\in[M]\\ &\Leftrightarrow \Omega_m \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0-\mathbf{\Gamma b})\,\forall\, m\in[M]. \qquad (11)\end{aligned}$$

Hence we can consider separately the inclusion of each Ω_m, formulate the theorem for $M=1$ and drop the index m.[8]

Theorem 2 (Inclusion formula for balls and half-spaces) *Let $\mathcal{F}_K$ be the vRKHS associated to a $\mathbb{R}^{Q\times Q}$-valued kernel K. Then the following statements are equivalent:*

1. $\emptyset \neq \Omega := \left(\bigcap_{j\in[J_B]}\mathring{\mathbb{B}}_K(\mathbf{c}_j,r_j)\right)\cap\left(\bigcap_{j\in[J_H]}\mathring{H}_K^-(\mathbf{v}_j,\rho_j)\right)\subseteq H_K^+\left(\mathbf{f}-\mathbf{f}_0, b_0-\mathbf{\Gamma b}\right)\neq\mathcal{F}_K.$
2. *There exists J_B functions $(\mathbf{g}_j)_{j\in[J_B]}\subset \operatorname{span}\left(\mathbf{f}-\mathbf{f}_0,\{\mathbf{c}_j\}_{j\in[J_B]},\{\mathbf{v}_j\}_{j\in[J_H]}\right)$ and J_H non-negative coefficients $(\xi_j)_{j\in[J_H]}\in\mathbb{R}_+^{J_H}$ such that*

$$\begin{aligned}-b_0+\mathbf{\Gamma b}+\sum_{j\in[J_B]}\langle\mathbf{g}_j,\mathbf{c}_j\rangle_K-\sum_{j\in[J_H]}\xi_j\rho_j-\sum_{j\in[J_B]}r_j\|\mathbf{g}_j\|_K\geq 0,\\ -(\mathbf{f}-\mathbf{f}_0)+\sum_{j\in[J_B]}\mathbf{g}_j-\sum_{j\in[J_H]}\xi_j\mathbf{v}_j=\mathbf{0}.\end{aligned}\qquad (12)$$

8. Since Ω_m is convex, the inclusion $\Omega_m\subseteq H_K^+(\mathbf{f}-\mathbf{f}_0,b_0-\mathbf{\Gamma b})$ in (11) is equivalent to $\Omega_m\cap\mathring{H}_K^-(\mathbf{f}-\mathbf{f}_0,b_0-\mathbf{\Gamma b})=\emptyset$ which can be interpreted as a convex separation problem.

Remarks:

- ($\mathcal{C}_{1,\Omega}$) is tighter than ($\mathcal{C}_1$): Theorem 2 provides a general finite-dimensional formula for separating convex sets combining balls and half-spaces. It can be of independent interest for studies in RKHSs. Specifically, using the notation

$$C_{1,\Omega} = \{(\mathbf{f}, \mathbf{b}) \,:\, (12) \text{ holds for all } m \in [M]\}, \tag{$\mathcal{C}_{1,\Omega}$}$$

requiring $(\mathbf{f}, \mathbf{b}) \in C_{1,\Omega}$ is equivalent to having $\bar{\Omega} \subseteq H_K^+(\mathbf{f} - \mathbf{f}_0, b_0 - \mathbf{\Gamma b})$ by Theorem 2 and (8). Hence, owing to (7), ($\mathcal{C}_{1,\Omega}$) is a tighter constraint than ($\mathcal{C}_1$), i.e. $C_{1,\Omega} \subseteq C_1$.

- Illustration: A visual illustration of the inclusion relation for a single ball ($J_B = 1, J_H = 0$), and for one ball and one half-space ($J_B = J_H = 1$) is given in Fig. 1(a) and Fig. 1(b), respectively.

- Case of a single ball ($J_B = 1$, $J_H = 0$): In the simplest case where there is a single ball and no half-spaces, i.e. $\Omega = \mathring{\mathbb{B}}_K(\mathbf{c}, r)$, then (12) reduces to $\mathbf{g} = \mathbf{f} - \mathbf{f}_0$ and $\langle \mathbf{g}, \mathbf{c}\rangle_K \geq r \|\mathbf{g}\|_K + b_0 - \mathbf{\Gamma b}$, thus

$$\langle \mathbf{f} - \mathbf{f}_0, \mathbf{c}\rangle_K \geq r \|\mathbf{f} - \mathbf{f}_0\|_K + b_0 - \mathbf{\Gamma b}. \tag{13}$$

- Case of one ball and one half-space ($J_B = J_H = 1$): In this case $\Omega = \mathring{\mathbb{B}}_K(\mathbf{c}, r) \cap \mathring{H}_K^-(\mathbf{v}, \rho)$ and (12) writes as $\mathbf{f} - \mathbf{f}_0 = \mathbf{g} - \xi \mathbf{v}$ and $\langle \mathbf{g}, \mathbf{c}\rangle_K \geq r \|\mathbf{g}\|_K + b_0 - \mathbf{\Gamma b} + \xi\rho$, thus

$$\langle \mathbf{f} - \mathbf{f}_0 + \xi\mathbf{v}, \mathbf{c}\rangle_K \geq r \|\mathbf{f} - \mathbf{f}_0 + \xi\mathbf{v}\|_K + b_0 - \mathbf{\Gamma b} + \xi\rho. \tag{14}$$

- Constructing Ω using the compactness of $\mathcal{K}$: A natural choice of Ω of the form (9) can be obtained by leveraging the compactness of $\mathcal{K}$. Indeed, let us take any finite covering of $\mathcal{K}$ through balls centered at M points $\{\tilde{\mathbf{x}}_m\}_{m\in[M]}$ with radius $\delta_m > 0$. Then one can cover the sets $\Phi_D(\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)) \subset \mathcal{F}_K$ by balls $\Omega_m = \mathring{\mathbb{B}}_K(DK(\cdot, \tilde{\mathbf{x}}_m), \eta_m)$ with radii

$$\eta_m = \sup_{\mathbf{x}\,\in\,\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)} \|DK(\cdot, \tilde{\mathbf{x}}_m) - DK(\cdot, \mathbf{x})\|_K,\ m \in [M]. \tag{15}$$

In other words, $\Phi_D(\mathcal{K}) \subseteq \bigcup_{m\in[M]} \Phi_D(\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)) \subseteq \bigcup_{m\in[M]} \bar{\Omega}_m =: \bar{\Omega}$, hence $\bar{\Omega}$ satisfies (8) and $(\mathbf{f}, \mathbf{b}) \in C_{1,\Omega}$. In this case ($\mathcal{C}_1$) has been strengthened to the SOC constraints

$$\langle \mathbf{f} - \mathbf{f}_0, \mathbf{c}_m\rangle_K \geq r_m \|\mathbf{f} - \mathbf{f}_0\|_K + b_0 - \mathbf{\Gamma b}, \quad \forall m \in [M], \tag{16}$$

where $c_m := DK(\cdot, \tilde{\mathbf{x}}_m)$ and $r_m := \eta_m$, by using (13).

The tightening we detailed in this section allows for a large class of coverings based on balls and half-spaces. However the reformulation (7) heavily relies on the assumption of $P = 1$.

3.2 Constraints by Upper Bounding the Modulus of Continuity

We now present a **second approach** capable of handling $P \geq 1$, i.e. the affine SDP constraint ($\mathcal{C}_P$). The method relies on an upper bound of the modulus of continuity of $\mathbf{D}(\mathbf{f} - \mathbf{f}_0)$ over a finite covering of a compact $\mathcal{K} \subseteq \bigcup_{m\in[M]} \mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$. For simplicity, we present the high-level idea for $P = 1$. Let the modulus of continuity of $D(\mathbf{f} - \mathbf{f}_0)$ on $\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$ be defined as

$$\omega_{D(\mathbf{f}-\mathbf{f}_0)}(\tilde{\mathbf{x}}_m, \delta_m) := \sup_{\mathbf{x}\,\in\,\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)} |D(\mathbf{f} - \mathbf{f}_0)(\mathbf{x}) - D(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m)|. \tag{17}$$

Assume that we have an exact finite covering, in other words $\mathcal{K} = \bigcup_{m\in[M]} \mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$. If $\omega_{D(\mathbf{f}-\mathbf{f}_0)}(\tilde{\mathbf{x}}_m, \delta_m)$ was known for every $m \in [M]$, then the constraint $(\mathbf{f}, \mathbf{b}) \in C_P$ would be equivalent to

$$\omega_{D(\mathbf{f}-\mathbf{f}_0)}(\tilde{\mathbf{x}}_m, \delta_m) \leq D(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m) + \mathbf{\Gamma b} - b_0, \, \forall \, m \in [M]. \tag{18}$$

The equivalence follows from (17) since the modulus of continuity is the smallest upper bound of the variations of the values. Applying the reproducing property for derivatives (Lemma 1) and the Cauchy-Schwarz inequality, we obtain an upper bound

$$\omega_{D(\mathbf{f}-\mathbf{f}_0)}(\tilde{\mathbf{x}}_m, \delta_m) = \sup_{\mathbf{x}\,\in\,\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m,\delta_m)} |\langle \mathbf{f} - \mathbf{f}_0, DK(\cdot, \mathbf{x}) - DK(\cdot, \tilde{\mathbf{x}}_m)\rangle_K| \leq \eta_m \|\mathbf{f} - \mathbf{f}_0\|_K \tag{19}$$

with η_m defined as in (15). While the original quantity $\omega_{D(\mathbf{f}-\mathbf{f}_0)}(\tilde{\mathbf{x}}_m, \delta_m)$ can be hard to evaluate, the bound $\eta_m \|\mathbf{f} - \mathbf{f}_0\|_K$ is much more favourable from a computational perspective. Indeed, the term η_m has an explicit finite-dimensional description (see Lemma 4 below), and combining (19) with (18) gives rise to the tightened second-order cone (SOC) constraints

$$\eta_m \|\mathbf{f} - \mathbf{f}_0\|_K \leq D(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m) + \mathbf{\Gamma b} - b_0, \, \forall \, m \in [M].$$

for which the term $\|\mathbf{f} - \mathbf{f}_0\|_K$ of (19) ensures that the problem is still convex and implementable.

The following theorem extends the idea presented in (19) to affine SDP constraints and states our result on how to translate a finite ball-covering of $\mathcal{K}$ (meant w.r.t. a norm $\|\cdot\|_{\mathcal{X}}$) into a SOC tightening of $(\mathcal{C}_P)$.

Theorem 3 (Tighter constraint for ball covering in $\mathcal{X}$ and $P \geq 1$) *Assume that the points $\{\tilde{\mathbf{x}}_m\}_{m\in[M]} \subset \mathcal{X}$ associated with radii $\delta_m > 0$ form a ball-covering of $\mathcal{K}$, i.e. $\mathcal{K} \subseteq \bigcup_{m\in[M]} \mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$. Let $\mathbf{D} = [D_{p_1,p_2}]_{p_1,p_2\in[P]}$ ($D_{p_1,p_2} \in O_{Q,s}$), and*

$$\eta_{m,P} := \sup_{\substack{\mathbf{x}\,\in\,\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m,\delta_m),\\ \mathbf{u}=[u_p]_{p\in[P]}\in\mathcal{S}^{P-1}}} \left\| \sum_{p_1,\,p_2\in[P]} u_{p_1} u_{p_2} \left[D_{p_1,p_2}K(\cdot, \tilde{\mathbf{x}}_m) - D_{p_1,p_2}K(\cdot, \mathbf{x})\right] \right\|_K, \tag{20}$$

$$C_{P,SOC} := \left\{(\mathbf{f}, \mathbf{b}) \,:\, \eta_{m,P}\|\mathbf{f} - \mathbf{f}_0\|_K \mathbf{I}_P \preccurlyeq \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m) + \operatorname{diag}(\mathbf{\Gamma b} - \mathbf{b}_0), \forall \, m \in [M]\right\}. \tag{$\mathcal{C}_{P,\mathrm{SOC}}$}$$

Then $(\mathcal{C}_{P,\mathrm{SOC}})$ is tighter than $(\mathcal{C}_P)$, i.e. $C_{P,SOC} \subseteq C_P$.

The following lemma provides a more explicit, finite-dimensional description of $\eta_{m,P}$.

Lemma 4 (Finite-dimensional description of $\eta_{m,P}$) *For $\mathbf{z} \in \mathcal{X}$, $\delta > 0$, and a differential operator $\mathbf{D} = [D_{p_1,p_2}]_{p_1,p_2\in[P]}$ ($D_{p_1,p_2} \in O_{Q,s}$), let*

$$\eta(\mathbf{z}, \delta; \mathbf{D}) := \sup_{\substack{\mathbf{x}\,\in\,\mathbb{B}_{\mathcal{X}}(\mathbf{z},\delta),\\ \mathbf{u}\in\mathcal{S}^{P-1}}} |\langle \mathbf{u} \otimes \mathbf{u}, [\boldsymbol{\mathcal{K}}(\mathbf{z}, \mathbf{z}) + \boldsymbol{\mathcal{K}}(\mathbf{x}, \mathbf{x}) - 2\boldsymbol{\mathcal{K}}(\mathbf{z}, \mathbf{x})] \, (\mathbf{u} \otimes \mathbf{u})\rangle_F|^{1/2}, \tag{21}$$

with the symmetric 4D-tensor $\boldsymbol{\mathcal{K}}(\mathbf{x}', \mathbf{x}) = \left[\boldsymbol{\mathcal{K}}(\mathbf{x}', \mathbf{x})_{p_1, p_2, p_1', p_2'}\right]_{p_1, p_2, p_1', p_2' \in [P]} \in \mathbb{R}^{P\times P\times P\times P}$*, having elements* $\boldsymbol{\mathcal{K}}(\mathbf{x}', \mathbf{x})_{p_1, p_2, p_1', p_2'} := D^\top_{p_1', p_2'} D_{p_1, p_2} K(\mathbf{x}', \mathbf{x})$ *and acting as a linear operator over matrices of* $\mathbb{R}^{P\times P}$*. Then, the quantity* $\eta_{m,P}$ *defined in* (20) *can be written as*

$$\eta_{m,P} = \eta\left(\tilde{\mathbf{x}}_m, \delta_m; \mathbf{D}\right). \tag{22}$$

Remarks:

- Relation of $\eta_{m,P}$ to the eigenvalues of $\boldsymbol{\mathcal{K}}$: Since $\mathbf{u} \in \mathcal{S}^{p-1}$, $\|\mathbf{u}\otimes\mathbf{u}\|_F^2 = 1$. This means that $\eta_{m,P}$ can be upper bounded by the supremum over the ball $\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$ of the square root $\lambda_{\max}^{1/2}$ of the maximal eigenvalue of the 4D-tensor $\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \tilde{\mathbf{x}}_m) + \boldsymbol{\mathcal{K}}(\mathbf{x}, \mathbf{x}) - 2\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \mathbf{x})$

$$\begin{aligned}\eta_{m,P} &= \sup_{\substack{\mathbf{x}\in\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m,\delta_m),\\ \mathbf{u}\in\mathcal{S}^{P-1}}} \left|\langle \mathbf{u}\otimes\mathbf{u}, \left[\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \tilde{\mathbf{x}}_m) + \boldsymbol{\mathcal{K}}(\mathbf{x}, \mathbf{x}) - 2\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \mathbf{x})\right](\mathbf{u}\otimes\mathbf{u})\rangle_F\right|^{1/2}\\ &\le \sup_{\substack{\mathbf{x}\in\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m,\delta_m),\\ \mathbf{U}\in\mathbb{R}^{P\times P}:\|\mathbf{U}\|_F=1}} \left|\langle \mathbf{U}, \left[\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \tilde{\mathbf{x}}_m) + \boldsymbol{\mathcal{K}}(\mathbf{x}, \mathbf{x}) - 2\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \mathbf{x})\right]\mathbf{U}\rangle_F\right|^{1/2}\\ &= \sup_{\mathbf{x}\in\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m,\delta_m)} \lambda_{\max}^{1/2}\left(\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \tilde{\mathbf{x}}_m) + \boldsymbol{\mathcal{K}}(\mathbf{x}, \mathbf{x}) - 2\boldsymbol{\mathcal{K}}(\tilde{\mathbf{x}}_m, \mathbf{x})\right).\end{aligned}$$

  In particular, by continuity of the spectral radius, this ensures that $\eta_{m,P} = \eta_{m,P}(\delta_m)$ converges to zero when δ_m goes to zero. Hence when the discretization steps $(\delta_m)_{m\in[M]}$ decrease to zero, we recover the original constraint $(\mathcal{C}_P)$.

- Equivalence of Theorem 2 and Theorem 3 for balls and $P = 1$: When $P = 1$, $u \in \mathcal{S}^0$ means that $|u| = 1$. Hence $|u_1 u_2| = 1$ can be pulled out from (20) and $\eta_{m,1}$ reduces to

$$\eta_{m,1} = \sup_{\mathbf{x}\in\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m,\delta_m)} \|DK(\cdot, \tilde{\mathbf{x}}_m) - DK(\cdot, \mathbf{x})\|_K,$$

  so we recover η_m as defined in (15), and as anticipated in (19). In other words, for $P = 1$, when choosing a ball covering $\Omega_m = \mathring{\mathbb{B}}_K(DK(\cdot, \tilde{\mathbf{x}}_m), \eta_m)$, Theorem 2 coincides with Theorem 3. This specific choice was followed by Aubin-Frankowski and Szabó (2020). The two theorems presented here have complementary advantages: for real-valued constraints, Theorem 2 allows more general coverings than just balls, whereas Theorem 3 is able to handle affine SDP constraints with $P > 1$.

- Computation of $\eta_{m,P}$: The value of $\eta_{m,P}$ can be computed analytically in various cases. For instance, for $P = 1$ and $D = \mathrm{Id}$, with a monotonically decreasing radial kernel $K(\mathbf{x}, \mathbf{y}) = K_0(\|\mathbf{x} - \mathbf{y}\|_{\mathcal{X}})$ (such as the Gaussian kernel), (22) simplifies to

$$\eta_{m,1}(\delta_m) = \sup_{\mathbf{x}\in\mathbb{B}_{\mathcal{X}}(\mathbf{0},\delta_m)} \sqrt{|2K_0(0) - 2K_0\left(\|\mathbf{x}\|_{\mathcal{X}}\right)|} = \sqrt{|2K_0(0) - 2K_0\left(\delta_m\right)|}. \tag{23}$$

  Depending on the choice of the kernel, similar computations could be carried out for higher-order derivatives. For translation-invariant kernels, $\eta_{m,P}$ can be computed on a single δ_m-ball around the origin as in (23). A fast approximation of $\eta_{m,P}$ can also for instance be performed by sampling $\mathbf{x}$ (resp. $\mathbf{u}$) in the ball $\mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$ (resp. sphere $\mathcal{S}^{P-1}$).

Moreover, as $\eta_{m,P}$ is related to the modulus of continuity of DK, the smoother the kernel, the smaller $\eta_{m,P}$ and the tighter the approximation of $\mathbf{\Phi}_D(\mathcal{K})$. As intuitively explained in (19), $\eta_{m,P}$ is *one* possible upper bound on the modulus of continuity, enabling guarantees for hard shape constraints. Depending on the objective function $\mathcal{L}$, this bound is also tight in the equality case of the Cauchy-Schwarz inequality.

4. Objective Function

In Section 3 we detailed how one can tighten an infinite number of affine SDP constraints over a compact set of $\mathcal{X}$ into finitely many convex constraints in RKHSs through finite coverings of compact sets in $\mathcal{X}$ or in $\mathcal{F}_K$. The proposed construction tightens the constraints ($\mathcal{C}$) into the ones defined in ($\mathcal{C}_{P,\text{SOC}}$) and ($\mathcal{C}_{1,\Omega}$). Our next theorem shows that the resulting optimization problem can be expressed as a finite-dimensional one (representer theorem) and when the tightening converges to the original constraint, the solutions of the constrained tasks converge as well to the solution of the original problem, provided that it was strongly convex.

Theorem 5 (Existence, representer theorem, performance guarantee) *Let $\mathcal{X} \subseteq \mathbb{R}^d$ be a set which is contained in the closure of its interior and is endowed with a matrix-valued kernel $K \in \mathcal{C}^{s,s}\left(\mathcal{X}\times\mathcal{X}, \mathbb{R}^{Q\times Q}\right)$ for some $s \in \mathbb{N}$. Let $\mathcal{B}$ be a closed convex set in $\mathbb{R}^B$, consider the samples $(\mathbf{x}_n)_{n\in N} \subset \mathcal{X}$, and $I \in \mathbb{N}$ with $[I]$ be partitioned into two disjoint index sets $\mathcal{I}_{SOC}$ and $\mathcal{I}_\Omega$ ($[I] = \mathcal{I}_{SOC} \cup \mathcal{I}_\Omega$). Define the optimization problem*

$$\left(\bar{\mathbf{f}}_{app}, \bar{\mathbf{b}}_{app}\right) \in \underset{\substack{\mathbf{f}\in\mathcal{F}_K,\, \mathbf{b}\in\mathcal{B}\\ (\mathbf{f},\mathbf{b})\in C_{app}}}{\arg\min}\ \mathcal{L}(\mathbf{f},\mathbf{b}) = L\left(\mathbf{b}, \left(\left(D^0_{n,j}(\mathbf{f})(\mathbf{x}_n)\right)_{j\in J_n}\right)_{n\in[N]}\right) + R\left(\|\mathbf{f}\|_K\right), \qquad (24)$$

where $C_{app} := \left(\bigcap_{i\in\mathcal{I}_{SOC}} C^i_{P_i,SOC}\right) \cap \left(\bigcap_{i\in\mathcal{I}_\Omega} C^i_{1,\Omega}\right)$, with loss $L : \mathbb{R}^B \times \mathbb{R}^{\sum_{n\in[N]}\#J_n} \to \mathbb{R}\cup\{\infty\}$, monotonically increasing regularizer $R : \mathbb{R}_+ \to \mathbb{R}$, differential operators $(D^0_{n,j})_{j\in J_n} \subset O_{Q,s}$, and $C^i_{P_i,SOC}$ and $C^i_{1,\Omega}$ defined as in ($\mathcal{C}_{P,\text{SOC}}$) and ($\mathcal{C}_{1,\Omega}$). Then

1. *Existence: Assume that (i) R is coercive (i.e. $\lim_{z\to\infty} R(z) = \infty$), (ii) L is "uniformly" coercive in $\mathbf{b}$: $\lim_{\|\mathbf{b}\|_2\to\infty} \inf_{\mathbf{y}\in\mathbb{B}_{\|\cdot\|_2}(\mathbf{0},r)} L(\mathbf{b},\mathbf{y}) + \chi_{\mathcal{B}}(\mathbf{b}) = \infty$ for any $r > 0$, (iii) $L + \chi_{C_{app}}$ is lower bounded, (iv) the functions L and R are lower semi-continuous[9], and (v) there exists an admissible pair $(\mathbf{f},\mathbf{b}) \in C_{app} \cap \operatorname{dom}(\mathcal{L}) \cap (\mathcal{F}_K \times \mathcal{B})$. Then there exists a minimizer $\left(\bar{\mathbf{f}}_{app}, \bar{\mathbf{b}}_{app}\right)$.*
2. *Representer theorem: If there exists a minimizer, then there also exists a minimizer $\bar{\mathbf{f}}_{app}$ and coefficients $\{a_{L,n,j}\}_{n\in[N],\, j\in J_n}$, $\{a_{S,i,p_1,p_2}\}_{i\in\mathcal{I}_{SOC},\, p_1,p_2\in[P_i]}$, $\{a_{B,i,m,j}\}_{i\in\mathcal{I}_\Omega,\, m\in[M_i],\, j\in[J_{B,i,m}]}$,*

9. An extended real-valued function $g : \mathcal{D} \subseteq \mathbb{R}^q \to \mathbb{R}\cup\{\infty\}$ is called lower semi-continuous (shortly l.s.c.) if $g(\mathbf{x}_0) \le \liminf_{\mathbf{x}\to\mathbf{x}_0} g(\mathbf{x})$ for all $\mathbf{x}_0 \in \operatorname{dom}(g) := \{\mathbf{x}\in\mathcal{D} : g(\mathbf{x}) < \infty\}$.

$\{a_{H,i,m,j}\}_{i\in\mathcal{I}_\Omega,\, m\in[M_i],\, j\in[J_{H,i,m}]}$, $\{a_{0,i}\}_{i\in[I]} \subset \mathbb{R}$ *such that*

$$\bar{\mathbf{f}}_{app} = \underbrace{\sum_{n\in[N]}\sum_{j\in J_n} a_{L,n,j} D^0_{n,j} K(\cdot,\mathbf{x}_n)}_{\text{input samples } \mathbf{x}_n} + \underbrace{\sum_{i\in\mathcal{I}_{SOC}}\sum_{p_1,p_2\in[P_i]}\sum_{m\in[M_i]} a_{S,i,p_1,p_2} D^i_{p_1,p_2} K(\cdot,\tilde{\mathbf{x}}_{i,m})}_{\text{virtual points } \tilde{\mathbf{x}}_{i,m} \text{ in } C^i_{P_i,SOC}}$$
$$+ \underbrace{\sum_{i\in\mathcal{I}_\Omega}\sum_{m\in[M_i]}\left[\sum_{j\in[J_{B,i,m}]} a_{B,i,m,j}\mathbf{c}_{i,m,j} + \sum_{j\in[J_{H,i,m}]} a_{H,i,m,j}\mathbf{v}_{i,m,j}\right]}_{\text{centers } \mathbf{c}_{i,m,j} \text{ and normal vectors } \mathbf{v}_{i,m,j} \text{ of } \Omega_{i,m} \text{ associated to } C^i_{1,\Omega}} + \underbrace{\sum_{i\in[I]} a_{0,i}\mathbf{f}_{0,i}}_{\text{affine biases } \mathbf{f}_{0,i}}, \quad (25)$$

where the functions $D^0_{n,j}K(\cdot,\mathbf{x}_n)$ *and* $D^i_{p_1,p_2}K(\cdot,\mathbf{x}_{i,m})$ *are defined as in* (5).

3. *Performance guarantee: Let* v_{relax} *be the optimal value of any relaxation of* ($\mathcal{P}$), *and* $v_{app} = \mathcal{L}\left(\bar{\mathbf{f}}_{app}, \bar{\mathbf{b}}_{app}\right)$. *If* $\mathcal{L}$ *is* $(\mu_\mathbf{f},\mu_\mathbf{b})$*-strongly convex w.r.t.* $(\mathbf{f},\mathbf{b})$*, then* $(\bar{\mathbf{f}},\bar{\mathbf{b}})$ *exists, unique and*

$$\left\|\bar{\mathbf{f}}_{app} - \bar{\mathbf{f}}\right\|_K \le \sqrt{\frac{2(v_{app}-v_{relax})}{\mu_\mathbf{f}}}, \qquad \left\|\mathbf{b}_{app} - \bar{\mathbf{b}}\right\|_2 \le \sqrt{\frac{2(v_{app}-v_{relax})}{\mu_\mathbf{b}}}. \quad (26)$$

Let us assume in addition that (i) $\mathcal{B} = \operatorname{dom}(\mathcal{L}(\bar{\mathbf{f}},\cdot)) = \mathbb{R}^B$*, (ii) there exists* $\boldsymbol{\beta}\in\mathbb{R}^B$ *such that* $\boldsymbol{\Gamma}_i\boldsymbol{\beta} > \mathbf{0}$ *for all* $i\in\mathcal{I}$*, (iii)* $\{\tilde{\mathbf{x}}_{i,m}\}_{m\in[M_i]} \subseteq \mathcal{K}_i$, $\forall i\in\mathcal{I}_{SOC}$*, and (iv)* $\mathcal{L}(\bar{\mathbf{f}},\cdot)$ *is* L_b-*Lipschitz continuous on* $\mathbb{B}_{\|\cdot\|_2}\left(\bar{\mathbf{b}}, \eta_\infty c_f\|\boldsymbol{\beta}\|_2\right)$ *where* $c_f := \frac{\max_{i\in[I]}\|\bar{\mathbf{f}}-\mathbf{f}_{0,i}\|_K}{\min_{i\in[I],p\in P_i}(\boldsymbol{\Gamma}_i\boldsymbol{\beta})_p}$ *and*

$$\eta_\infty := \max\left(\max_{i\in\mathcal{I}_{SOC},\, m\in[M_i]} \eta_{i,m,P_i}, \max_{i\in\mathcal{I}_\Omega,\, m\in[M_i]} \operatorname{diam}(\Omega_{i,m})\right). \quad (27)$$

Then

$$\left\|\bar{\mathbf{f}}_{app} - \bar{\mathbf{f}}\right\|_K \le \sqrt{\frac{2L_b c_f\eta_\infty\|\boldsymbol{\beta}\|_2}{\mu_\mathbf{f}}}, \qquad \left\|\bar{\mathbf{b}}_{app} - \bar{\mathbf{b}}\right\|_2 \le \sqrt{\frac{2L_b c_f\eta_\infty\|\boldsymbol{\beta}\|_2}{\mu_\mathbf{b}}}. \quad (28)$$

Remarks:

- Existence for our examples: All the examples provided at the end of Section 2 satisfy the conditions of our existence result. For instance, for the JQR problem, R is quadratic, L is continuous, nonnegative and $L(\mathbf{b},\mathbf{y})/\|\mathbf{b}\|_2 \xrightarrow{\|\mathbf{b}\|_2\to\infty} \infty$ when $\mathbf{y}\in\mathbb{B}_{\|\cdot\|_2}(\mathbf{0},r)$ for any $r>0$ (this property is often referred to as (super)coercivity of L in the variable $\mathbf{b}$).
- Tightness of assumptions for existence: Below we illustrate that the statement on the existence is tight. Particularly, we give examples (with $\mathcal{B}=\{0\}$) showing that if the coercivity of R or the lower bounded property of $L+\chi_{C_{\text{app}}}$ does not hold, then there might not be solutions.
  - $L+\chi_{C_{\text{app}}}$ is not lower bounded: Consider the unconstrained problem with $\mathcal{L}(f) = 2f(\mathbf{x}_0)/\sqrt{K(\mathbf{x}_0,\mathbf{x}_0)} + \|f\|_K$ with $\mathbf{x}_0$ taken such that $K(\mathbf{x}_0,\mathbf{x}_0)>0$. In this case $R(z)=z$, hence the coercivity of R holds. However, L is not lower bounded as for $f_n = -2^n K(\cdot,\mathbf{x}_0)\in\mathcal{F}_K$, we have $\mathcal{L}(f_n) = -2^n\sqrt{K(\mathbf{x}_0,\mathbf{x}_0)} \xrightarrow{n\to\infty} -\infty$.

- R is not coercive: Let $\mathcal{L}(f) = 2\arctan\left(f(\mathbf{x}_0)/\sqrt{K(\mathbf{x}_0,\mathbf{x}_0)}\right) + \arctan\left(\|f\|_K\right)$ with $\mathbf{x}_0$ as above. In this case $L(f) > -\pi$. However $R(z) = \arctan(z) \le \frac{\pi}{2}$, hence the coercivity of R does not hold. With the same f_n as in the previous example, one gets that $\mathcal{L}(f_n) = -\arctan\left(2^n\sqrt{K(\mathbf{x}_0,\mathbf{x}_0)}\right) \xrightarrow{n\to\infty} -\pi/2$.

- Representer theorem $\Rightarrow$ finite-dimensional optimization task: Using the parameterization of $\bar{\mathbf{f}}_{\text{app}}$ in (25) with the reproducing property (Lemma 1), the finite-dimensional optimization problem over the coefficients of (25) immediately follows. Such a reformulation was exemplified by Aubin-Frankowski and Szabó (2020) for $Q = P = 1$.

- Performance bound:
  - Assumption on $\mathbf{\Gamma}_i$: When $P_i = 1$ for all $i \in [I]$, the surjectivity of $[\mathbf{\Gamma}_1; \ldots; \mathbf{\Gamma}_I]$ (assumed by Aubin-Frankowski and Szabó 2020) implies the existence of $\boldsymbol{\beta} \in \mathbb{R}^B$ such that $\mathbf{\Gamma}_i\boldsymbol{\beta} > \mathbf{0}$ for all $i \in \mathcal{I}$; hence the assumption on $\mathbf{\Gamma}_i$-s made in Theorem 5 is weaker than the one imposed by Aubin-Frankowski and Szabó (2020).
  - Bound (28), role of η_∞: Notice that one gets a non-trivial bound in (28) if $\operatorname{diam}(\Omega_{i,m}) < \infty$, i.e. $J_{B,i,m} \in \mathbb{N}^*$ for all $i \in \mathcal{I}_\Omega$ and $m \in [M_i]$. Moreover, (28) shows that the error of the presented tightening is controlled by the value of η_∞. Shrinking all the radii η_{i,m,P_i} and the diameters $\operatorname{diam}(\Omega_{i,m})$ to zero, forces η_∞ to zero; the former can be achieved by a *uniformly* refined covering in $\mathcal{F}_K$.

In the next section, we present the "soap bubble" algorithm which is capable of achieving convergence *without* having to refine the covering everywhere.

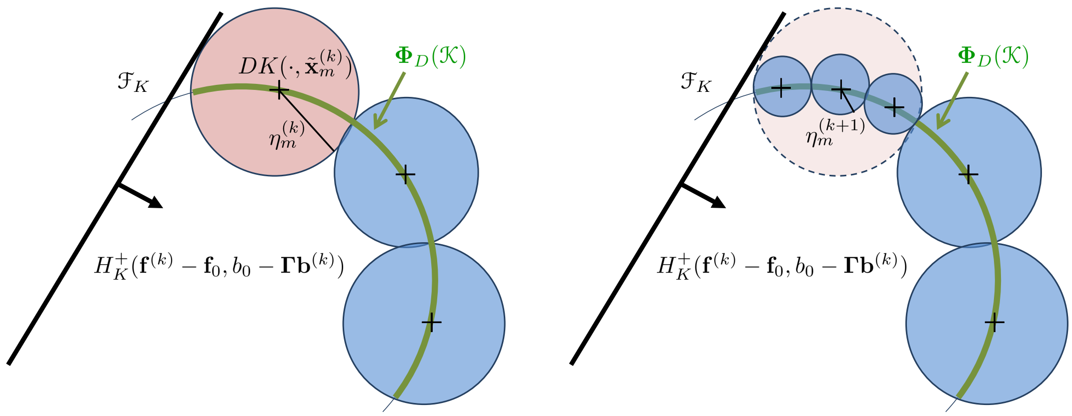
5. Adaptive Covering Algorithm of Compact Sets in RKHSs

In this section we present an adaptive approach, the soap bubble algorithm which provides a non-uniform covering relying on the objective $\mathcal{L}$. The rationale behind this algorithm is to avoid (i) applying a uniformly refined covering and (ii) tightening ($\mathcal{P}$) independently of $\mathcal{L}$. Instead, the soap bubble algorithm starts from a coarse covering (which allows faster computation), and then it gradually refines the covering where the constraints are saturated.

Throughout this section we assume to have access to some covering oracles: Alg. 1 and Alg. 2. Alg. 1 operates in $\mathcal{X}$, and for any compact set $\mathcal{K} \subseteq \mathcal{X}$ and radius $\delta_{\max}$ it outputs a covering of $\mathcal{K}$ with balls of radius at most $\delta_{\max}$. Alg. 2 works in $\mathcal{F}_K$, and for any compact set $\mathcal{K} \subseteq \mathcal{X}$ and diameter $d_{\max}$ it outputs a covering of $\mathbf{\Phi}_D(\mathcal{K})$ with sets $\bar{\Omega}_m$ of diameter at most $d_{\max}$.

The soap bubble algorithm iterates between solving a tightened optimization problem given a covering of $\mathbf{\Phi}_D(\mathcal{K})$ and refining the covering by a factor of γ for the covering subsets in $\mathcal{F}_K$ which saturate the constraints. The resulting algorithm (Alg. 3) is instantiated in the framework of Theorem 2 with sets $\bar{\Omega}_m$ and using the covering oracle Alg. 2. The method writes as Alg. 4 in the framework of Theorem 3 with ball-coverings and using the covering oracle Alg. 1.

Remark: For $P = I = 1$ and ball covering $\bar{\Omega}_m^{(k)} = \mathbb{B}_K\left(DK\left(\cdot, \tilde{\mathbf{x}}_m^{(k)}\right), \eta_{m,1}^{(k)}\right)$, Alg. 3 and Alg. 4 coincide. In this case saturating the constraints at the k^{th} iteration corresponds to



(a) (b)

Figure 2: Illustration of one iteration of the soap bubble algorithm Alg. 3 with ball covering (corresponding to Alg. 4 with $P = I = 1$). (a): After computing the optimal $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)$ for a given covering at step k, the elements of the covering that are tangent to the hyperplane burst (red). The other elements (blue) are kept for the next iteration. (b): The elements that are tangent are replaced by a new covering of the subset of $\Phi_D(\mathcal{K})$ that they covered. This covering is chosen such that its radii are smaller by at least a factor γ than the previous radii. The covering at step $k+1$ of $\Phi_D(\mathcal{K})$ is formed by combining the elements untouched at step k with the new elements. These new constraints define a new optimization problem leading to $\left(\mathbf{f}^{(k+1)}, \mathbf{b}^{(k+1)}\right)$.

being tangent to the affine hyperplane $H_K\left(\mathbf{f}^{(k)} - \mathbf{f}_0, b_0 - \mathbf{\Gamma b}^{(k)}\right)$. For an illustration, see Fig. 2.

Algorithm 1 Ball covering in $\mathcal{X}$ (shortly Cover)

Input: Compact set $\mathcal{K} \subseteq \mathcal{X}$, maximal covering radius $\delta_{\max} > 0$.

Output: Covering $(\mathbf{x}_m, \delta_m)_{m\in[M]}$ s.t. $\mathcal{K} \subseteq \cup_{m\in[M]} \mathbb{B}_{\mathcal{X}}(\mathbf{x}_m, \delta_m)$ and $\max_{m\in[M]} \delta_m \leq \delta_{\max}$.[a]

a. We assume that superfluous covering sets, i.e. for which $\mathbb{B}_{\mathcal{X}}(\mathbf{x}_m, \delta_m) \cap \mathcal{K} = \emptyset$ are not generated.

Algorithm 2 Ω-covering in $\mathcal{F}_K$ (shortly Ω-Cover)

Input: Compact set $\mathcal{K} \subseteq \mathcal{X}$, kernel K, differential operator D, maximal covering diameter $d_{\max} > 0$.

Output: Covering $\left(\bar{\Omega}_m\right)_{m\in[M]}$ s.t. $\mathbf{\Phi}_D(\mathcal{K}) \subseteq \bar{\Omega} := \cup_{m\in[M]} \bar{\Omega}_m$ and $\max_{m\in[M]} \operatorname{diam}\left(\bar{\Omega}_m\right) \leq d_{\max}$, with $\bar{\Omega}_m$ of the form (10).[a]

a. We assume that superfluous covering sets, i.e. for which $\bar{\Omega}_m \cap \mathbf{\Phi}_D(\mathcal{K}) = \emptyset$ are not generated.

Our next result shows the convergence of the soap bubble algorithm when $I = P = 1$ for general covering sets of the form (9)-(10).

Algorithm 3 Soap Bubble Algorithm with Ω-covering ($I = P = 1$)

Input: Compact set $\mathcal{K} \subseteq \mathcal{X}$, kernel K, constraint set $\mathcal{B}$, bias $\mathbf{f}_0$ and b_0, linear transformation $\mathbf{\Gamma} \in \mathbb{R}^{1\times B}$, differential operator D, refinement rate $\gamma \in (0,1)$, number of iterations $k_{\max} \in \mathbb{N}$, maximal initial covering diameter $d_{\max}^{(0)} > 0$.

Initialization: $\left(\bar{\Omega}_m^{(0)}\right)_{m\in\left[M^{(0)}\right]} := \Omega\text{-Cover}\left(\mathbf{\Phi}_D(\mathcal{K}), d_{\max}^{(0)}\right)$.

for $k = 0$ **to** $k_{\max}$ **do**

Solve the tightening with Ω-covering $\bar{\Omega}^{(k)} = \bigcup_{m\in\left[M^{(k)}\right]} \bar{\Omega}_m^{(k)}$:

$$\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) = \underset{\mathbf{f}\in\mathcal{F}_K, \mathbf{b}\in\mathcal{B}}{\arg\min}\ \mathcal{L}(\mathbf{f}, \mathbf{b}), \qquad \text{s.t. } \bar{\Omega}_m^{(k)} \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})\ \forall\, m \in \left[M^{(k)}\right]. \tag{$\mathcal{P}\left(\bar{\Omega}^{(k)}\right)$}$$

Find the indices $\mathcal{I}^{(k)} \subseteq \left[M^{(k)}\right]$ for which the sets intersect the hyperplane:

$$\mathcal{I}^{(k)} := \left\{m \in \left[M^{(k)}\right] \,:\, \bar{\Omega}_m^{(k)} \cap H_K\left(\mathbf{f}^{(k)} - \mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b}^{(k)}\right) \neq \emptyset\right\}.$$

The associated $\left(\bar{\Omega}_m^{(k)}\right)_{m\in\mathcal{I}^{(k)}}$ burst and give rise to a finer covering:

for $j \in \mathcal{I}^{(k)}$ **do**

New Ω-covering: $\left(\bar{\Omega}_{j,m}^{(k+1)}\right)_{m\in\left[M_j^{(k+1)}\right]} := \Omega\text{-Cover}\left(\mathbf{\Phi}_D(\mathcal{K}) \cap \bar{\Omega}_j^{(k)}, \gamma\, \mathrm{diam}\left(\bar{\Omega}_j^{(k)}\right)\right)$

end for

$$\left(\bar{\Omega}_m^{(k+1)}\right)_{m\in\left[M^{(k+1)}\right]} = \underbrace{\left(\bar{\Omega}_m^{(k)}\right)_{m\in\left[M^{(k)}\right]\setminus\mathcal{I}^{(k)}}}_{\text{non-burst coverings}} \cup \underbrace{\bigcup_{j\in\mathcal{I}^{(k)}} \left(\bar{\Omega}_{j,m}^{(k+1)}\right)_{m\in\left[M_j^{(k+1)}\right]}}_{\text{burst} \Rightarrow \text{refined coverings}}$$

end for

Output: Ω-covering $\left(\bar{\Omega}_m^{(k_{\max})}\right)_{m\in\left[M^{(k_{\max}+1)}\right]}$

Algorithm 4 Soap Bubble Algorithm with ball coverings $I \geq 1$, $P_i \geq 1$

Input: Compact sets $\{\mathcal{K}_i\}_{i\in[I]}$, kernel K, constraint set $\mathcal{B}$, biases $\{\mathbf{f}_{0,i}\}_{i\in[I]}$ and $\{\mathbf{b}_{0,i}\}_{i\in[I]}$, linear transformations $\{\mathbf{\Gamma}_i\}_{i\in[I]}$, differential operators $\{\mathbf{D}_i\}_{i\in[I]}$, refinement rate $\gamma \in (0,1)$, number of iterations $k_{\max} \in \mathbb{N}$, maximal initial covering radii $\left\{\delta_{i,\max}^{(0)}\right\}_{i\in[I]}$.

Initialization: $\left(\tilde{\mathbf{x}}_{i,m}^{(0)}, \delta_{i,m}^{(0)}\right)_{m\in\left[M_i^{(0)}\right]} := \operatorname{Cover}\left(\mathcal{K}_i, \delta_{i,\max}^{(0)}\right)$ for all $i \in [I]$.

for $k = 0$ **to** $k_{\max}$ **do**

Compute buffers using (22):

$$\boldsymbol{\eta}_i^{(k)} := \left(\eta_{i,m,P_i}^{(k)}\right)_{m\in\left[M_i^{(k)}\right]} = \left(\eta\left(\tilde{\mathbf{x}}_{i,m}^{(k)}, \delta_{i,m}^{(k)}; \mathbf{D}_i\right)\right)_{m\in\left[M_i^{(k)}\right]} \quad \forall i \in [I].$$

Solve the tightening with buffers $\left\{\boldsymbol{\eta}_i^{(k)}\right\}_{i\in[I]}$ and anchors $\left\{\tilde{\mathbf{x}}_{i,m}^{(k)}\right\}_{i\in[I],\, m\in\left[M_i^{(k)}\right]}$:

$$\begin{aligned}\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) = \underset{\mathbf{f}\in\mathcal{F}_K, \mathbf{b}\in\mathcal{B}}{\arg\min}\ & \mathcal{L}(\mathbf{f}, \mathbf{b}),\\ \text{s.t. } & \eta_{i,m,P_i}^{(k)}\|\mathbf{f}-\mathbf{f}_0\|_K \mathbf{I}_{P_i} \preccurlyeq \mathbf{D}_i\left(\mathbf{f}-\mathbf{f}_{0,i}\right)\left(\tilde{\mathbf{x}}_{i,m}^{(k)}\right) + \operatorname{diag}\left(\mathbf{\Gamma}_i\mathbf{b}-\mathbf{b}_{0,i}\right)\\ & \forall i \in [I], \forall m \in \left[M_i^{(k)}\right].\end{aligned}$$

Find the indices $\mathcal{I}_i^{(k)} \subseteq \left[M_i^{(k)}\right]$ for which the constraints are saturated; the associated $\mathbb{B}_K\left(DK\left(\cdot, \tilde{\mathbf{x}}_{i,m}^{(k)}\right), \eta_{i,m,P_i}^{(k)}\right)$ balls burst and give rise to a finer covering:

for $i \in [I]$ **do**

$$\begin{aligned}\mathcal{I}_i^{(k)} := \Big\{m \in \left[M_i^{(k)}\right] \,:\, \eta_{i,m,P_i}^{(k)}\left\|\mathbf{f}^{(k)}-\mathbf{f}_{0,i}\right\|_K \mathbf{I}_{P_i} = \mathbf{D}_i\left(\mathbf{f}^{(k)}-\mathbf{f}_{0,i}\right)\left(\tilde{\mathbf{x}}_{i,m}^{(k)}\right)\\ + \operatorname{diag}\left(\mathbf{\Gamma}_i\mathbf{b}^{(k)}-\mathbf{b}_{0,i}\right)\Big\}.\end{aligned}$$

Refine the covering on $\mathcal{I}_i^{(k)}$:

for $j \in \mathcal{I}_i^{(k)}$ **do**

$\delta_{i,j,\max}^{(k+1)} :=$ largest solution of the equation over δ: $\eta\left(\tilde{\mathbf{x}}_{i,j}^{(k)}, \delta; \mathbf{D}_i\right) = \gamma\eta_i^{(k)}$ with η defined in (21).

Implied covering in $\mathcal{X}$: $\left(\tilde{\mathbf{x}}_{i,j,m}^{(k+1)}, \delta_{i,j}^{(k+1)}\right)_{m\in\left[M_{i,j}^{(k+1)}\right]} :=\operatorname{Cover}\left(\mathcal{K}\cap\mathbb{B}\left(\tilde{\mathbf{x}}_{i,j}^{(k)}, \delta_{i,j}^{(k)}\right), \delta_{i,j,\max}^{(k+1)}\right)$

end for

$$\left(\tilde{\mathbf{x}}_{i,m}^{(k+1)}, \delta_{i,m}^{(k+1)}\right)_{m\in\left[M_i^{(k+1)}\right]} = \underbrace{\left(\tilde{\mathbf{x}}_{i,m}^{(k)}, \delta_{i,m}^{(k)}\right)_{m\in\left[M_i^{(k)}\right]\setminus\mathcal{I}_i^{(k)}}}_{\text{non-burst coverings}} \cup \underbrace{\bigcup_{j\in\mathcal{I}_i^{(k)}}\left(\tilde{\mathbf{x}}_{i,j,m}^{(k+1)}, \delta_{i,j}^{(k+1)}\right)_{m\in\left[M_{i,j}^{(k+1)}\right]}}_{\text{burst} \Rightarrow \text{refined coverings}}$$

end for

end for

Output: covering $\left\{\left(\tilde{\mathbf{x}}_{i,m}^{(k_{\max}+1)}, \delta_{i,m}^{(k_{\max}+1)}\right)_{m\in\left[M_i^{(k_{\max}+1)}\right]}\right\}_{i\in[I]}$

Theorem 6 (Convergence of Alg. 3) *Let us assume that Alg. 3 is written for* Ω*-coverings (Alg. 2) with elements defined as in* (9)-(10)*, in other words, with balls and half-spaces.*

1. *Limit covering: If all the iterates* $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ *of Alg. 3 exist, then the corresponding coverings* $\left(\bar{\Omega}^{(k)}\right)_{k\in\mathbb{N}}$ *converge in Hausdorff distance to a limit set* $\bar{\Omega}^{(\infty)}$ *containing* $\mathbf{\Phi}_D(\mathcal{K})$*. Moreover the solutions of* $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$ *also solve the original problem.*

2. *Convergence of* $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$*: Assume that (i) R is monotonically increasing and coercive, (ii) L is "uniformly" coercive in* $\mathbf{b}$*,* $\lim_{\|\mathbf{b}\|_2\to\infty} \inf_{\mathbf{y}\in\mathbb{B}_{\|\cdot\|_2}(\mathbf{0},r)} L\left(\mathbf{b},\mathbf{y}\right) = \infty$ *for any* $r > 0$*, (iii) L is lower bounded, (iv) the functions L and R are lower semi-continuous, (v) there exists an admissible pair* $\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}\right)$ *for* $\mathcal{P}\left(\bar{\Omega}^{(0)}\right)$*, (vi)* $\mathcal{B} = \mathrm{dom}(\mathcal{L}(\mathbf{f},\cdot)) = \mathbb{R}^B$ *and* $L\left(\cdot, \left(\left(D^0_{n,j}(\mathbf{f})(\mathbf{x}_n)\right)_{j\in J_n}\right)_{n\in[N]}\right)$ *is continuous for all* $\mathbf{f}$ *in its domain, and (vii)* $\mathbf{\Gamma} \neq \mathbf{0}$*.*
Then the sequence of iterates $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ *exists and is bounded in* $\mathcal{F}_K \times \mathbb{R}^B$*. Moreover every weakly-converging sub-sequence converges to a solution of the original problem. If* $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$ *is unique, then the iterates* $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ *converge weakly to* $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$*.*

Remark: The assumptions (i)-(vii) are stronger than that of Theorem 5 as instead of having a single problem (24) to solve, we consider a sequence of tasks $\left(\mathcal{P}\left(\bar{\Omega}^{(k)}\right)\right)_{k\in\mathbb{N}}$. This requires additional regularity on the objective.

6. Numerical Experiments

In this section we demonstrate the efficiency of the proposed tightened schemes. Particularly, we designed the following experiments:

- **Experiment-1**: We show that the soap bubble algorithm (Section 5) can be more efficient both in terms of accuracy and of computation time when compared to non-adaptive techniques (Section 4). We illustrate this result on a 1D-shape optimization problem ($Q = 1$) with a single constraint over a large domain.
- **Experiment-2**: In our second application we tackle a linear-quadratic optimal control problem with state constraints. This is a vector-valued example ($Q > 1$) where we show how the proposed hard shape-constrained technique enables one to guarantee obstacle avoidance when piloting an underwater vehicle, in contrast to classical discretization-based approaches.
- **Experiment-3**: Our third example pertains to econometrics, the goal being to learn of production functions based on only a few samples. This example underlines how shape constraints interpreted as side information can empirically improve generalization properties. In this case the function to be determined is real-valued ($Q = 1$) with several shape constraints including an SDP one (joint convexity, $P_i > 1$).

6.1 Experiment-1: Soap Bubble Algorithm

In our **first experiment** we demonstrate the efficiency of the soap bubble algorithm (Alg. 3) compared to non-adaptive schemes. Our benchmark task corresponds to a shape optimiza-

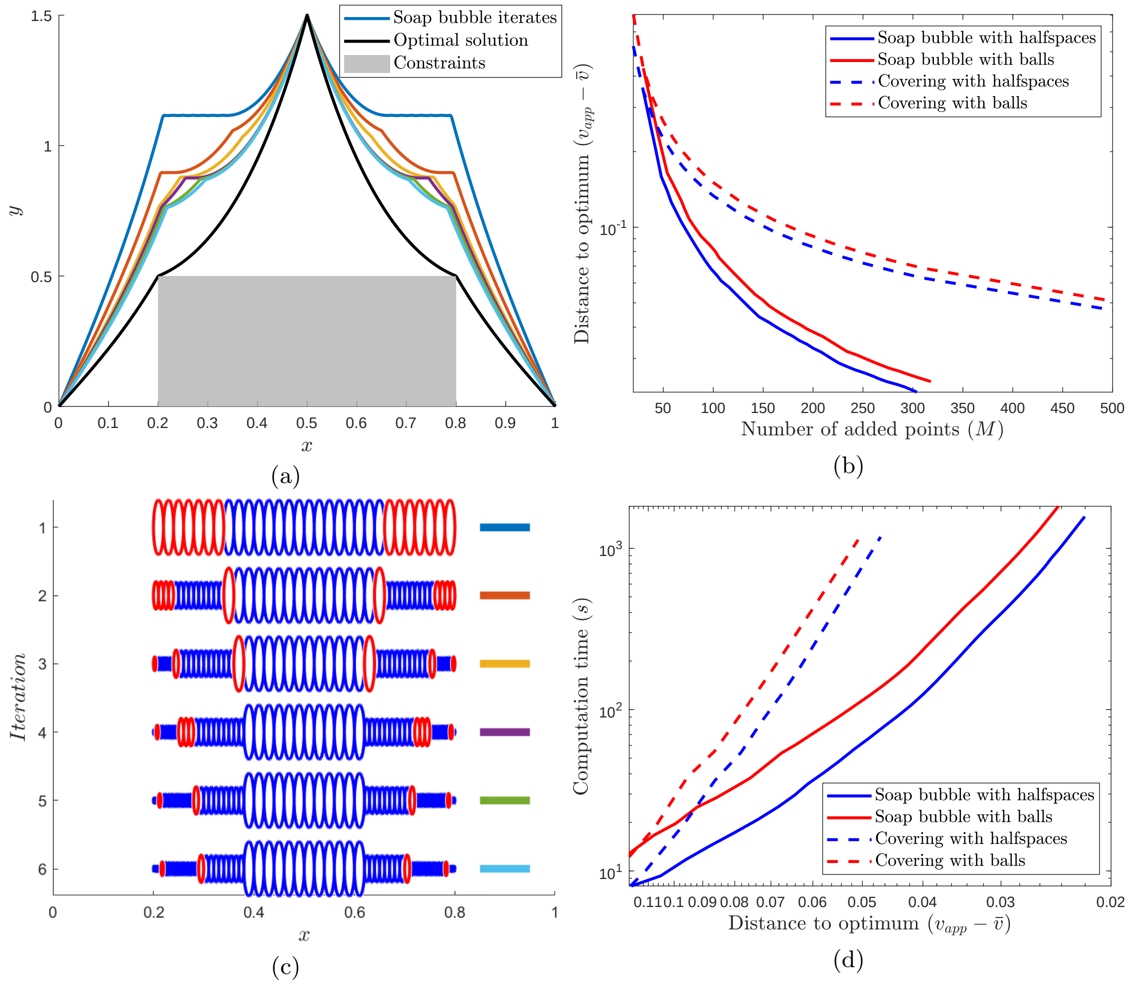


Figure 3: Illustration of the soap bubble algorithm to optimize the shape of a constrained catenary. Compared techniques: (uniform) covering with balls, covering with balls and half-spaces, soap bubble covering with balls, soap bubble covering with balls and half-spaces. (a): Shape constraint on $[0.2, 0.8]$ (grey), optimal solution (black), first 6 iterates of the estimates using the soap bubble technique with balls (coloured curves, first: blue, sixth: cyan). (b): Performance as a function of the number of elements in the covering (M). (c): Illustration of bursting in (a); kept balls (blue); burst balls (red). (d): Computational time as a function of accuracy.

tion problem. Particularly, the goal is to determine the deformation of a catenary under its weight. This is equivalent to minimizing the potential energy of its shape. Our domain is $\mathcal{X} = [0, 1]$, the form of the catenary is described by a function $f \in \mathcal{F}_K$ where $K(x, x') = e^{-\lambda|x-x'|}$ ($\lambda > 0$) is the Laplacian kernel. This form is constrained at 3 points $x \in \{0, 0.5, 1\}$ to be equal to 0, 1.5 and 0 respectively, and the catenary has to be above the value 0.5 on the whole interval $[0.2, 0.8]$. The resulting optimization problem can be expressed as

$$\begin{aligned} \min_{f\in\mathcal{F}_K} \quad & \|f\|_K \\ \text{s.t.} \quad & f(0) = 0,\ f(0.5) = 1.5,\ f(1) = 0, \\ & 0.5 \leq f(x),\ \forall\, x \in [0.2, 0.8]. \end{aligned}$$

This task can be written equivalently as

$$\begin{aligned} \min_{f\in\mathcal{F}_K} \quad & \mathcal{L}(f) := \|f\|_K + \chi_{\{0\}}(f(0)) + \chi_{\{1.5\}}(f(0.5)) + \chi_{\{0\}}(f(1)) \\ \text{s.t.} \quad & 0.5 \leq f(x),\ \forall\, x \in [0.2, 0.8], \end{aligned}$$

which falls within the framework ($\mathcal{P}$) with $Q = I = P = 1$, $\mathcal{K} = [0.2, 0.8]$, $D(f) = f$, $f_0 = 0$, $b_0 = 0.5$, $\Gamma = 0$ and $\mathcal{B} = \{0\}$. One of the advantages of this problem is that its solution can be computed analytically for some values of λ (for an illustration, see the black solid curve in Fig. 3(a)). This optimal solution can be thought of as the tilt of a circus tent, and is used as the ground truth.

In our experiments we chose the bandwidth parameter to be $\lambda = 5$. We compared the efficiency (in terms of time and accuracy) of four different covering schemes which we detail in the following.

1. Covering with balls only: In this case the M points of the covering of $\mathcal{K}$ were equidistant over the interval $\mathcal{K}$, i.e. $\tilde{x}_m = 0.2 + \frac{1}{2M} + (j-1)\frac{1}{M}$ and $\delta_m = \frac{0.8-0.2}{2M}$ with $m \in [M]$. The shape constraint $0.5 \leq f(x)$ for all $x \in \mathcal{K}$ was tightened to the SOC one ($\eta_m\|f\|_K + 0.5 \leq f(\tilde{x}_m)$ for all $m \in [M]$) with $\eta_m = \sqrt{|2 - 2\tilde{\rho}_m|} = \sqrt{2 - 2\tilde{\rho}_m}$ and $\tilde{\rho}_m := e^{-\lambda\delta_m}$ according to (23). This choice corresponds to the ball covering
$$\mathbf{\Phi}(\mathbb{B}_{|\cdot|}(\tilde{x}_m, \delta_m)) \subseteq \mathbb{B}_K\big(\underbrace{K(\cdot, \tilde{x}_m)}_{\mathbf{c}_m}, \underbrace{\eta_m}_{r_m}\big) \tag{29}$$
in the RKHS $\mathcal{F}_K$, with $J_{B,m} = 1, J_{H,m} = 0$ ($\forall m \in [M]$) in accordance with (9)-(10) and (16). The resulting convex optimization problem was solved directly using the representer theorem (Theorem 5).

2. Covering with balls and half-spaces: This method corresponds to the coverings (9)-(10) with $J_{B,m} = J_{H,m} = 1$, as depicted on Fig. 1(b). The rationale behind this scheme is to provide a finer covering compared to the previous one, and thus a more accurate approximation. As mentioned in footnote 6, since for the Laplacian kernel $K(x, x) = 1$ for all $x \in \mathcal{X}$, we have that $\mathbf{\Phi}(\mathcal{K}) \subseteq \mathbb{B}_K(\mathbf{0}, 1)$. Moreover for $x \in \mathbb{B}_{|\cdot|}(\tilde{x}_m, \delta_m)$, $K(\tilde{x}_m, x) = e^{-\lambda|x-\tilde{x}_m|} \geq e^{-\lambda\delta_m} = \tilde{\rho}_m$. Hence $-K(x, \tilde{x}_m) = \langle K(\cdot, x), -K(\cdot, \tilde{x}_m)\rangle_K \leq -\tilde{\rho}_m$, i.e. $K(\cdot, x) \in H_K^-(-K(\cdot, \tilde{x}_m), -\tilde{\rho}_m)$, consequently
$$\mathbf{\Phi}(\mathbb{B}_{|\cdot|}(\tilde{x}_m, \delta_m)) \subseteq \mathbb{B}_K\big(\underbrace{\mathbf{0}}_{\mathbf{c}_m}, \underbrace{1}_{r_m}\big) \cap H_K^-\big(\underbrace{-K(\cdot, \tilde{x}_m)}_{\mathbf{v}_m}, \underbrace{-\tilde{\rho}_m}_{\rho_m}\big) \tag{30}$$

in line with (14). This is indeed a covering at least as tight as (29), as, when considering an element $\mathbf{g}$ in the r.h.s. of (30), then

$$\|\mathbf{g} - K\left(\cdot, \tilde{x}_m\right)\|_K^2 = \|\mathbf{g}\|_K^2 + K\left(\tilde{x}_m\, \tilde{x}_m\right) - 2\langle \mathbf{g}, K\left(\cdot, \tilde{x}_m\right)\rangle_K \leq 2 - 2\tilde{\rho}_m = \eta_m^2,$$

which gives that

$$\mathbb{B}_K\big(\mathbf{0}, 1\big) \cap H_K^-\big(-K(\cdot, \tilde{x}_m), -\tilde{\rho}_m\big) \subseteq \mathbb{B}_K\big(K\left(\cdot, \tilde{x}_m\right), \eta_m\big).$$

The values of $\tilde{x}_m$, δ_m, $\tilde{\rho}_m$ and η_m were chosen similarly as in the previous point.

3. Soap bubble covering with balls only: In contrast to the direct solution with a fine covering, our first soap bubble scheme using balls (Alg. 4) is initialized with a coarser uniform covering with an initial covering radius $\delta_{\max}^{(0)} = 0.01$; the latter results in $M = \frac{0.8-0.2}{2\times 0.01} = 30$ anchor points at the beginning. This initial covering is then iteratively refined in our experiments using a rate $\gamma = 0.8$. The shape constraint were considered to be saturated when the condition $|\eta_m\|f\|_k + 0.5 - f(\tilde{x}_m)| \leq 10^{-8}$ held, determining the bursting condition of the balls in Alg. 4.
4. Soap bubble covering with balls and half-spaces: A combination of balls and half spaces were considered as in the second covering scheme, to which the soap bubble algorithm (Alg. 3) was applied. The initialization was the same as in the third scheme.

Our results are summarized in Fig. 3. The figure shows that the adaptive soap bubble technique (i) converges to the optimal solution as the iteration proceeds (in accordance with Theorem 6; see Fig. 3(a)) with illustration of the bursts in Fig. 3(c). (ii) It achieves the same accuracy with smaller number of covering points (Fig. 3(c)) and faster (Fig. 3(d)) compared to the non-adaptive schemes. These experiments demonstrate the efficiency of the adaptive soap bubble algorithm in the context of shape optimization.

6.2 Experiment-2: Safety-Critical Control

In our **second experiment** we focus on a constrained path-planning problem. Particularly, in this task the trajectory of an underwater vehicle navigating in a two-dimensional cavern is described by a curve $t \in \mathcal{T} := [0, 1] \mapsto [x(t); z(t)] \in \mathbb{R}^2$ describing its lateral (x) and depth (z) coordinates at time $t \in \mathcal{T}$. For simplicity, we assume that the lateral component satisfies $x(0) = 0$ and $\dot{x}(t) = 1$ for all $t \in \mathcal{T}$.[10] In this case, $x(t) = t$ for all $t \in \mathcal{T}$ and the control problem reduces to that of ensuring that the depth $z(t)$ stays between the floor and ceiling of the cavern ($z(t) \in [z_{\text{low}}(t), z_{\text{up}}(t)]$ for all $t \in \mathcal{T}$). We take as initial conditions $z(0) = 0$ and $\dot{z}(0) = 0$. By denoting the control with $u \in L^2(\mathcal{T}, \mathbb{R})$ where $L^2(\mathcal{T}, \mathbb{R})$ is the set of square-integrable real-valued functions on $\mathcal{T}$, our control task can be formulated as

$$\begin{aligned} \min_{u(\cdot)\in L^2(\mathcal{T},\mathbb{R})} \quad & \int_{\mathcal{T}} |u(t)|^2 \mathrm{d}t \\ \text{s.t.} \quad & z(0) = 0, \quad \dot{z}(0) = 0, \\ & \ddot{z}(t) = -\dot{z}(t) + u(t),\ \forall\, t \in \mathcal{T}, \\ & z_{\text{low}}(t) \leq z(t) \leq z_{\text{up}}(t),\ \forall\, t \in \mathcal{T}. \end{aligned} \qquad (\mathcal{P}_{\text{cave}})$$

10. The notations $\dot{\mathbf{g}}(t)$ and $\ddot{\mathbf{g}}(t)$ stand for the first and second-order derivative of a function $\mathbf{g}$ at time t.

The task ($\mathcal{P}_{\text{cave}}$) belongs to the class of linearly-constrained linear quadratic regulator problems. As shown by Aubin-Frankowski (2020), these tasks can be rephrased as a shape-constrained kernel regression for a kernel K defined by the objective and the dynamics. By defining the full state of the vehicle as $\mathbf{f}(t) := [z(t); \dot{z}(t)] \in \mathbb{R}^2$, $\mathbf{f}$ evolves according to the linear dynamics

$$\dot{\mathbf{f}}(t) = \mathbf{A}\mathbf{f}(t) + \mathbf{B}u(t) \in \mathbb{R}^2, \quad \mathbf{f}(0) = \mathbf{0}, \quad \mathbf{A} = \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \in \mathbb{R}^{2\times 2}, \quad \mathbf{B} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \in \mathbb{R}^2.$$

Using that $\mathbf{f}(0) = \mathbf{0}$ the controlled trajectories $\mathbf{f}$ belong to a $\mathbb{R}^2$-valued RKHS $\mathcal{F}_K$ defined over $\mathcal{T}$ with the matrix-valued kernel[11]

$$K(s,t) := \int_0^{\min(s,t)} e^{(s-\tau)\mathbf{A}}\mathbf{B}\mathbf{B}^\top e^{(t-\tau)\mathbf{A}^\top} \mathrm{d}\tau, \quad s,t \in \mathcal{T}, \tag{31}$$

where $e^{\mathbf{M}}$ denotes the matrix exponential. With this kernel-based formulation, the problem ($\mathcal{P}_{\text{cave}}$) can be rewritten as an optimization problem over full-state trajectories

$$\begin{aligned} \min_{\mathbf{f}=[f_1;f_2]\in\mathcal{F}_K} \quad & \|\mathbf{f}\|_K^2 \\ \text{s.t.} \quad & z_{\text{low}}(t) \le f_1(t) \le z_{\text{up}}(t), \, \forall\, t \in \mathcal{T}. \end{aligned}$$

In our experiment we assume that the given bounds z_{low} and z_{up} are piece-wise constant: taking a uniform δ-covering $\mathcal{T} = \cup_{m\in[M]}\mathcal{T}_m$ with $\mathcal{T}_m := [t_m - \delta, t_m + \delta]$ and $t_{m+1} = t_m + 2\delta$ for $m \in [M-1]$, this means that $z_{\text{low}}(t) = z_{\text{low},m}$ for all $t \in \mathcal{T}_m$; similarly $z_{\text{up}}(t) = z_{\text{up},m}$ for all $t \in \mathcal{T}_m$. Hence, with the piece-wise constant assumption, the control task ($\mathcal{P}_{\text{cave}}$) reduces to

$$\begin{aligned} \min_{\mathbf{f}=[f_1;f_2]\in\mathcal{F}_K} \quad & \|\mathbf{f}\|_K^2 \\ \text{s.t.} \quad & z_{\text{low},m} \le f_1(t) \le z_{\text{up},m}, \; \forall\, t \in \mathcal{T}_m, \, \forall m \in [M]. \end{aligned}$$

This optimization problem belongs to the family ($\mathcal{P}$) with $Q = 2$, $P = 1$, $D_m(\mathbf{f}) = f_1$ and $b_{0,m} = z_{\text{low},m}$ for $m \in [M]$ ($z_{\text{low},m} \le f_1(t)$ for $t \in \mathcal{T}_m$ and $m \in [M]$), $D_{M+m}(\mathbf{f}) = -f_1$ and $b_{0,M+m} = -z_{\text{up},m}$ for $m \in [M]$ ($-z_{\text{up},m} \le -f_1(t)$ for $t \in \mathcal{T}_m$ and $m \in [M]$), $\mathbf{f}_{0,m} = \mathbf{0}$ and $\Gamma_m = 0$ for $m \in [2M]$, $I = 2M$ and $\mathcal{B} = \{0\}$.

In Fig. 4 we compare the optimal trajectory obtained with the proposed SOC tightening (using ball covering) to the one derived when applying discretized constraints (formally corresponding to taking $\eta_m = 0$). Here the piece-wise constants bounds were obtained as piece-wise approximations of random functions drawn in a Gaussian RKHS. As illustrated in Fig. 4(a), the vehicle guided with discretized constraints crashes into the blue wall at multiple locations, whereas the trajectory resulting from the SOC-based tightening stays within the bounds at all times. The SOC trajectory can be described as solving a problem where $z_{\text{low},m}$ (resp. $z_{\text{up},m}$) was replaced by $z_{\text{low},m} + \eta_{m,1} \left\|\bar{\mathbf{f}}\right\|_K$ (resp. $z_{\text{up},m} - \eta_{m,1} \left\|\bar{\mathbf{f}}\right\|_K$). This acts as a supplementary buffer which we illustrate in Fig. 4(b) (green solid line). Even

11. The Hilbert space $\mathcal{F}_K$ corresponding to (31) is the one of controlled trajectories with zero initial condition ($\mathbf{f}(0) = \mathbf{0}$) such that $\|\mathbf{f}\|_K = \|u\|_{L^2(\mathcal{T},\mathbb{R})}$.

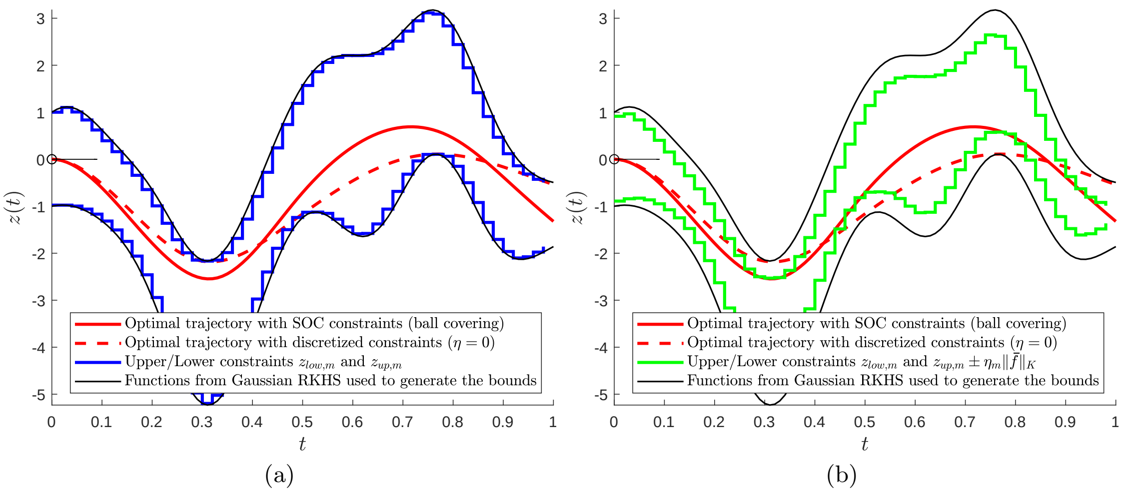


Figure 4: Illustration of the optimal control problem ($\mathcal{P}_{\text{cave}}$) of piloting a vehicle staying between the ceiling (z_{up}) and the floor (z_{low}) of a cavern. Red solid line: SOC-based approach. Red dashed line: solution based on a discretization (formally setting $\eta = 0$). Blue solid lines: constraints ($z_{\text{low},m}$ and $z_{\text{up},m}$). Black solid lines: functions used to generate the constraints. Green solid lines: constraints with buffer $\pm\eta_{m,1} \left\|\bar{\mathbf{f}}\right\|_K$.

though the SOC trajectory intersects the green boundary, the buffer $\eta_{m,1} \left\|\bar{\mathbf{f}}\right\|_K$ is guaranteed to be large enough for the SOC trajectory to never collide with the blue boundary. This experiment demonstrates the efficiency of the SOC approach in a safety-critical application where the constraints have to be met at all times.

Remark (encoding of the bounds z_{low} and z_{high}): In this control application we assumed that the prescribed bounds are piecewise constant and we generated them using functions which do not necessarily belong to $\mathcal{F}_K$. If one faces instead boundaries z_{low} and $z_{\text{high}} \in \mathcal{F}_K$, then these bounds could be treated as biases $\mathbf{f}_{0,i} = [z_{\text{up}}; z_{\text{low}}]$-s. While this would reduce the number of shape constraints from $I = 2M$ to $I = 2$, our current choice allows us to investigate the efficiency of the proposed approach in a complementary setting. Indeed, in contrast to the considered shape optimization task with one shape constraint ($I = 1$) on a large $\mathcal{K}$ which is refined by the soap bubble algorithm, the path-planning task involves $I = 2M$ constraints on an already refined grid.

6.3 Experiment-3: Econometrics

Our **third** example belongs to econometrics; our goal is to estimate production functions based on very few samples and additional side information. Particularly, let us consider a firm which produces an output from d different goods/inputs/factors. Let the quantity corresponding to the i^{th} input be written as $x_i \in \mathbb{R}_+$ ($i \in [d]$). Then the corresponding output can be modelled by a production function $f : \mathcal{X} \subseteq \mathbb{R}_+^d \to \mathbb{R}_+$. Classical assumptions on the production function (Varian, 1984; Allon et al., 2007) are (i) non-negativity ($f(\mathbf{x}) \geq 0$ $\forall \mathbf{x}$), (ii) monotonically increasing property (i.e., more inputs gives rise to more output; $\partial^{\mathbf{e}_i} f(\mathbf{x}) \geq 0$ $\forall \mathbf{x}$ and $\forall i \in [d]$), (iii) $f(\mathbf{0}) = 0$ (zero input gives no output) and (iv) concavity (also called diminishing marginal returns; $\left[\left(\partial^{\mathbf{e}_i+\mathbf{e}_j} f\right)(\mathbf{x})\right]_{i,j\in[d]} \preccurlyeq \mathbf{0}_{d\times d}$ $\forall \mathbf{x}$). Having access to N input-output samples $\{\mathbf{x}_n, y_n\}_{n\in[N]}$, the learning of a production function can be addressed by solving

$$\begin{aligned}
\min_{f\in\mathcal{F}_K} \quad & \mathcal{L}(f) := \frac{1}{N}\sum_{n\in[N]} [y_n - f(\mathbf{x}_n)]^2 + \lambda \|f\|_K^2, \quad (\lambda > 0)\\
\text{s.t.} \quad & 0 \le f(\mathbf{x}) \quad \forall \mathbf{x}\in\mathcal{K},\\
& 0 \le \partial^{\mathbf{e}_i} f(\mathbf{x}) \quad \forall \mathbf{x}\in\mathcal{K}, \forall i\in[d],\\
& 0 = f(\mathbf{0}),\\
& \mathbf{0}_{d\times d} \preccurlyeq -\left[\left(\partial^{\mathbf{e}_i+\mathbf{e}_j} f\right)(\mathbf{x})\right]_{i,j\in[d]} \quad \forall \mathbf{x}\in\mathcal{K},
\end{aligned}$$

where $\mathcal{K} \subset (\mathbb{R}_+)^d$ is a compact set containing the samples. This problem belongs to the family $(\mathcal{P})$ with the choice $s = 2$, $I = d+2$, $D_1(f) = f$ and $P_1 = 1$, $D_i = \partial^{\mathbf{e}_{i-1}}$ and $P_i = 1$ for $i \in \{2, 3, \ldots, d+1\}$, $\mathbf{D}_{d+2} = -\left[\partial^{\mathbf{e}_i+\mathbf{e}_j}\right]_{i,j\in[d]}$, $P_{d+2} = d$, $\mathbf{\Gamma}_i = \mathbf{0}$, $\mathbf{b}_{0,i} = \mathbf{0}$ and $f_{0,i} = 0$ for all $i \in [d+2]$. The requirement $f(\mathbf{0}) = 0$ can be encoded by incorporating an indicator function to the loss function.

For our experiment, we considered a benchmark dataset containing the production data of 569 Belgian firms.[12] The input $\mathbf{x}$ is two-dimensional ($d = 2$), describing the capital expressed in euros (x_1) and the labour involved, interpreted as the number of workers (x_2). The output y is one-dimensional ($Q = 1$), and is the added value in euros. We applied a standard pre-processing of the data (Mazumder et al., 2019) by (i) considering the negative logarithm of the output[13], (ii) mean-centering and standardizing each component of the input and of the output to have zero mean and unit variance, and (iii) removing some outliers, resulting in $N_{tot} = 543$ points kept. The final optimization problem[14] contains two monotonicity and one joint convexity constraint:

$$\min_{g\in\mathcal{F}_K} \quad \mathcal{L}(g) := \frac{1}{N}\sum_{n\in[N]} [y_n - g(\mathbf{x}_n)]^2 \tag{32a}$$

$$\text{s.t.} \quad \|g\|_K \le \tilde{\lambda}, \tag{32b}$$

$$0 \le -\partial^{\mathbf{e}_1} g(\mathbf{x}) \quad \forall \mathbf{x}\in\mathcal{K}, \tag{32c}$$

$$0 \le -\partial^{\mathbf{e}_2} g(\mathbf{x}) \quad \forall \mathbf{x}\in\mathcal{K}, \tag{32d}$$

$$\mathbf{0}_{2\times 2} \preccurlyeq \left[\left(\partial^{\mathbf{e}_i+\mathbf{e}_j} g\right)(\mathbf{x})\right]_{i,j\in[2]} \quad \forall \mathbf{x}\in\mathcal{K}. \tag{32e}$$

To demonstrate the importance of imposing the shape constraints we made the problem even more challenging and fixed $\mathcal{K} = \prod_{j\in[2]} \left[\min_{n\in[N_{tot}]}(\mathbf{x}_n)_j, 2\right]$. This choice allows us to illustrate how the imposed shape constraints are satisfied outside of $\mathcal{K}$, which here does not contain all the points. The covering of $\mathcal{K}$ was uniform, performed through rectangles of size $\delta_1 \times \delta_2$. The values of δ_1 and δ_2 were chosen to have 15 added points per dimension, resulting in $M = 225$ $\tilde{\mathbf{x}}_m$-s. The chosen kernel was Gaussian with bandwidth σ set to the

12. The dataset is available at `https://vincentarelbundock.github.io/Rdatasets/doc/Ecdat/Labour.html`.
13. Taking the logarithm of the output improves the numerical stability at the price of discarding the constraint $f(\mathbf{0}) = 0$.
14. Imposing the quadratic regularization $\lambda \|g\|_K^2$ as an equivalent constraint $\|g\|_K \le \tilde{\lambda}$ is in line with the implementation of conic convex problems through interior point methods.

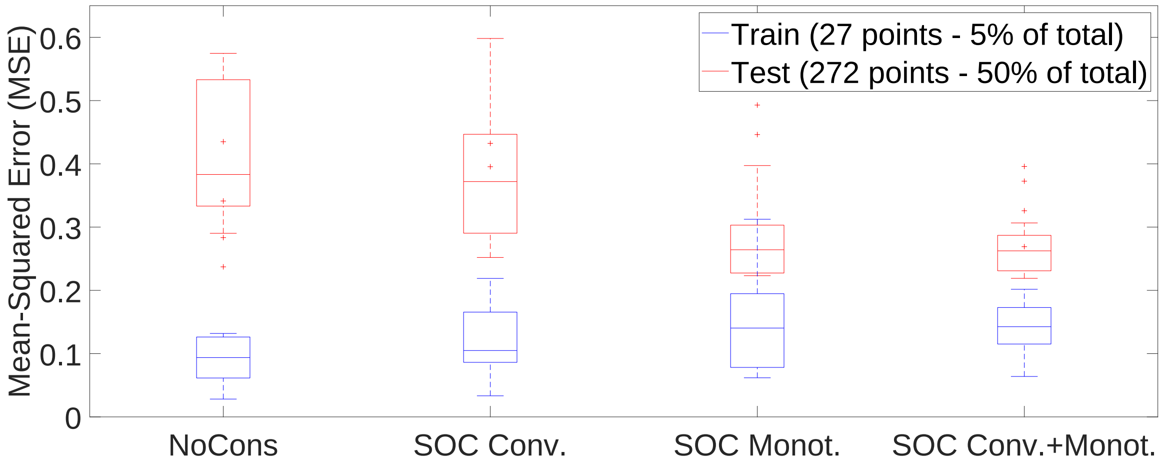


Figure 5: MSE as a function of incorporating shape constraints with the proposed SOC technique. NoCons: no constraint. SOC Monot.: two monotonicity constraints. SOC Conv.: one convexity constraint. SOC Conv.+Monot.: one convexity and two monotonicity constraints.

square root of the eighth decile of the squared pairwise distances of the points $\{\mathbf{x}_n\}_{n\in[N_{tot}]}$. As discussed after (23), the Gaussian kernel being translation-invariant, the computation of η_{m,P_i} can be centered at the origin, and it is sufficient to evaluate $\eta(\mathbf{0},\delta;D_i)$ defined in (21). These values were approximated numerically by taking 50 $\mathcal{X}$-points uniformly at random in $[-\delta_1,\delta_1]\times[-\delta_2,\delta_2]$. For the convexity constraint ($P_i=2$), we applied additionally a $\mathbf{u}=[\cos(\theta);\sin(\theta)]$ parameterization with 20 equidistant values of θ from $[0,\pi)$, by the invariance of $\eta(\mathbf{0},\delta;D_i)$ when replacing $\mathbf{u}$ by $-\mathbf{u}$. We considered four scenarios in terms of the shape constraints imposed: (i) no shape constraint [(32b)], (ii) two SOC-based monotonicity constraints [(32b)-(32d)], (iii) one SOC-based convexity constraint [(32b), (32e)], (iv) two SOC-based monotonicity and one SOC-based convexity constraint [(32b)-(32e)]. In our experiments, we partitioned randomly the dataset $\{(\mathbf{x}_n,y_n)\}_{n\in[N_{tot}]}$ into a validation set $\mathcal{D}_{val}$ and a test set $\mathcal{D}_{test}$ of approximately equal size ($\#\mathcal{D}_{val}=271$, $\#\mathcal{D}_{test}=272$) corresponding each to 50% of the total dataset. 20-fold cross-validation was performed on $\mathcal{D}_{val}$ to estimate the optimal value of $\tilde{\lambda}$ on a logarithmic grid. We then selected randomly 10% of $\mathcal{D}_{val}$ (referred to as $\mathcal{D}'_{val}$) to optimize $\mathcal{L}$ over this small training set using one of the four constraint settings detailed above for the estimated $\tilde{\lambda}$.[15] The efficiency of the resulting estimate for g was evaluated by the mean-squared error (MSE) over $\mathcal{D}'_{val}$ and $\mathcal{D}_{test}$. The whole experiment was repeated 20 times. The resulting statistics on the MSE values are summarized in Fig. 5, with a visual illustration of the underlying curves in Fig. 6. As it can be observed, adding shape constraints gradually improves the generalization performance (Fig. 5) while mitigating overfitting on the training set, and also helps satisfying the shape requirements outside of the constraint set $\mathcal{K}$ (Fig. 6).

These three applications demonstrate the efficiency of the proposed SOC approach in the context of shape optimization tasks, safety-critical control, and econometrics.

15. The rationale behind selecting only 10% of $\mathcal{D}_{val}$ is to make the problem more challenging and to illustrate the usefulness of considering shape constraints for small sample size.

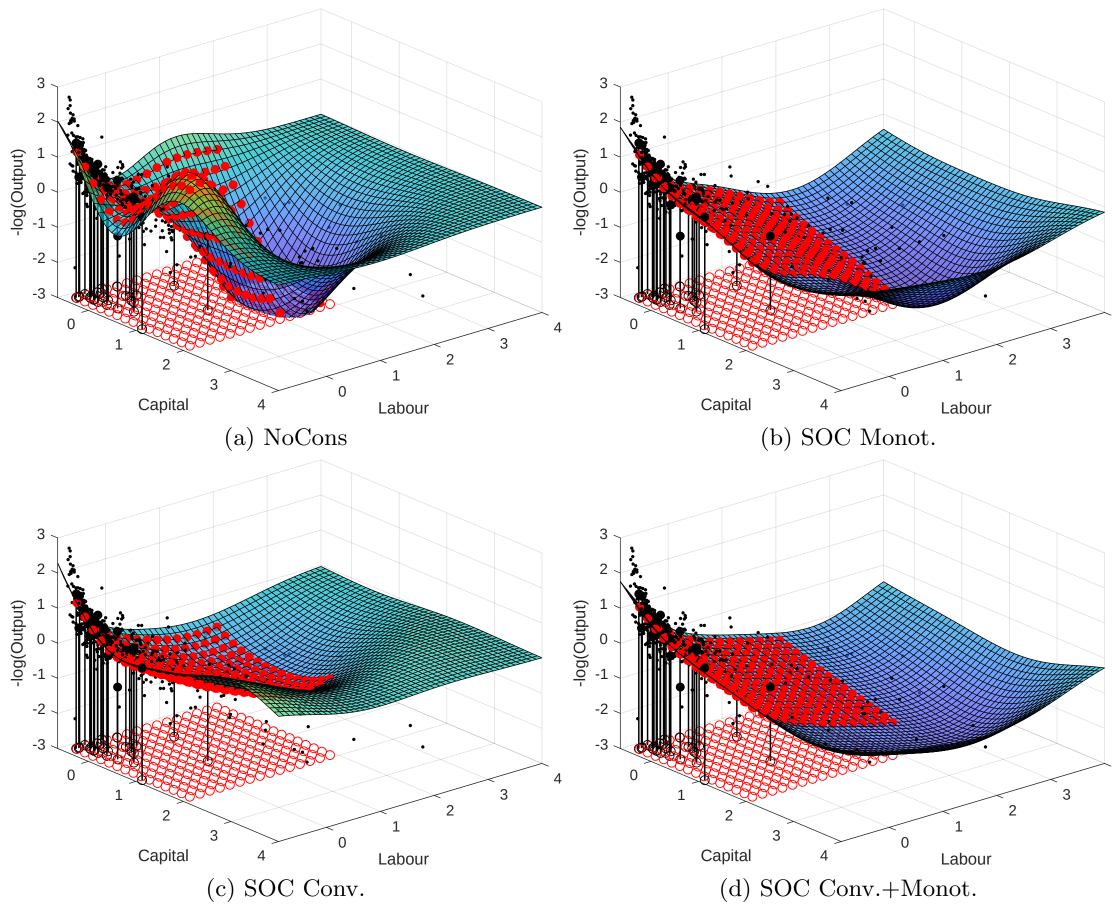


Figure 6: Illustration of the production function estimates with different shape constraints. Notation of the methods: as in Fig. 5. Red circles: covering points of $\mathcal{K}$. Red points on the surface: resulting y values. Black circles with vertical lines: N_{te} test points. Black circles without vertical lines: remaining $(\mathbf{x}, y)$ points.

7. Conclusions

In this paper we focused on the problem of incorporating hard affine SDP shape constraints on function derivatives into optimization problems over vector-valued reproducing kernel Hilbert spaces. We proposed a unified and modular second-order cone (SOC) based convex optimization framework to tackle this task. We designed and analysed two complementary approaches to derive SOC-based tightenings; they build upon a convex separation theorem in RKHSs (Theorem 2) and on an upper bound of the modulus of continuity (Theorem 3). We established the consistency of the techniques in terms of the refinement of the covering (Theorem 5). In addition, we proposed the soap bubble algorithm which guarantees hard shape constraints while adaptively refining the covering, and proved it convergence (Theorem 6). The efficiency of the approach was demonstrated in three applications (Section 6): in the context of shape optimization, safety-critical control and econometrics.

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Appendix A. Proofs

Section A.2 contains the proofs of our results (detailed in Section 3 – Section 5). Section A.1 is dedicated to auxiliary lemmas used in Section A.2.

A.1 Auxiliary Lemmas

In this section we provide auxiliary lemmas with their proofs.

Lemma 7 (Infimum over balls) *Let $\mathcal{F}$ be a Hilbert space, $\mathbf{g}, \mathbf{c} \in \mathcal{F}$ and $r > 0$. Then*

$$\inf_{\mathbf{w}\in\mathring{\mathbb{B}}_{\mathcal{F}}(\mathbf{c},r)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}} = \langle \mathbf{g}, \mathbf{c}\rangle_{\mathcal{F}} - r\|\mathbf{g}\|_{\mathcal{F}}.$$

Proof (Lemma 7) The statement follows by noting that

$$\inf_{\mathbf{w}\in\mathring{\mathbb{B}}_{\mathcal{F}}(\mathbf{c},r)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}} = \langle \mathbf{g}, \mathbf{c}\rangle_{\mathcal{F}} + \inf_{\mathbf{w}\in\mathbb{B}_{\mathcal{F}}(\mathbf{0},r)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}} = \langle \mathbf{g}, \mathbf{c}\rangle_{\mathcal{F}} - r\|\mathbf{g}\|_{\mathcal{F}}.$$

■

Lemma 8 (Infimum over half-spaces) *Let $\mathcal{F}$ be a Hilbert space, $\mathbf{g}, \mathbf{v} \in \mathcal{F}$, $\mathbf{v} \neq \mathbf{0}$, $\rho > 0$ and assume that $\inf_{\mathbf{w}\in\mathring{H}^-_{\mathcal{F}}(\mathbf{v},\rho)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}}$ is finite. Then there exists $\xi \in \mathbb{R}_+$ such that*

$$\mathbf{g} = -\xi\mathbf{v} \text{ and } -\xi\rho = \inf_{\mathbf{w}\in H^-_{\mathcal{F}}(\mathbf{v},\rho)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}}.$$

Proof (Lemma 8) Let us decompose $\mathbf{g}$ along the one-dimensional subspace spanned by $\mathbf{v}$: $\mathbf{g} = -\xi\mathbf{v} + \mathbf{u}$ where $\xi \in \mathbb{R}$, $\mathbf{u} \in \mathcal{F}$ and $\langle \mathbf{u}, \mathbf{v}\rangle_{\mathcal{F}} = 0$. We show that a finite infimum implies that in this decomposition $\xi \geq 0$ and $\mathbf{u} = \mathbf{0}$. Indeed,

- $\xi \geq 0$:

$$-\infty \overset{(a)}{<} \inf_{\mathbf{w}\in H^-_{\mathcal{F}}(\mathbf{v},\rho)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}} \overset{(b)}{\leq} \inf_{\tau\in\mathbb{R}_+} \left\langle -\xi\mathbf{v} + \mathbf{u}, \frac{\rho}{\|\mathbf{v}\|^2_{\mathcal{F}}}\mathbf{v} - \tau\mathbf{v} \right\rangle_{\mathcal{F}} \overset{(c)}{=} -\xi\rho + \inf_{\tau\in\mathbb{R}_+} \xi\tau\|\mathbf{v}\|^2_{\mathcal{F}}. \quad (33)$$

  where (a) holds by our assumption on the finiteness of the infimum. (b) is implied by the fact that for all $\tau \geq 0$, $\rho - \tau\|\mathbf{v}\|^2_{\mathcal{F}} \leq \rho$, so $\langle \frac{\rho}{\|\mathbf{v}\|^2_{\mathcal{F}}}\mathbf{v} - \tau\mathbf{v}, \mathbf{v}\rangle_{\mathcal{F}} \leq \rho$, hence $\frac{\rho}{\|\mathbf{v}\|^2}\mathbf{v} - \tau\mathbf{v} \in H^-_{\mathcal{F}}(\mathbf{v},\rho)$. (c) follows from $\langle \mathbf{u}, \mathbf{v}\rangle_{\mathcal{F}} = 0$. As $\mathbf{v} \neq \mathbf{0}$, (33) implies that $\xi \geq 0$.

- $\mathbf{u} = \mathbf{0}$:

$$-\infty \overset{(a)}{<} \inf_{\mathbf{w}\in H^-_{\mathcal{F}}(\mathbf{v},\rho)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}} \overset{(b)}{\leq} \inf_{\tau\in\mathbb{R}_+} \left\langle -\xi\mathbf{v} + \mathbf{u}, \frac{\rho}{\|\mathbf{v}\|^2_{\mathcal{F}}}\mathbf{v} - \tau\mathbf{u} \right\rangle_{\mathcal{F}} \overset{(c)}{=} -\xi\rho + \inf_{\tau\in\mathbb{R}_+} -\tau\|\mathbf{u}\|^2_{\mathcal{F}}. \quad (34)$$

  Our assumption on the finiteness of the infimum implies (a). (b) follows from $\frac{\rho}{\|\mathbf{v}\|^2_{\mathcal{F}}}\mathbf{v} - \tau\mathbf{u} \in H^-_{\mathcal{F}}(\mathbf{v},\rho)$ since $\langle \frac{\rho}{\|\mathbf{v}\|^2_{\mathcal{F}}}\mathbf{v} - \tau\mathbf{u}, \mathbf{v}\rangle_{\mathcal{F}} = \rho$ for any $\tau \in \mathbb{R}$. (c) is again a consequence of $\langle \mathbf{u}, \mathbf{v}\rangle_{\mathcal{F}} = 0$. Hence (34) means that $\mathbf{u} = \mathbf{0}$.

Applying the obtained $\mathbf{g} = -\xi\mathbf{v}$ relation ($\xi \geq 0$), we conclude that

$$\inf_{\mathbf{w}\in H^-_{\mathcal{F}}(\mathbf{v},\rho)} \langle \mathbf{g}, \mathbf{w}\rangle_{\mathcal{F}} = \inf_{\mathbf{w}\in H^-_{\mathcal{F}}(\mathbf{v},0)} \left\langle -\xi\mathbf{v}, \frac{\rho}{\|\mathbf{v}\|^2_{\mathcal{F}}}\mathbf{v} + \mathbf{w} \right\rangle_{\mathcal{F}} = \inf_{\mathbf{w}\in H^-_{\mathcal{F}}(\mathbf{v},0)} \left(-\xi\rho + \langle -\xi\mathbf{v}, \mathbf{w}\rangle_{\mathcal{F}}\right) = -\xi\rho$$

using that $\langle -\xi\mathbf{v}, \mathbf{w}\rangle_{\mathcal{F}} \geq 0$ since $\xi \geq 0$ and $\mathbf{w} \in H^-_{\mathcal{F}}(\mathbf{v},0)$, with the infimum attained at $\mathbf{w} = \mathbf{0}$. ■

Lemma 9 (Closed convex constraints) *Let* $C_{app} = \left(\bigcap_{i\in\mathcal{I}_{SOC}} C^i_{P_i,SOC}\right) \cap \left(\bigcap_{i\in\mathcal{I}_\Omega} C^i_{1,\Omega}\right)$ *with* $C^i_{P_i,SOC}$ *and* $C^i_{1,\Omega}$ *defined as in* ($\mathcal{C}_{P,\mathrm{SOC}}$) *and* ($\mathcal{C}_{1,\Omega}$), *then* C_{app} *is a closed convex set of* $\mathcal{F}_K \times \mathbb{R}^B$.

Proof (Lemma 9) The set C_{app} is closed and convex as it is the intersection of the closed convex sets $\left\{C^i_{P_i,\mathrm{SOC}}\right\}_{i\in\mathcal{I}_{\mathrm{SOC}}}$ and $\left\{C^i_{1,\Omega}\right\}_{i\in i\in\mathcal{I}_\Omega}$. The closedness of the latter sets can be proved as follows.

- Closedness of $C^i_{P_i,\mathrm{SOC}}$: Since $\|\cdot\|_K$ is lower semicontinuous, the SOC constraints define closed sets, thus any $C^i_{P_i,\mathrm{SOC}}$ is closed.
- Closedness of $C^i_{1,\Omega}$: Let $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}} \in \left(C^i_{1,\Omega}\right)^{\mathbb{N}}$ converge to some $(\mathbf{f}, \mathbf{b}) \in \mathcal{F}_K \times \mathbb{R}^B$. We show that $(\mathbf{f}, \mathbf{b}) \in C^i_{1,\Omega}$ which is equivalent to $\Omega_{i,m} \subseteq H^+_K(\mathbf{f} - \mathbf{f}_{0,i}, b_{0,i} - \mathbf{\Gamma}_i\mathbf{b})$ for every $m \in [M_i]$ by (11). Since the sequence $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}} \in \left(C^i_{1,\Omega}\right)^{\mathbb{N}}$, one has $\Omega_{i,m} \subseteq H^+_K\left(\mathbf{f}^{(k)} - \mathbf{f}_{0,i}, b_{0,i} - \mathbf{\Gamma}_i\mathbf{b}^{(k)}\right)$ for all $k \in \mathbb{N}$ and $m \in [M_i]$ by (11), i.e. $\langle \mathbf{g}, \mathbf{f}^{(k)} - \mathbf{f}_{0,i}\rangle_K \geq$

$b_{0,i} - \mathbf{\Gamma}_i \mathbf{b}^{(k)}$ for all $k \in \mathbb{N}$ and any $\mathbf{g} \in \Omega_{i,m}$. This implies that $\langle \mathbf{g}, \mathbf{f} - \mathbf{f}_{0,i} \rangle_K \geq b_{0,i} - \mathbf{\Gamma}_i \mathbf{b}$ also holds for all $\mathbf{g} \in \Omega_{i,m}$ by continuity. Hence $\Omega_{i,m} \subseteq H_K^+(\mathbf{f} - \mathbf{f}_{0,i}, b_{0,i} - \mathbf{\Gamma}_i \mathbf{b})$ for all $m \in [M_i]$ which means that $(\mathbf{f}, \mathbf{b}) \in C^i_{1,\Omega}$ by (11).

■

A.2 Proofs of Our Results

This section contains the proofs of the results presented in Section 3, Section 4, and Section 5: Lemma 1 (Section A.2.1), Theorem 2 (Section A.2.2), Theorem 3 (Section A.2.3), Lemma 4 (Section A.2.4), Theorem 5 (Section A.2.5), Theorem 6 (Section A.2.6).

A.2.1 Proof of Lemma 1

By the reproducing property of matrix-valued kernels

$$f_q(\mathbf{x}) = \mathbf{e}_q^\top \mathbf{f}(\mathbf{x}) = \langle \mathbf{f}, K(\cdot, \mathbf{x}) \mathbf{e}_q \rangle_K \overset{(*)}{\Rightarrow} D_q f_q(\mathbf{x}) = \langle \mathbf{f}, D_q K(\cdot, \mathbf{x}) \mathbf{e}_q \rangle_K$$

provided that the terms on the r.h.s. of the implication $(*)$ exist, which is proved below. Hence

$$D(\mathbf{f})(\mathbf{x}) = \sum_{q \in [Q]} \beta_q D_q f_q(\mathbf{x}) = \sum_{q \in [Q]} \beta_q \langle \mathbf{f}, D_q K(\cdot, \mathbf{x}) \mathbf{e}_q \rangle_K = \left\langle \mathbf{f}, \sum_{q \in [Q]} D_q K(\cdot, \mathbf{x}) \beta_q \mathbf{e}_q \right\rangle_K.$$

For $(*)$ to be valid, one has to show that for any $\mathbf{r} \in \mathbb{N}^d$ satisfying $|\mathbf{r}| \leq s$ and any $q \in [Q]$ we have

$$\mathbf{f} \in \mathcal{C}^s(\mathcal{X}, \mathbb{R}^Q), \tag{35a}$$

$$\partial_2^{\mathbf{r}} K(\cdot, \mathbf{x}) \mathbf{e}_q \in \mathcal{F}_K, \tag{35b}$$

$$\partial^{\mathbf{r}}(f_q)(\mathbf{x}) = \langle \mathbf{f}, \partial_2^{\mathbf{r}} K(\cdot, \mathbf{x}) \mathbf{e}_q \rangle_K \;\; (\forall\, \mathbf{f} \in \mathcal{F}_K,\, \mathbf{x} \in \mathcal{X}), \tag{35c}$$

where $\partial_2^{\mathbf{r}} K(\mathbf{x}', \mathbf{x}) := \partial^{\mathbf{r}}[\mathbf{x} \mapsto K(\mathbf{x}', \mathbf{x})] \in \mathbb{R}^{Q \times Q}$; this extends to general D_q by taking linear combinations. We prove (35a), (35b), (35c) by induction over $s_0 \in [\![0, s-1]\!]$, assuming the property to be satisfied for all $\mathbf{r}$ such that $|\mathbf{r}| \leq s_0$. For $s_0 = 0$, the assertion is true. Fix $p, q \in [Q]$ and $\mathbf{r}$ satisfying $|\mathbf{r}| = s_0$. Let $\mathbf{r}' := \mathbf{r} + \mathbf{e}_p$, $|\mathbf{r}'| = |\mathbf{r}| + 1 = s_0 + 1$ where $p, q \in [Q]$ are fixed and $\mathbf{e}_p \in \mathbb{R}^d$ is the p-th canonical basis vector. We show the statement first for the interior $\mathring{\mathcal{X}}$, then for the whole $\mathcal{X}$, extending by continuity. For all $h \neq 0$ and $\mathbf{x} \in \mathcal{X}$, let us introduce the difference quotient $\Delta_{h,\mathbf{x}}$, the limits of which shall give (35a), (35b), (35c)

$$\Delta_{h,\mathbf{x}} := \frac{\partial_2^{\mathbf{r}} K(\cdot, \mathbf{x} + h\mathbf{e}_p) \mathbf{e}_q - \partial_2^{\mathbf{r}} K(\cdot, \mathbf{x}) \mathbf{e}_q}{h}. \tag{36}$$

• Case of $\mathring{\mathcal{X}}$: Take $\mathbf{x}_1, \mathbf{x}_2 \in \mathring{\mathcal{X}}$ and $\rho > 0$ such that $\mathbb{B}_{\mathcal{X}}(\mathbf{x}_1, \rho) \cup \mathbb{B}_{\mathcal{X}}(\mathbf{x}_2, \rho) \subset \mathring{\mathcal{X}}$. Let $h_1, h_2 \in [-\rho, \rho] \backslash \{0\}$. By induction, for any $\mathbf{x}, \mathbf{x}' \in \mathcal{X}$,

$$\mathbf{e}_q^\top \partial_1^{\mathbf{r}} \partial_2^{\mathbf{r}} K(\mathbf{x}', \mathbf{x}) \mathbf{e}_q = \partial^{\mathbf{r}}(\mathbf{e}_q^\top \partial_2^{\mathbf{r}} K(\cdot, \mathbf{x}) \mathbf{e}_q)(\mathbf{x}') = \left\langle \partial_2^{\mathbf{r}} K(\cdot, \mathbf{x}) \mathbf{e}_q, \partial_2^{\mathbf{r}} K(\cdot, \mathbf{x}') \mathbf{e}_q \right\rangle_K, \tag{37}$$

where $\partial_1^{\mathbf{r}}$ is defined analogously to $\partial_2^{\mathbf{r}}$. Let us derive Cauchy sequences based on $\Delta_{h,\mathbf{x}}$. Since

$$\|\Delta_{h_1,\mathbf{x}_1} - \Delta_{h_2,\mathbf{x}_2}\|_K^2 = \|\Delta_{h_1,\mathbf{x}_1}\|_K^2 + \|\Delta_{h_2,\mathbf{x}_2}\|_K^2 - 2\langle \Delta_{h_1,\mathbf{x}_1}, \Delta_{h_2,\mathbf{x}_2}\rangle_K, \tag{38}$$

it is sufficient to consider quantities of the form

$$\begin{aligned}
&\langle \Delta_{h_1,\mathbf{x}_1}, \Delta_{h_2,\mathbf{x}_2}\rangle_K \\
&= \frac{1}{h_1h_2}\left[\langle \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_1+h_1\mathbf{e}_p)\mathbf{e}_q, \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_2+h_2\mathbf{e}_p)\mathbf{e}_q\rangle_K + \langle \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_1)\mathbf{e}_q, \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_2)\mathbf{e}_q\rangle_K\right. \\
&\qquad \left. - \langle \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_1)\mathbf{e}_q, \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_2+h_2\mathbf{e}_p)\mathbf{e}_q\rangle_K - \langle \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_1+h_1\mathbf{e}_p)\mathbf{e}_q, \partial_2^{\mathbf{r}}K(\cdot,\mathbf{x}_2)\mathbf{e}_q\rangle_K\right]. \\
&= \frac{1}{h_1h_2}\mathbf{e}_q^\top\left[\partial_1^{\mathbf{r}}\partial_2^{\mathbf{r}}K(\mathbf{x}_2+h_2\mathbf{e}_p,\mathbf{x}_1+h_1\mathbf{e}_p) + \partial_1^{\mathbf{r}}\partial_2^{\mathbf{r}}K(\mathbf{x}_2,\mathbf{x}_1)\right. \\
&\qquad \left. - \partial_1^{\mathbf{r}}\partial_2^{\mathbf{r}}K(\mathbf{x}_2+h_2\mathbf{e}_p,\mathbf{x}_1) - \partial_1^{\mathbf{r}}\partial_2^{\mathbf{r}}K(\mathbf{x}_2,\mathbf{x}_1+h_1\mathbf{e}_p)\right]\mathbf{e}_q \\
&= \int_0^1\int_0^1 \mathbf{e}_q^\top \partial_1^{\mathbf{r}'}\partial_2^{\mathbf{r}'}K(\mathbf{x}_1+\alpha h_1\mathbf{e}_p, \mathbf{x}_2+\beta h_2\mathbf{e}_p)\mathbf{e}_q \mathrm{d}\alpha\mathrm{d}\beta,
\end{aligned} \tag{39}$$

where (39) follows from integration by parts and by the fact that $K \in \mathcal{C}^{s,s}\left(\mathcal{X}\times\mathcal{X}, \mathbb{R}^{Q\times Q}\right)$. Applying the resulting expression (39) in (38), we obtain that

$$\|\Delta_{h_1,\mathbf{x}_1} - \Delta_{h_2,\mathbf{x}_2}\|_K^2 = \sum_{i,j\in[2]}(-1)^{i+j}\int_0^1\int_0^1 \mathbf{e}_q^\top \partial_1^{\mathbf{r}'}\partial_2^{\mathbf{r}'}K(\mathbf{x}_i+\alpha h_i\mathbf{e}_p, \mathbf{x}_j+\beta h_j\mathbf{e}_p)\mathbf{e}_q\mathrm{d}\alpha\mathrm{d}\beta. \tag{40}$$

To upper bound (40), since $K \in \mathcal{C}^{s,s}\left(\mathcal{X}\times\mathcal{X}, \mathbb{R}^{Q\times Q}\right)$, one can define the modulus of continuity for any $\delta \ge 0$

$$\omega\left(\mathbf{e}_q^\top\partial_1^{\mathbf{r}'}\partial_2^{\mathbf{r}'}K(\cdot,\cdot)\mathbf{e}_q, \delta\right) = \sup_{\substack{\mathbf{x},\mathbf{x}',\mathbf{y},\mathbf{y}'\in\mathcal{X},\\ \|\mathbf{x}-\mathbf{x}'\|_2\le\delta,\, \|\mathbf{y}-\mathbf{y}'\|_2\le\delta}} \left|\mathbf{e}_q^\top\partial_1^{\mathbf{r}'}\partial_2^{\mathbf{r}'}K(\mathbf{x}',\mathbf{x})\mathbf{e}_q - \mathbf{e}_q^\top\partial_1^{\mathbf{r}'}\partial_2^{\mathbf{r}'}K(\mathbf{y}',\mathbf{y})\mathbf{e}_q\right|$$

which is a continuous function of δ, with limit 0 at 0. Forming two groups in (40) with $(i,j) \in \{(1,1),(1,2)\}$ and $(i,j)\in\{(2,2),(2,1)\}$ one gets the bound

$$\|\Delta_{h_1,\mathbf{x}_1} - \Delta_{h_2,\mathbf{x}_2}\|_K \le \sqrt{2\omega\left(\mathbf{e}_q^\top\partial_1^{\mathbf{r}}\partial_2^{\mathbf{r}}K(\cdot,\cdot)\mathbf{e}_q, \|\mathbf{x}_1-\mathbf{x}_2\|_2 + |h_1| + |h_2|\right)} \tag{41}$$

depending on $\omega(\mathbf{e}_q^\top\partial_1^{\mathbf{r}}\partial_2^{\mathbf{r}}K(\cdot,\cdot)\mathbf{e}_q,\cdot)$, since

$$\begin{aligned}
\|(\mathbf{x}_1+\beta h_1\mathbf{e}_p) - (\mathbf{x}_2+\beta h_2\mathbf{e}_p)\|_2 &\le \|\mathbf{x}_1-\mathbf{x}_2\|_2 + \underbrace{\beta}_{\in[0,1]}|h_1-h_2|\underbrace{\|\mathbf{e}_p\|_2}_{=1} \\
&\le \|\mathbf{x}_1-\mathbf{x}_2\|_2 + |h_1| + |h_2|.
\end{aligned}$$

Having derived the upper bound (41) to control $\|\Delta_{h_1,\mathbf{x}_1} - \Delta_{h_2,\mathbf{x}_2}\|_K$, let us choose $\mathbf{x}_1 = \mathbf{x}_2 = \mathbf{x} \in \mathring{\mathcal{X}}$ and any sequence $(h_n)_{n\in\mathbb{N}} \subset [-\rho,\rho]\backslash\{0\}$ such that $h_n \xrightarrow{n\to\infty} 0$. In this case, (41) shows that $(\Delta_{h_n,\mathbf{x}})_{n\in\mathbb{N}}$ is a Cauchy sequence in the Hilbert space $\mathcal{F}_K$ so it converges by the completeness of $\mathcal{F}_K$. Moreover (41) ensures that all the sequences — independently of the choice of $(h_n)_{n\in\mathbb{N}}$ — have the same limit which we denote formally by $\Delta_{0,\mathbf{x}} \in \mathcal{F}_K$. Since strong convergence in $\mathcal{F}_K$ implies weak convergence, for any $\mathbf{f} \in \mathcal{F}_K$, we have

$$\lim_{h\to 0} \frac{\partial^{\mathbf{r}} f_q(\mathbf{x}+h\mathbf{e}_p) - \partial^{\mathbf{r}} f_q(\mathbf{x})}{h} = \lim_{h\to 0} \langle \mathbf{f}, \Delta_{h,\mathbf{x}} \rangle_K = \langle \mathbf{f}, \Delta_{0,\mathbf{x}} \rangle_K . \tag{42}$$

Consequently $\partial^{\mathbf{r}'} f_q(\mathbf{x})$ exists. Moreover, by choosing $\mathbf{f} = K(\cdot,\mathbf{x}')\mathbf{e}_{q'}$ in (42), we deduce that $\Delta_{0,\mathbf{x}} \in \mathcal{F}_K$ equals to $\partial_2^{\mathbf{r}'} K(\cdot,\mathbf{x})\mathbf{e}_q$ which establishes (35b) and (35c) for $\mathbf{r}'$. The continuity of $\partial^{\mathbf{r}'} f_q(\mathbf{x})$ on $\mathring{\mathcal{X}}$, hence (35a) for $\mathbf{r}'$ follows from the Cauchy-Schwarz inequality

$$\left|\partial^{\mathbf{r}'} f_q(\mathbf{x}_1) - \partial^{\mathbf{r}'} f_q(\mathbf{x}_2)\right| \le \|\mathbf{f}\|_K \|\Delta_{0,\mathbf{x}_1} - \Delta_{0,\mathbf{x}_2}\|_K$$

combined with (41).

• Case of $\mathcal{X}$: Let us consider an arbitrary point $\mathbf{x} \in \mathcal{X}$. Then there exists a sequence $(\mathbf{x}'_n)_{n\in\mathbb{N}} \in (\mathring{\mathcal{X}})^{\mathbb{N}}$ converging to $\mathbf{x}$ since $\mathcal{X}$ is contained in the closure of its interior. For any such sequence $(\mathbf{x}'_n)_{n\in\mathbb{N}}$, $(\Delta_{0,\mathbf{x}'_n})_{n\in\mathbb{N}}$ is a Cauchy sequence by (41) applied with $h_1 = h_2 = 0$ (hence convergent by the completeness of $\mathcal{F}_K$), with the same limit which we again denote formally by $\Delta_{0,\mathbf{x}} \in \mathcal{F}_K$. Consequently,

$$\lim_{\mathbf{x}'\to\mathbf{x}} \partial^{\mathbf{r}'} f_q(\mathbf{x}') = \lim_{\mathbf{x}'\to\mathbf{x}} \langle \mathbf{f}, \Delta_{0,\mathbf{x}'} \rangle_K = \langle \mathbf{f}, \Delta_{0,\mathbf{x}} \rangle_K ,$$

so $\partial^{\mathbf{r}'} f_q(\mathbf{x})$ exists and $\Delta_{0,\mathbf{x}} \in \mathcal{F}_K$ can be identified with $\partial_2^{\mathbf{r}'} K(\cdot,\mathbf{x})\mathbf{e}_q$ which establishes (35b) and (35c) for $\mathbf{r}'$. Let $f_q^{[\mathbf{r}']}(\mathbf{x}') := \langle \mathbf{f}, \Delta_{0,\mathbf{x}'} \rangle_K$ for $\mathbf{x}' \in \mathcal{X}$. Again by the Cauchy-Schwarz inequality, we obtain that $f_q^{[\mathbf{r}']}$ is continuous on $\mathcal{X}$, and it is the continuous extension of $\partial^{\mathbf{r}'} f_q$ from $\mathring{\mathcal{X}}$ to $\mathcal{X}$. This proves (35a) for $\mathbf{r}'$ and concludes the induction.

A.2.2 Proof of Theorem 2

By the convex separation formula of Dubovitskii and Milyutin (1965), the first statement is equivalent to the existence of $\mathbf{g}_{\mathbf{f}}, (\mathbf{g}_{B,j})_{j\in[J_B]}, (\mathbf{g}_{H,j})_{j\in[J_H]} \in \mathcal{F}_K$ not vanishing simultaneously and satisfying

$$\inf_{\mathbf{w}\in \mathring{H}_K^-(\mathbf{f}-\mathbf{f}_0, b_0-\boldsymbol{\Gamma}\mathbf{b})} \langle \mathbf{g}_{\mathbf{f}}, \mathbf{w}\rangle_K + \sum_{j\in[J_B]} \inf_{\mathbf{w}\in\mathring{\mathbb{B}}_K(\mathbf{c}_j,r_j)} \langle \mathbf{g}_{B,j}, \mathbf{w}\rangle_K + \sum_{j\in[J_H]} \inf_{\mathbf{w}\in\mathring{H}_K^-(\mathbf{v}_j,\rho_j)} \langle \mathbf{g}_{H,j}, \mathbf{w}\rangle_K \ge 0,$$
$$\mathbf{g}_{\mathbf{f}} + \sum_{j\in[J_B]} \mathbf{g}_{B,j} + \sum_{j\in[J_H]} \mathbf{g}_{H,j} = \mathbf{0}.$$

Since the sum of the infima is nonnegative, each infimum is finite. Hence by Lemma 7 and Lemma 8 we get that the inclusion $\Omega \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0-\boldsymbol{\Gamma}\mathbf{b})$ holds if and only if there exist $[\xi_{\mathbf{f}};\xi_1;\ldots;\xi_{J_H}] \in \mathbb{R}_+^{J_H+1}$ and $(\mathbf{g}_{B,j})_{j\in[J_B]} \in \mathcal{F}_K^{J_B}$ not vanishing simultaneously (since $\xi_{\mathbf{f}} = 0 \Leftrightarrow \mathbf{g}_{\mathbf{f}} = \mathbf{0}$, and $\xi_j = 0 \Leftrightarrow \mathbf{g}_{H,j} = \mathbf{0}$) such that

$$\begin{aligned} -\xi_{\mathbf{f}} b_0 - \boldsymbol{\Gamma}\mathbf{b} + \sum_{j\in[J_B]} \langle \mathbf{g}_{B,j}, \mathbf{c}_j\rangle_K - \sum_{j\in[J_H]} \xi_j\rho_j - \sum_{j\in[J_B]} r_j \|\mathbf{g}_{B,j}\|_K \ge 0, \\ -\xi_{\mathbf{f}}(\mathbf{f}-\mathbf{f}_0) + \sum_{j\in[J_B]} \mathbf{g}_{B,j} - \sum_{j\in[J_H]} \xi_j \mathbf{v}_j = \mathbf{0}. \end{aligned} \tag{43}$$

Let $\mathcal{V} = \text{span}\left(\mathbf{f} - \mathbf{f}_0, \{\mathbf{c}_j\}_{j\in[J_B]}, \{\mathbf{v}_j\}_{j\in[J_H]}\right)$ and $\mathbf{g}_j = \text{proj}_{\mathcal{V}}(\mathbf{g}_{B,j})$ where $\text{proj}_{\mathcal{V}}$ denotes the projection onto the subspace $\mathcal{V}$. Since $\langle \mathbf{g}_{B,j}, \mathbf{c}_j\rangle_K = \langle \mathbf{g}_j, \mathbf{c}_j\rangle_K$ and $\|\mathbf{g}_j\|_K \leq \|\mathbf{g}_{B,j}\|_K$, this family also satisfies (43). Here, again $[\xi_{\mathbf{f}}; \xi_1; \ldots; \xi_{J_H}] \in \mathbb{R}_+^{J_H+1}$ and $(\mathbf{g}_j)_{j\in[J_B]} \in \mathcal{F}_K^{J_B}$ cannot all vanish. Indeed, if it were the case, then by $\langle \mathbf{g}_{B,j}, \mathbf{c}_j\rangle_K = \langle \mathbf{g}_j, \mathbf{c}_j\rangle_K = 0$, (43) would give $-\sum_{j\in[J_B]} r_j \|\mathbf{g}_{B,j}\|_K \geq 0$, so, since $r_j > 0$ $(\forall j \in [J_B])$, $(\mathbf{g}_{B,j})_{j\in[J_B]}$ would all vanish too.

The nonnegative number $\xi_{\mathbf{f}}$ cannot be zero since in this case either $H_K^-(\mathbf{f} - \mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})$ or Ω would be empty by (43) (Dubovitskii and Milyutin, 1965), both cases being excluded by assumption. Hence, we can divide (43) by $\xi_{\mathbf{f}} > 0$; replacing ξ_j with $\xi_j/\xi_{\mathbf{f}}$ and $\mathbf{g}_j$ with $\mathbf{g}_j/\xi_{\mathbf{f}}$, the claimed equation (12) follows.

A.2.3 Proof of Theorem 3

In accordance with the r.h.s. of (20) let us define

$$\mathbf{g}_{\mathbf{x},\mathbf{u}}(\cdot) := \mathbf{u}^\top \mathbf{D}K(\cdot, \mathbf{x})\mathbf{u} := \sum_{p_1,\, p_2\in[P]} u_{p_1} u_{p_2} D_{p_1,\, p_2} K(\cdot, \mathbf{x}) \in \mathcal{F}_K, \tag{44}$$

where $\mathbf{x} \in \mathcal{X}$ and $\mathbf{u} \in \mathcal{S}^{P-1}$. Since $\mathcal{K} \subseteq \bigcup_{m\in[M]} \mathbb{B}_{\mathcal{X}}(\tilde{\mathbf{x}}_m, \delta_m)$, for any $\mathbf{x} \in \mathcal{K}$ let us take $\tilde{\mathbf{x}}_m$ for which $\|\mathbf{x} - \tilde{\mathbf{x}}_m\|_{\mathcal{X}} \leq \delta_m$. Applying the reproducing formula (6) and the Cauchy-Schwartz inequality, for any $\mathbf{f} \in \mathcal{F}_k$ one gets the lower bound

$$\begin{aligned}
\mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\mathbf{x})\mathbf{u} &= \langle \mathbf{f} - \mathbf{f}_0, \mathbf{u}^\top \mathbf{D}K(\cdot, \mathbf{x})\mathbf{u}\rangle_K \\
&= \mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m)\mathbf{u} + \langle \mathbf{f} - \mathbf{f}_0, \mathbf{u}^\top [\mathbf{D}K(\cdot, \mathbf{x}) - \mathbf{D}K(\cdot, \tilde{\mathbf{x}}_m)]\, \mathbf{u}\rangle_K \\
&\geq \mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m)\mathbf{u} - \|\mathbf{f} - \mathbf{f}_0\|_K \left\| \mathbf{u}^\top [\mathbf{D}K(\cdot, \mathbf{x}) - \mathbf{D}K(\cdot, \tilde{\mathbf{x}}_m)]\, \mathbf{u} \right\|_K \\
&\geq \mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m)\mathbf{u} - \eta_{m,P}\|\mathbf{f} - \mathbf{f}_0\|_K.
\end{aligned} \tag{45}$$

This means that for $(\mathbf{f}, \mathbf{b}) \in C_{P,\text{SOC}}$ and for any $\mathbf{u} \in \mathcal{S}^{P-1}$,

$$\begin{aligned}
\eta_{m,P}\|\mathbf{f} - \mathbf{f}_0\|_K \underbrace{\mathbf{u}^\top \mathbf{u}}_{=1} &\leq \mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m)\mathbf{u} + \mathbf{u}^\top \operatorname{diag}(\mathbf{\Gamma}\mathbf{b} - \mathbf{b}_0)\mathbf{u} \\
0 &\leq \mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\tilde{\mathbf{x}}_m)\mathbf{u} - \eta_{m,P}\|\mathbf{f} - \mathbf{f}_0\|_K + \mathbf{u}^\top \operatorname{diag}(\mathbf{\Gamma}\mathbf{b} - \mathbf{b}_0)\mathbf{u} \\
0 &\overset{(45)}{\leq} \mathbf{u}^\top \mathbf{D}(\mathbf{f} - \mathbf{f}_0)(\mathbf{x})\mathbf{u} + \mathbf{u}^\top \operatorname{diag}(\mathbf{\Gamma}\mathbf{b} - \mathbf{b}_0)\mathbf{u},
\end{aligned}$$

in other words, $(\mathbf{f}, \mathbf{b}) \in C_P$; this proves Theorem 3.

A.2.4 Proof of Lemma 4

Taking the square of the argument of the supremum in (20), by (44) we have

$$\begin{aligned}
&\left\| \sum_{p_1,\, p_2\in[P]} u_{p_1} u_{p_2} D_{p_1,p_2} K(\cdot, \tilde{\mathbf{x}}_m) - \sum_{p_1,\, p_2\in[P]} u_{p_1} u_{p_2} D_{p_1,p_2} K(\cdot, \mathbf{x}) \right\|_K^2 = \\
&\quad = \|g_{\tilde{\mathbf{x}}_m,\mathbf{u}} - g_{\mathbf{x},\mathbf{u}}\|_K^2 = \|g_{\tilde{\mathbf{x}}_m,\mathbf{u}}\|_K^2 + \|g_{\mathbf{x},\mathbf{u}}\|_K^2 - 2\,\langle g_{\tilde{\mathbf{x}}_m,\mathbf{u}}, g_{\mathbf{x},\mathbf{u}}\rangle_K^2 .
\end{aligned} \tag{46}$$

This means that it is sufficient to compute expressions of the form $\langle g_{\mathbf{x}',\mathbf{u}}, g_{\mathbf{x},\mathbf{u}}\rangle_K$ where $\mathbf{x}', \mathbf{x} \in \mathcal{X}$.

$$\begin{aligned}\langle g_{\mathbf{x}',\mathbf{u}}, g_{\mathbf{x},\mathbf{u}}\rangle_K &= \left\langle \sum_{p_1,\,p_2\in[P]} u_{p_1}u_{p_2}D_{p_1,\,p_2}K(\cdot,\mathbf{x}'), \sum_{p_1,\,p_2\in[P]} u_{p_1}u_{p_2}D_{p_1,\,p_2}K(\cdot,\mathbf{x})\right\rangle_K \\ &= \sum_{p'_1,\,p'_2,\,p_1,\,p_2\in[P]} u_{p'_1}u_{p'_2}u_{p_1}u_{p_2} \underbrace{\left\langle D_{p'_1,\,p'_2}K(\cdot,\mathbf{x}'), D_{p_1,\,p_2}K(\cdot,\mathbf{x})\right\rangle_K}_{\overset{(*)}{=} D^\top_{p'_1,p'_2}D_{p_1,p_2}K(\mathbf{x}',\mathbf{x}) = \boldsymbol{\mathcal{K}}(\mathbf{x}',\mathbf{x})_{p_1,p_2,p'_1,p'_2}} \\ &= \langle \mathbf{u}\otimes\mathbf{u}, \boldsymbol{\mathcal{K}}(\mathbf{x}',\mathbf{x})(\mathbf{u}\otimes\mathbf{u})\rangle_F. \end{aligned} \tag{47}$$

$(*)$ follows from the fact that for any point $\mathbf{x}', \mathbf{x} \in \mathcal{X}$ and differential operator $\tilde{D}, D \in O_{Q,s}$ with parameterization $D(\mathbf{f})(\mathbf{x}) = \sum_{q\in[Q]} \beta_q D_{q,\mathbf{x}}(f_q)(\mathbf{x})$ and $\tilde{D}(\mathbf{f})(\mathbf{x}') = \sum_{q\in[Q]} \tilde{\beta}_q \tilde{D}_{q,\mathbf{x}'}(f_q)(\mathbf{x}')$

$$\left\langle \tilde{D}K(\cdot,\mathbf{x}'), DK(\cdot,\mathbf{x})\right\rangle_K = \sum_{q,q'\in[Q]} \beta_q\tilde{\beta}_{q'}\mathbf{e}_{q'}^\top \tilde{D}_{q',\mathbf{x}'}D_{q,\mathbf{x}}K(\mathbf{x}',\mathbf{x})\mathbf{e}_q = \tilde{D}^\top DK(\mathbf{x}',\mathbf{x})$$

as implied by the reproducing property (6). Combining (46) and (47) concludes the proof.

A.2.5 Proof of Theorem 5

Existence: Define the domain $\mathcal{D} := C_{\text{app}} \cap \operatorname{dom}(\mathcal{L}) \cap (\mathcal{F}_K \times \mathcal{B})$ and

$$v_{\text{app}} = \inf_{\substack{\mathbf{f}\in\mathcal{F}_K,\,\mathbf{b}\in\mathcal{B}\\ (\mathbf{f},\mathbf{b})\in C_{\text{app}}}} \mathcal{L}(\mathbf{f},\mathbf{b}).$$

By definition of the infimum, there exists a sequence $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}} \in \mathcal{D}^{\mathbb{N}}$ such that

$$\lim_{k\to\infty} \mathcal{L}\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) = v_{\text{app}}. \tag{48}$$

Using this sequence we will construct a pair $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) \in \mathcal{D}$ for which $\mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) = v_{\text{app}}$.

- Finiteness of v_{app}: By Assumption (v) there exists an admissible pair $(\mathbf{f},\mathbf{b}) \in C_{\text{app}}$ which implies that $v_{\text{app}} < \infty$. Using that both $L + \chi_{C_{\text{app}}}$ and R are lower bounded (the former is Assumption (iii), the latter is larger than $R(0)$ since R is monotonically increasing), one gets that $v_{\text{app}} > -\infty$; so v_{app} is finite.
- Construction of $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$: Since $L + \chi_{C_{\text{app}}}$ is lower bounded by Assumption (iii) and v_{app} is finite, the sequence $\left(R\left(\|\mathbf{f}^{(k)}\|_K\right)\right)_{k\in\mathbb{N}}$ is necessarily upper bounded. This implies the boundedness of $\left(\|\mathbf{f}^{(k)}\|_K\right)_{k\in\mathbb{N}}$ by Assumption (i). In other words, there exists $r > 0$ such that $\left(\|\mathbf{f}^{(k)}\|_K\right)_{k\in\mathbb{N}} \subset \mathbb{B}_K(\mathbf{0}, r)$. Let $\tilde{L}(\mathbf{f},\mathbf{b}) := L\left(\mathbf{b}, \left(\left(D^0_{n,j}(\mathbf{f})(\mathbf{x}_n)\right)_{j\in J_n}\right)_{n\in[N]}\right) + \chi_{\mathbb{B}_K(\mathbf{0},r)}(\mathbf{f})$, $\tilde{L}$ is l.s.c. since it is the composition of the l.s.c. L (Assumption (iv)) with the continuous maps $\mathbf{f} \mapsto D^0_{n,j}(\mathbf{f})(\mathbf{x}_n)$. Moreover, $\lim_{\|\mathbf{f}\|_K + \|\mathbf{b}\|_2 \to\infty} \tilde{L}(\mathbf{f},\mathbf{b}) = \infty$ by Assumption (ii). Hence, $\tilde{L}$ is coercive over the Hilbert space $\mathcal{F}_K \times \mathbb{R}^B$ equipped with the

sum of the inner products. However $\tilde{L}(\mathbf{f}^{(k)},\mathbf{b}^{(k)}) \le L(\mathbf{f}^{(k)},\mathbf{b}^{(k)}) + R(\|\mathbf{f}^{(k)}\|_K) - R(0) \le \sup_{k\in\mathbb{N}} \mathcal{L}(\mathbf{f}^{(k)},\mathbf{b}^{(k)}) - R(0)$. Consequently $\left(\mathbf{f}^{(k)},\mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ belongs to a bounded closed level set of $\tilde{L}$. As $\left(\mathbf{f}^{(k)},\mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ is bounded in the Hilbert space $\mathcal{F}_K \times \mathbb{R}^B$, it has a subsequence (w.l.o.g. one can assume that it is the sequence itself) converging weakly to some $\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) \in \mathcal{F}_K \times \mathbb{R}^B$; by the closedness of the level set and of $\mathcal{B}$, we have that $\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) \in \operatorname{dom}(\tilde{L}) \cap (\mathcal{F}_K \times \mathcal{B}) \subseteq \operatorname{dom}(\mathcal{L})$.

- $\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) \in C_{\text{app}}$, $\mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) = v_{\text{app}}$: One has

$$L\left(\bar{\mathbf{b}}_{\text{app}}, \left(\left(D^0_{n,j}(\bar{\mathbf{f}}_{\text{app}})(\mathbf{x}_n)\right)_{j\in J_n}\right)_{n\in[N]}\right) \overset{(a)}{\le} \liminf_{k\to\infty} L\left(\mathbf{b}^{(k)}, \left(\left(D^0_{n,j}\left(\mathbf{f}^{(k)}\right)(\mathbf{x}_n)\right)_{j\in J_n}\right)_{n\in[N]}\right), \tag{49}$$

$$R\left(\left\|\bar{\mathbf{f}}_{\text{app}}\right\|_K\right) \overset{(b)}{\le} R\left(\liminf_{k\to\infty}\left\|\mathbf{f}^{(k)}\right\|_K\right) \overset{(c)}{\le} \liminf_{k\to\infty} R\left(\left\|\mathbf{f}^{(k)}\right\|_K\right). \tag{50}$$

(a) follows from the fact that in finite-dimensional Euclidean spaces strong and weak convergence coincide, from the lower semi-continuity of L (Assumption (iv)), and by the fact that $\lim_{k\to\infty} D^0_{n,j}\left(\mathbf{f}^{(k)}\right)(\mathbf{x}_n) = D^0_{n,j}\left(\bar{\mathbf{f}}_{\text{app}}\right)(\mathbf{x}_n)$ ($\forall n \in [N]$, $j \in J_n$); the latter is implied by the weak convergence of $\left(\mathbf{f}^{(k)}\right)_{k\in\mathbb{N}}$ to $\bar{\mathbf{f}}_{\text{app}}$ and the reproducing property (Lemma 1). (b) comes from the (sequentially) weakly l.s.c. property of $\|\cdot\|_K$ and the monotonicity of R. The l.s.c. property of R (Assumption (iv)) gives (c): by the definition of the lim inf, there exists a subsequence $\left(\mathbf{f}^{(k_n)}\right)_{n\in\mathbb{N}}$ such that $\liminf_{k\to\infty}\left\|\mathbf{f}^{(k)}\right\|_K = \lim_{n\to\infty}\left\|\mathbf{f}^{(k_n)}\right\|_K$ and $R\left(\lim_{n\to\infty}\left\|\mathbf{f}^{(k_n)}\right\|_K\right) \le \liminf_{n\to\infty} R\left(\left\|\mathbf{f}^{(k_n)}\right\|_K\right)$ as R is l.s.c.; again the reasoning can be restricted w.l.o.g. to the subsequence $\left(\mathbf{f}^{(k_n)}\right)_{n\in\mathbb{N}}$.
The set C_{app} is a closed convex subset of $\mathcal{F}_k \times \mathbb{R}^B$ by Lemma 9. Hence it also closed w.r.t. weak convergence and $\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) \in C_{\text{app}}$ since it is a weak limit of a sequence $\left(\mathbf{f}^{(k)},\mathbf{b}^{(k)}\right)_{k\in\mathbb{N}} \subset C_{\text{app}}$. Therefore

$$\begin{aligned}
v_{\text{app}} &\le \mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right)\\
&\overset{(a)}{\le} \liminf_{k\to\infty} L\left(\mathbf{b}^{(k)}, \left(\left(D^0_{n,j}\left(\mathbf{f}^{(k)}\right)(\mathbf{x}_n)\right)_{j\in J_n}\right)_{n\in[N]}\right) + \liminf_{k\to\infty} R\left(\left\|\mathbf{f}^{(k)}\right\|_K\right)\\
&\overset{(b)}{\le} \liminf_{k\to\infty}\mathcal{L}\left(\mathbf{f}^{(k)},\mathbf{b}^{(k)}\right) = \lim_{k\to\infty}\mathcal{L}\left(\mathbf{f}^{(k)},\mathbf{b}^{(k)}\right) = v_{\text{app}},
\end{aligned}$$

where (a) is implied by (49) and (50), and (b) holds by the superadditivity of lim inf. This means that $\mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) = v_{\text{app}}$ which combined with the established $\left(\bar{\mathbf{f}}_{\text{app}},\bar{\mathbf{b}}_{\text{app}}\right) \in \mathcal{D} = C_{\text{app}} \cap \operatorname{dom}(\mathcal{L}) \cap (\mathcal{F}_K \times \mathcal{B})$ concludes the proof.

Finite-dimensional description: Let us consider the finite-dimensional subspace

$$\begin{aligned}
V := \operatorname{span}\Big(&\{\mathbf{f}_{0,i}\}_{i\in[I]}, \left\{D^0_{n,j}K(\cdot,\mathbf{x}_n)\right\}_{n\in[N],j\in J_n}, \{D^i_{p_1,p_2}K(\cdot,\tilde{\mathbf{x}}_{i,m})\}_{i\in\mathcal{I}_{\text{SOC}},\,p_1,\,p_2\in[P_i],\,m\in[M_i]},\\
&\{\mathbf{c}_{i,m,j}\}_{i\in\mathcal{I}_\Omega,\,m\in[M_i],\ j\in[J_{B,i,m}],}, \{\mathbf{v}_{i,m,j}\}_{i\in\mathcal{I}_\Omega,\,m\in[M_i],\,j\in[J_{H,i,m}]}\Big).
\end{aligned}$$

Let $(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}})$ be an optimal solution, which we decompose as $\bar{\mathbf{f}}_{\text{app}} = \mathbf{z} + \mathbf{w}$ where $\mathbf{z} = \text{proj}_V\left(\bar{\mathbf{f}}_{\text{app}}\right) \in V$ and $\mathbf{w} \in V^{\perp}$. We show that $\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right)$ is then also an optimal solution.

- $L\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) = L\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right)$: By the linearity of the differential operators $D^0_{n,j}$, the reproducing property (Lemma 1) and the orthogonality of $\mathbf{w} \in V^{\perp}$ and $D^0_{n,j}K(\cdot, \mathbf{x}_n) \in V$, one gets

$$D^0_{n,j}\left(\bar{\mathbf{f}}_{\text{app}}\right)(\mathbf{x}_n) = D^0_{n,j}\left(\mathbf{z}+\mathbf{w}\right)(\mathbf{x}_n) = D^0_{n,j}\left(\mathbf{z}\right)(\mathbf{x}_n) + \underbrace{D^0_{n,j}\left(\mathbf{w}\right)(\mathbf{x}_n)}_{\left\langle \mathbf{w}, D^0_{n,j}K(\cdot,\mathbf{x}_n)\right\rangle_K = 0} .$$

  This implies that the terms appearing in L are the same for $\bar{\mathbf{f}}_{\text{app}}$ and for $\mathbf{z}$, and hence $L\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) = L\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right)$.

- $R\left(\|\mathbf{z}\|_K\right) \le R\left(\left\|\bar{\mathbf{f}}_{\text{app}}\right\|_K\right)$: This inequality follows from $\|\mathbf{z}\|_K \le \left\|\bar{\mathbf{f}}_{\text{app}}\right\|_K$ by the monotonicity of R.

- $\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right) \in C^i_{P_i,\text{SOC}}$ for all $i \in \mathcal{I}_{\text{SOC}}$: Let $i \in \mathcal{I}_{\text{SOC}}$. Similarly to the previous point, $D^i_{p_1,p_2}(\bar{\mathbf{f}}_{\text{app}})(\tilde{\mathbf{x}}_{i,m}) = D^i_{p_1,p_2}(\mathbf{z})(\tilde{\mathbf{x}}_{i,m})$ for all $p_1, p_2 \in [P_i]$ and $m \in [M_i]$, so the r.h.s. in the inequalities in $C^i_{P_i,\text{SOC}}$ are the same for $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ and $\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right)$. Considering the l.h.s.-s, $\|\mathbf{z} - \mathbf{f}_{0,i}\|_K \le \left\|\bar{\mathbf{f}}_{app} - \mathbf{f}_{0,i}\right\|_K$ since by the Pythagorean theorem $\left\|\bar{\mathbf{f}}_{app} - \mathbf{f}_{0,i}\right\|^2_K = \|\mathbf{z} - \mathbf{f}_{0,i}\|^2_K + \|\mathbf{w}\|^2_K$. This shows that $\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right) \in C^i_{P_i,\text{SOC}}$ for all $i \in \mathcal{I}_{\text{SOC}}$.

- $(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}) \in C^i_{1,\Omega}$ for all $i \in \mathcal{I}_\Omega$: By (11) it is sufficient to prove that $\Omega_{i,m} \subseteq H^+_K(\mathbf{z} - \mathbf{f}_{0,i}, b_{0,i} - \mathbf{\Gamma}_i\mathbf{b})$ for all $i \in \mathcal{I}_\Omega$ and $m \in [M_i]$. In the following the i and m indices are assumed to be fixed; in the notations we make them implicit. By Theorem 2, we have to show the existence of J_B functions $(\mathbf{g}'_j)_{j\in[J_B]} \subset \text{span}\left(\mathbf{z} - \mathbf{f}_0, \{\mathbf{c}_j\}_{j\in[J_B]}, \{\mathbf{v}_j\}_{j\in[J_H]}\right)$ and J_H non-negative coefficients $(\xi'_j)_{j\in[J_H]} \in \mathbb{R}^{J_H}_+$ satisfying (12). Consider $(\mathbf{g}_j)_{j\in[J_B]}$ and $(\xi_j)_{j\in[J_H]}$ for which (12) holds for $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$. Let us define $\mathbf{g}'_j := \text{proj}_V(\mathbf{g}_j)$ (in other words, $\mathbf{g}_j = \mathbf{g}'_j + \mathbf{g}'^{\perp}_j$ with $\mathbf{g}'_j \in V$, $\mathbf{g}'^{\perp}_j \in V^{\perp}$) and $\xi'_j := \xi_j \in \mathbb{R}_+$. With this choice of $(\mathbf{g}'_j)_{j\in[J_B]}$ and $(\xi'_j)_{j\in[J_H]}$, the pair $\left(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}\right)$ satisfies (12). Indeed, the inequality in (12) holds by

$$\langle \mathbf{g}_j, \mathbf{c}_j\rangle_K = \left\langle \mathbf{g}'_j + \mathbf{g}'^{\perp}_j, \mathbf{c}_j\right\rangle_K = \langle \mathbf{g}'_j, \mathbf{c}_j\rangle_K + \langle \underbrace{\mathbf{g}'^{\perp}_j}_{\in V^{\perp}}, \underbrace{\mathbf{c}_j}_{\in V}\rangle_K = \langle \mathbf{g}'_j, \mathbf{c}_j\rangle_K , \; \left\|\mathbf{g}'_j\right\|_K \le \|\mathbf{g}_j\|_K .$$

  The equality in (12) is satisfied since

$$\begin{aligned}\mathbf{0} = \text{proj}_V(\mathbf{0}) &= \text{proj}_V\left(-\left(\bar{\mathbf{f}}_{app} - \mathbf{f}_0\right) + \sum_{j\in[J_B]}\mathbf{g}_j - \sum_{j\in[J_H]}\xi_j\mathbf{v}_j\right)\\ &= -\Big[\underbrace{\text{proj}_V\left(\bar{\mathbf{f}}_{app}\right)}_{=\mathbf{z}} - \underbrace{\text{proj}_V\left(\mathbf{f}_0\right)}_{=\mathbf{f}_0 \Leftarrow \mathbf{f}_0\in V}\Big] + \sum_{j\in[J_B]}\underbrace{\text{proj}_V(\mathbf{g}_j)}_{=\mathbf{g}'_j} - \sum_{j\in[J_H]}\underbrace{\xi_j}_{=\xi'_j}\underbrace{\text{proj}_V(\mathbf{v}_j)}_{=\mathbf{v}_j \Leftarrow \mathbf{v}_j\in V} .\end{aligned}$$

Finally let us fix any $j \in [J_B]$ and show that $\mathbf{g}'_j \in \operatorname{span}\left(\mathbf{z} - \mathbf{f}_0, \{\mathbf{c}_i\}_{i\in[J_B]}, \{\mathbf{v}_i\}_{i\in[J_H]}\right)$. This relation follows from

$$\begin{aligned}
&\mathbf{g}_j \in \operatorname{span}\left(\mathbf{f} - \mathbf{f}_0, \{\mathbf{c}_i\}_{i\in[J_B]}, \{\mathbf{v}_i\}_{i\in[J_H]}\right) \Rightarrow \exists a \in \mathbb{R}, (b_i)_{i\in[J_B]} \in \mathbb{R}^{J_B}, (d_i)_{i\in[J_H]} \in \mathbb{R}^{J_H} \text{ s.t.}\\
&\mathbf{g}_j = a(\mathbf{f} - \mathbf{f}_0) + \sum_{i\in[J_B]} b_i \mathbf{c}_i + \sum_{i\in[J_H]} d_i \mathbf{v}_i \Rightarrow\\
&\mathbf{g}'_j = \operatorname{proj}_V(\mathbf{g}_j) = \operatorname{proj}_V\left(a(\mathbf{f} - \mathbf{f}_0) + \sum_{i\in[J_B]} b_i \mathbf{c}_i + \sum_{i\in[J_H]} d_i \mathbf{v}_i\right)\\
&\quad = a\Big[\underbrace{\operatorname{proj}_V(\mathbf{f})}_{=\mathbf{z}} - \underbrace{\operatorname{proj}_V(\mathbf{f}_0)}_{=\mathbf{f}_0 \Leftarrow \mathbf{f}_0\in V}\Big] + \sum_{i\in[J_B]} b_i \underbrace{\operatorname{proj}_V(\mathbf{c}_i)}_{=\mathbf{c}_i \Leftarrow \mathbf{c}_i\in V} + \sum_{i\in[J_H]} d_i \underbrace{\operatorname{proj}_V(\mathbf{v}_i)}_{=\mathbf{v}_i \Leftarrow \mathbf{v}_i\in V}.
\end{aligned}$$

This means that $(\mathbf{z}, \bar{\mathbf{b}}_{\text{app}}) \in C_{\text{app}}$ and that it is necessarily optimal.

Performance guarantee: By assumption (iv), L and R are l.s.c. so $\mathcal{L}$ is weakly l.s.c. thus strongly l.s.c. Since by construction $C_{\text{app}} \subseteq C$, we know that the solution $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is also admissible for $(\mathcal{P})$. Hence

$$v_{\text{relax}} \le \bar{v} \le v_{\text{app}}, \tag{51}$$

where $\bar{v} := \mathcal{L}\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$ as $(\bar{\mathbf{f}}, \bar{\mathbf{b}})$ exists and is unique by the strong convexity assumption over the l.s.c. $\mathcal{L}$.

- Bound (26): Let us fix any $(\mathbf{p}_f, \mathbf{p}_b) \in \mathcal{F}_K \times \mathbb{R}^B$ belonging to the subdifferential of $\mathcal{L}(\cdot,\cdot) + \chi_{\mathcal{C}}(\cdot,\cdot)$ at point $(\bar{\mathbf{f}}, \bar{\mathbf{b}})$, where $\chi_{\mathcal{C}}$ is the characteristic function of $\mathcal{C}$, i.e. $\chi_{\mathcal{C}}(\mathbf{u}, \mathbf{v}) = 0$ if $(\mathbf{u}, \mathbf{v}) \in \mathcal{C}$ and $\chi_{\mathcal{C}}(\mathbf{u}, \mathbf{v}) = \infty$ otherwise. Using the $(\mu_{\mathbf{f}}, \mu_{\mathbf{b}})$-strong convexity of $\mathcal{L}$ w.r.t. $(\mathbf{f}, \mathbf{b})$ we get

$$\begin{aligned}
\mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) \ge{}& \mathcal{L}\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)\\
&+ \underbrace{\langle \mathbf{p}_f, \bar{\mathbf{f}}_{\text{app}} - \bar{\mathbf{f}}\rangle_K + \langle \mathbf{p}_b, \bar{\mathbf{b}}_{\text{app}} - \bar{\mathbf{b}}\rangle_2}_{\ge 0} + \frac{\mu_{\mathbf{f}}}{2}\left\|\bar{\mathbf{f}}_{\text{app}} - \bar{\mathbf{f}}\right\|_K^2 + \frac{\mu_{\mathbf{b}}}{2}\left\|\mathbf{b}_{\text{app}} - \bar{\mathbf{b}}\right\|_2^2,
\end{aligned} \tag{52}$$

  where the non-negativity holds since $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$ is the optimum of $(\mathcal{P})$ and $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is admissible for $(\mathcal{P})$. One gets the claimed bound (26) by

$$\begin{aligned}
v_{\text{app}} - v_{\text{relax}} &\overset{(51)}{\ge} \mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) - \bar{v}\\
&= \mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) - \mathcal{L}\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right) \overset{(52)}{\ge} \frac{\mu_{\mathbf{f}}}{2}\left\|\bar{\mathbf{f}}_{\text{app}} - \bar{\mathbf{f}}\right\|_K^2 + \frac{\mu_{\mathbf{b}}}{2}\left\|\mathbf{b}_{\text{app}} - \bar{\mathbf{b}}\right\|_2^2.
\end{aligned} \tag{53}$$

- Bound (28): Recall that $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$ satisfies $(\mathcal{C})$ and that we assume $\mathcal{B} = \mathbb{R}^B$. Let η_∞ be defined according to (27), let $\boldsymbol{\beta} \in \mathbb{R}^B$ such that $\boldsymbol{\Gamma}_i \boldsymbol{\beta} > \mathbf{0}$ for all $i \in \mathcal{I}$, and define

$$\tilde{\boldsymbol{\beta}} := \eta_\infty c_f \boldsymbol{\beta} = \eta_\infty \frac{\max_{i\in[I]} \left\|\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right\|_K}{\min_{i\in[I],\, p\in P_i} \left(\boldsymbol{\Gamma}_i \boldsymbol{\beta}\right)_p} \boldsymbol{\beta}. \tag{54}$$

Applying $\boldsymbol{\Gamma}_i$ to (54) results in the bound (used below)

$$\boldsymbol{\Gamma}_i\tilde{\boldsymbol{\beta}} = \eta_\infty \max_{i\in[I]} \left\|\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right\|_K \underbrace{\frac{\boldsymbol{\Gamma}_i\boldsymbol{\beta}}{\min_{i\in[I],\, p\in P_i}\left(\boldsymbol{\Gamma}_i\boldsymbol{\beta}\right)_p}}_{\geq 1 \Leftarrow \boldsymbol{\Gamma}_i\boldsymbol{\beta}>\mathbf{0},\ \forall i\in[I]} \geq \eta_\infty \left\|\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right\|_K \mathbf{1}_{P_i},\ \forall i \in [I] \tag{55}$$

with $\mathbf{1}_{P_i} \in \mathbb{R}^{P_i}$ being the vector of ones.
Next we show that $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) \in C_{\text{app}}$.

– $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) \in C^i_{P_i,\text{SOC}}$ for all $i \in \mathcal{I}_{\text{SOC}}$: Let $i \in \mathcal{I}_{\text{SOC}}$. Then for all $\mathbf{x} \in \mathcal{K}_i$

$$\begin{aligned}
\eta_{i,m,P_i}\left\|\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right\|_K \mathbf{I}_{P_i} &\overset{(a)}{\preccurlyeq} \eta_\infty \left\|\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right\|_K \mathbf{I}_{P_i} \overset{(b)}{\preccurlyeq} \operatorname{diag}\left(\boldsymbol{\Gamma}_i\tilde{\boldsymbol{\beta}}\right)\\
&\preccurlyeq \operatorname{diag}\left(\boldsymbol{\Gamma}_i\tilde{\boldsymbol{\beta}}\right) + \underbrace{\mathbf{D}_i\left(\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right)(\mathbf{x}) + \operatorname{diag}\left(\boldsymbol{\Gamma}_i\bar{\mathbf{b}} - \mathbf{b}_{0,i}\right)}_{\succcurlyeq 0 \text{ for } \forall \mathbf{x}\in\mathcal{K}_i \Leftarrow \left(\bar{\mathbf{f}},\bar{\mathbf{b}}\right)\in C}\\
&= \mathbf{D}_i\left(\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right)(\mathbf{x}) + \operatorname{diag}\left(\boldsymbol{\Gamma}_i\left(\bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) - \mathbf{b}_{0,i}\right),
\end{aligned} \tag{56}$$

where (a) comes from the definition of η_∞ and (b) follows from (55). Since $\tilde{\mathbf{x}}_{i,m} \in \mathcal{K}_i$, (56) means that $(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}) \in C^i_{P_i,\text{SOC}}$.

– $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) \in C^i_{1,\Omega}$ for all $i \in \mathcal{I}_\Omega$: Let $i \in \mathcal{I}_\Omega$. By the definition of η_∞, $\Phi_{D_i}(\mathcal{K}_i) \subseteq \bar{\Omega}_i \subseteq \Phi_{D_i}(\mathcal{K}_i) + \mathbb{B}_K(0, \eta_\infty)$. This inclusion with (8) means that for $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) \in C^i_{1,\Omega}$ to hold it is sufficient to prove that $\Phi_{D_i}(\mathcal{K}_i) + \mathbb{B}_K(0, \eta_\infty) \subseteq H^+_K\left(\bar{\mathbf{f}} - \mathbf{f}_{0,i}, b_{0,i} - \boldsymbol{\Gamma}_i\left(\bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right)\right)$. The latter holds since for any $\mathbf{x} \in \mathcal{K}_i$ and $\mathbf{g} \in \mathbb{B}_K(0, \eta_\infty)$ we have

$$\begin{aligned}
&\langle \bar{\mathbf{f}} - \mathbf{f}_{0,i}, D_i K(\cdot, \mathbf{x}) + \mathbf{g}\rangle_K + \boldsymbol{\Gamma}_i(\bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}) - b_{0,i}\\
&\overset{(a)}{=} D_i\left(\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right)(\mathbf{x}) + \boldsymbol{\Gamma}_i\bar{\mathbf{b}} - b_{0,i} + \boldsymbol{\Gamma}_i\tilde{\boldsymbol{\beta}} + \langle \bar{\mathbf{f}} - \mathbf{f}_{0,i}, \mathbf{g}\rangle_K\\
&\overset{(b)}{\geq} \underbrace{D_i\left(\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right)(\mathbf{x}) + \boldsymbol{\Gamma}_i\bar{\mathbf{b}} - b_{0,i}}_{\geq 0 \text{ for } \forall \mathbf{x}\in\mathcal{K}_i \Leftarrow \left(\bar{\mathbf{f}},\bar{\mathbf{b}}\right)\in C} + \underbrace{\boldsymbol{\Gamma}_i\tilde{\boldsymbol{\beta}} - \left\|\bar{\mathbf{f}} - \mathbf{f}_{0,i}\right\|_K \underbrace{\|\mathbf{g}\|_K}_{\leq \eta_\infty}}_{\geq 0 \Leftarrow (55)} \geq 0.
\end{aligned}$$

In (a) we applied the reproducing formula (Lemma 1), (b) follows from the Cauchy-Schwarz inequality.

The proved relation $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) \in C_{\text{app}}$ implies that $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right)$ is admissible for (24) since $\bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}} \in \operatorname{dom}(\mathcal{L}(\bar{\mathbf{f}}, \cdot)) = \mathbb{R}^B$. Thus

$$\mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) - \mathcal{L}\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right) \overset{(a)}{\leq} \mathcal{L}\left(\bar{\mathbf{f}}, \bar{\mathbf{b}} + \tilde{\boldsymbol{\beta}}\right) - \mathcal{L}\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right) \overset{(b)}{\leq} L_b\left\|\tilde{\boldsymbol{\beta}}\right\|_2 \overset{(c)}{\leq} L_b\eta_\infty c_f\left\|\boldsymbol{\beta}\right\|_2, \tag{57}$$

where (a) follows from the fact that $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is an optimal solution of (24), (b) is implied by the local Lipschitz property of $\mathcal{L}$, and (c) holds by (54). Combining (57) with (53) results in the bound (28).

A.2.6 Proof of Theorem 6

Part 1 (limit covering): The properties we exploit are that $\operatorname{diam}\left(\Omega^{(0)}\right) < \infty$ and that the diameters of the bursting sets decrease by a factor of γ. Recall that at the k^{th} iteration of Alg. 3 we have

$$\mathbf{\Phi}_D(\mathcal{K}) \subseteq \bar{\Omega}^{(k)} = \cup_{m\in\left[M^{(k)}\right]}\bar{\Omega}_m^{(k)} \subseteq H_K^+\left(\mathbf{f}^{(k)} - \mathbf{f}_0, b_0 - \mathbf{\Gamma b}^{(k)}\right). \tag{58}$$

We say that a set $\bar{\Omega}_m^{(j)}$ present at the j^{th} iteration is k-persistent if $j \le k$ and $\bar{\Omega}_m^{(j)}$ does not burst at all in Alg. 3. Let us define

$$\bar{\Omega}_{\text{pers}}^{(k)} \subseteq \bar{\Omega}^{(k)} \subseteq \mathcal{F}_K \tag{59}$$

as the union of the k-persistent sets. By definition one gets an increasing sequence of sets $(\bar{\Omega}_{\text{pers}}^{(1)} \subseteq \bar{\Omega}_{\text{pers}}^{(2)} \subseteq \bar{\Omega}_{\text{pers}}^{(3)} \subseteq \ldots)$, hence we can take the closed limit of these sets and define $\bar{\Omega}_{\text{pers}}^{(\infty)} := \overline{\bigcup_{k\in\mathbb{N}} \bar{\Omega}_{\text{pers}}^{(k)}}$. We show that

$$\lim_{k\to\infty} \bar{\Omega}^{(k)} = \mathbf{\Phi}_D(\mathcal{K}) \cup \bar{\Omega}_{\text{pers}}^{(\infty)}. \tag{60}$$

Notice that by definition $\bar{\Omega}^{(k)}$ is a closed and bounded set. The set $\mathbf{\Phi}_D(\mathcal{K})$ is compact (thus closed and bounded) as Φ_D is continuous and $\mathcal{K}$ is compact. The set $\bar{\Omega}_{\text{pers}}^{(\infty)}$ is closed by definition; it is also bounded as $\bar{\Omega}_{\text{pers}}^{(\infty)} \subseteq \mathbf{\Phi}_D(\mathcal{K}) + \mathbb{B}_K\left(\mathbf{0}, \operatorname{diam}\left(\Omega^{(0)}\right)\right)$. Hence the terms in (60) are elements of the complete (Price, 1940) metric space of closed, bounded, non-empty sets of $\mathcal{F}_K$ equipped with the Hausdorff distance

$$d_{\mathrm{H}}(S_1, S_2) = \inf\left\{\epsilon > 0 \,:\, S_1 \subseteq S_2 + \mathbb{B}_K(\mathbf{0}, \epsilon) \text{ and } S_2 \subseteq S_1 + \mathbb{B}_K(\mathbf{0}, \epsilon)\right\}$$

where '+' denotes the Minkowski sum. The limit in (60) is meant in this d_{H} sense.

Indeed (60) can be proved as follows. Let $\mathcal{C}_{\text{no-pers}}^{(k)}$ denote the covering elements of the k-th iteration that are not k-persistent; in other words, each of these sets $\bar{\Omega}_m^{(k)}$ will burst after $N_m^{(k)} \in \mathbb{N}$ iterations. Let $A^{(k)} \subseteq \mathbb{R}_+$ be the finite set of the diameters of the elements in $\mathcal{C}_{\text{no-pers}}^{(k)}$ and $\alpha^{(k)} := \max\left(A^{(k)}\right)$. Since at each iteration, the diameters can only decrease, $\left(\alpha^{(k)}\right)_{k\in\mathbb{N}}$ is a non-negative decreasing sequence which thus converges to some $\alpha \in \mathbb{R}_+$. We show that $\alpha = 0$ by contradiction. Assume that $\alpha > 0$, and take k such that $0 \le \alpha^{(k)} - \alpha < (1-\gamma)\alpha$ which is possible since $\alpha > 0$ and $\gamma \in (0,1)$. As $\alpha \le \alpha^{(k)}$, this choice of k implies that $\alpha^{(k)} - \alpha < (1-\gamma)\alpha^{(k)}$, in other words that $\gamma\alpha^{(k)} < \alpha$. By taking $N^{(k)} := \max_m N_m^{(k)}$, we get that

$$\alpha^{\left(k+N^{(k)}\right)} \le \gamma\alpha^{(k)} < \alpha.$$

However, the obtained relation $\alpha^{\left(k+N^{(k)}\right)} < \alpha$ contradicts the fact that $\left(\alpha^{(k)}\right)_{k\in\mathbb{N}}$ converges decreasingly to α; this contradiction establishes that $\alpha = 0$.

We have that

$$\bar{\Omega}_{\text{pers}}^{(k)} \cup \mathbf{\Phi}_D(\mathcal{K}) \overset{(a)}{\subseteq} \bar{\Omega}^{(k)} \overset{(b)}{\subseteq} \bar{\Omega}_{\text{pers}}^{(k)} \cup \left(\mathbf{\Phi}_D(\mathcal{K}) + \mathbb{B}_K\left(\mathbf{0}, \alpha^{(k)}\right)\right), \tag{61}$$

The inclusion (a) holds since $\mathbf{\Phi}_D(\mathcal{K}) \subseteq \bar{\Omega}^{(k)}$ by (58) and $\bar{\Omega}^{(k)}_{\text{pers}} \subseteq \bar{\Omega}^{(k)}$ by (59), while (b) holds given that at each iteration k, $\bar{\Omega}^{(k)}_m \cap \mathbf{\Phi}_D(\mathcal{K}) \neq \emptyset$ for any m (recall that superfluous covering elements were discarded in Alg. 1). This means by the previously proved relation $\lim_{k\to\infty} \alpha^{(k)} = 0$ that

$$\lim_{k\to\infty} \bar{\Omega}^{(k)}_{\text{pers}} \cup \mathbf{\Phi}_D(\mathcal{K}) = \lim_{k\to\infty} \bar{\Omega}^{(k)} = \lim_{k\to\infty} \bar{\Omega}^{(k)}_{\text{pers}} \cup \left(\mathbf{\Phi}_D(\mathcal{K}) + \mathbb{B}_K\left(\mathbf{0}, \alpha^{(k)}\right)\right) = \mathbf{\Phi}_D(\mathcal{K}) \cup \bar{\Omega}^{(\infty)}_{\text{pers}}$$

in Hausdorff distance sense; this establishes (60).

Let $\Theta^{(k)} := \bar{\Omega}^{(k)} \setminus \bar{\Omega}^{(k)}_{\text{pers}}$. Since the constraints associated to $\bar{\Omega}^{(k)}_{\text{pers}}$ are never active by definition, they can be removed from the problem:

$$\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) \in \underset{\substack{\mathbf{f} \in \mathcal{F}_K, \mathbf{b} \in \mathcal{B} \\ \bar{\Omega}^{(k)} \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})}}{\arg\min} \mathcal{L}(\mathbf{f}, \mathbf{b}) = \underset{\substack{\mathbf{f} \in \mathcal{F}_K, \mathbf{b} \in \mathcal{B} \\ \Theta^{(k)} \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})}}{\arg\min} \mathcal{L}(\mathbf{f}, \mathbf{b}). \tag{62}$$

However by (61) and by using the fact that $(A \cup B) \backslash B \subseteq A$ for any sets A, B, we have that $\bar{\Theta}^{(\infty)} := \overline{\lim_{k\to\infty} \Theta^{(k)}} \subseteq \mathbf{\Phi}_D(\mathcal{K})$, where the limit is again meant in Hausdorff distance sense. Hence, considering the limit constraint sets in (62), any

$$\left(\mathbf{f}^{(\infty)}, \mathbf{b}^{(\infty)}\right) \in \underset{\substack{\mathbf{f} \in \mathcal{F}_K, \mathbf{b} \in \mathcal{B} \\ \bar{\Omega}^{(\infty)} \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})}}{\arg\min} \mathcal{L}(\mathbf{f}, \mathbf{b}) = \underset{\substack{\mathbf{f} \in \mathcal{F}_K, \mathbf{b} \in \mathcal{B} \\ \bar{\Theta}^{(\infty)} \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})}}{\arg\min} \mathcal{L}(\mathbf{f}, \mathbf{b}) \tag{63}$$

is the solution of both a tightening ($\bar{\Omega}^{(\infty)} \supseteq \Phi_D(\mathcal{K})$) and a relaxation ($\bar{\Theta}^{(\infty)} \subseteq \Phi_D(\mathcal{K})$) of the original problem; hence

$$\left(\mathbf{f}^{(\infty)}, \mathbf{b}^{(\infty)}\right) \in \underset{\substack{\mathbf{f} \in \mathcal{F}_K, \mathbf{b} \in \mathcal{B} \\ \mathbf{\Phi}_D(\mathcal{K}) \subseteq H_K^+(\mathbf{f}-\mathbf{f}_0, b_0 - \mathbf{\Gamma}\mathbf{b})}}{\arg\min} \mathcal{L}(\mathbf{f}, \mathbf{b}). \tag{64}$$

This establishes the first statement of Theorem 6.

Part 2 (convergence of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$): Suppose that Assumptions (i)-(vii) hold.

- Existence of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$: First we prove the existence of the iterates $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)$ by induction over k. For $k = 0$, the existence of $(\mathbf{f}^{(0)}, \mathbf{b}^{(0)})$ is guaranteed by Assumptions (i)-(v) and Theorem 5(1). Suppose we reached the k-th step, and let $d_k := d_H\left(\bar{\Omega}^{(0)}, \bar{\Omega}^{(k)}\right)$. Let us recall that $\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}\right)$ is an admissible pair for $\mathcal{P}\left(\bar{\Omega}^{(0)}\right)$ (see Assumption (v)), and let us define $\hat{\mathbf{b}}_k := \hat{\mathbf{b}} + \frac{d_k \|\hat{\mathbf{f}}-\mathbf{f}_0\|_K}{\|\mathbf{\Gamma}\|_2^2} \mathbf{\Gamma}^\top \in \mathbb{R}^B$ which exists since $\mathbf{\Gamma} \neq \mathbf{0}$ by Assumption (vii). With this choice, we show that

$$\bar{\Omega}^{(k)} \subseteq H_K^+\left(\hat{\mathbf{f}} - \mathbf{f}_0, b_0 - \mathbf{\Gamma}\hat{\mathbf{b}}_k\right). \tag{65}$$

Indeed, by the definition of the Hausdorff distance for any $\mathbf{g} \in \bar{\Omega}^{(k)}$ there exists some $\mathbf{u} \in \mathbb{B}_K(\mathbf{0}, 1)$ and $\mathbf{g}_0 \in \bar{\Omega}^{(0)}$ such that $\mathbf{g} = \mathbf{g}_0 + d_k\mathbf{u}$. This implies (65) as

$$\left\langle \hat{\mathbf{f}} - \mathbf{f}_0, \mathbf{g} \right\rangle_K + \boldsymbol{\Gamma}\hat{\mathbf{b}}_k - b_0 = \left\langle \hat{\mathbf{f}} - \mathbf{f}_0, \mathbf{g}_0 + d_k\mathbf{u} \right\rangle_K + \boldsymbol{\Gamma}\left(\hat{\mathbf{b}} + \frac{d_k \left\| \hat{\mathbf{f}} - \mathbf{f}_0 \right\|_K}{\|\boldsymbol{\Gamma}\|_2^2}\boldsymbol{\Gamma}^\top\right) - b_0$$
$$= \underbrace{\left\langle \hat{\mathbf{f}} - \mathbf{f}_0, \mathbf{g}_0 \right\rangle_K + \boldsymbol{\Gamma}\hat{\mathbf{b}} - b_0}_{\geq 0 \text{ by Assumption (v)}} + \underbrace{d_k \left\langle \hat{\mathbf{f}} - \mathbf{f}_0, \mathbf{u} \right\rangle_K + d_k \left\| \hat{\mathbf{f}} - \mathbf{f}_0 \right\|_K}_{\geq 0 \text{ by } \mathbf{u} \in \mathbb{B}_K(\mathbf{0},1) \text{ and the Cauchy-Schwartz inequality}} \geq 0. \tag{66}$$

(65) means that $\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}_k\right)$ is admissible for $\mathcal{P}\left(\bar{\Omega}^{(k)}\right)$ as $\hat{\mathbf{b}}_k \in \mathcal{B} \cap \operatorname{dom}\left(\mathcal{L}\left(\hat{\mathbf{f}}, \cdot\right)\right) = \mathbb{R}^B$ by Assumption (vi). The existence of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)$ follows from the proved admissibility of $\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}_k\right)$ and since the conditions of Theorem 5(1) hold.

- Boundedness of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$: Let us define the bound $d_{\max} := \sup_{k\in\mathbb{N}} d_k < \infty$ with $d_k = d_H\left(\bar{\Omega}^{(0)}, \bar{\Omega}^{(k)}\right)$; $d_{\max}$ exists since $\left(\bar{\Omega}^{(k)}\right)_{k\in\mathbb{N}}$ converges as it was proved in (60). Let $\hat{\mathbf{b}}_{\max} := \hat{\mathbf{b}} + \frac{d_{\max}\left\|\hat{\mathbf{f}} - \mathbf{f}_0\right\|_K}{\|\boldsymbol{\Gamma}\|_2^2}\boldsymbol{\Gamma}^\top$. Then $\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}_{\max}\right)$ is admissible for $\mathcal{P}\left(\bar{\Omega}^{(k)}\right)$ for all $k \in \mathbb{N}$ by a computation analogous to (65)-(66) and by using Assumption (vi). This admissibility means that $\mathcal{L}\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) \leq \mathcal{L}\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}_{\max}\right)$, in other words $\left\{\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)\right\}_{k\in\mathbb{N}} \subseteq \mathcal{L}^{-1}\left(\left(-\infty, \mathcal{L}\left(\hat{\mathbf{f}}, \hat{\mathbf{b}}_{\max}\right)\right]\right) =: S$. The set S is closed and bounded as Assumption (i)-(ii) imply the coercivity of $\mathcal{L}$ over the Hilbert space $\mathcal{F}_K \times \mathbb{R}^B$ equipped with the sum of the inner products, this can be shown similarly to the construction of $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ in the proof of Theorem 5. By the boundedness of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$, it has a weakly converging subsequence (w.l.o.g. it is the sequence itself) to some $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$.
- $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is admissible for $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$: Next we show that $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is admissible for $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$. Indeed, let $\epsilon > 0$. Then for any $\mathbf{g} \in \bar{\Omega}^{(\infty)}$, one can find $k \in \mathbb{N}$, $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)$ and $\mathbf{g}_k \in \bar{\Omega}^{(k)}$ such that

$$\left|\left\langle \mathbf{f}^{(k)} - \mathbf{f}_0, \mathbf{g}_k - \mathbf{g} \right\rangle_K\right| + \left|\left\langle \mathbf{f}^{(k)} - \bar{\mathbf{f}}_{\text{app}}, \mathbf{g} \right\rangle_K\right| + \left|\boldsymbol{\Gamma}\left(\mathbf{b}^{(k)} - \bar{\mathbf{b}}_{\text{app}}\right)\right| \leq \epsilon \tag{67}$$

using the boundedness of $\left(\mathbf{f}^{(k)}\right)_{k\in\mathbb{N}}$ and the convergence of $\left(\bar{\Omega}^{(k)}\right)_{k\in\mathbb{N}}$ to $\bar{\Omega}^{(\infty)}$ in Hausdorff distance (in the first term), and the weak convergence of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ to $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ (in the 2nd and the 3rd terms). Notice that

$$b_0 - \boldsymbol{\Gamma}\bar{\mathbf{b}}_{\text{app}} - \boldsymbol{\Gamma}\left(\mathbf{b}^{(k)} - \bar{\mathbf{b}}_{\text{app}}\right) = b_0 - \boldsymbol{\Gamma}\mathbf{b}^{(k)} \overset{(a)}{\leq} \left\langle \mathbf{f}^{(k)} - \mathbf{f}_0, \mathbf{g}_k \right\rangle_K$$
$$= \left\langle \mathbf{f}^{(k)} - \mathbf{f}_0, \mathbf{g}_k - \mathbf{g} \right\rangle_K + \left\langle \mathbf{f}^{(k)} - \bar{\mathbf{f}}_{\text{app}}, \mathbf{g} \right\rangle_K + \left\langle \bar{\mathbf{f}}_{\text{app}} - \mathbf{f}_0, \mathbf{g} \right\rangle_K, \tag{68}$$

where (a) holds since $\mathbf{g}_k \in \bar{\Omega}^{(k)}$. Rearranging (68) leads to

$$\left\langle \bar{\mathbf{f}}_{\text{app}} - \mathbf{f}_0, \mathbf{g} \right\rangle_K \geq b_0 - \boldsymbol{\Gamma}\bar{\mathbf{b}}_{\text{app}} - \boldsymbol{\Gamma}\left(\mathbf{b}^{(k)} - \bar{\mathbf{b}}_{\text{app}}\right) - \left\langle \mathbf{f}^{(k)} - \mathbf{f}_0, \mathbf{g}_k - \mathbf{g} \right\rangle_K - \left\langle \mathbf{f}^{(k)} - \bar{\mathbf{f}}_{\text{app}}, \mathbf{g} \right\rangle_K$$
$$\overset{(67)}{\geq} b_0 - \boldsymbol{\Gamma}\bar{\mathbf{b}}_{\text{app}} - \epsilon.$$

Taking the limit $\epsilon \to 0$, we get that $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is admissible for $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$.

- $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is an optimal solution of $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$: Let $\xi > 0$. Since our assumptions are stronger than those of Theorem 5(1), equations (49)-(50) hold; hence, there exists N_0 such that

$$\mathcal{L}\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) \geq \mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) - \xi \text{ for all } k \geq N_0. \tag{69}$$

Let us fix any arbitrary pair $(\mathbf{f}, \mathbf{b})$ which is admissible for $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$. Let us define $c_{\mathbf{f}} := \frac{\|\mathbf{f}-\mathbf{f}_0\|_K}{\|\mathbf{\Gamma}\|_2^2}\mathbf{\Gamma}^\top$ and $\epsilon_k := d_H\left(\bar{\Omega}^{(\infty)}, \bar{\Omega}^{(k)}\right)$. A computation similar to (66) combined with Assumption (vi) implies that $(\mathbf{f}, \mathbf{b} + \epsilon_k c_{\mathbf{f}})$ is admissible for $\mathcal{P}(\bar{\Omega}^{(k)})$ for all $k \in \mathbb{N}$, and that

$$\mathcal{L}(\mathbf{f}, \mathbf{b} + \epsilon_k c_{\mathbf{f}}) \geq \mathcal{L}\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right) \overset{(a)}{\geq} \mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) - \xi, \tag{70}$$

where (a) holds by (69) for $k \geq N_0$. This inequality shows that

$$\mathcal{L}(\mathbf{f}, \mathbf{b}) \geq \mathcal{L}\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) - \xi \tag{71}$$

by taking the limit $k \to \infty$ (in which case $\epsilon_k \to 0$) of (70). Taking the limit of (71) as $\xi \to 0$ shows that $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ is a solution of $\mathcal{P}\left(\bar{\Omega}^{(\infty)}\right)$. This means that $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right)$ also solves the original problem $(\mathcal{P})$

$$\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) \in \underset{\substack{\mathbf{f} \in \mathcal{F}_K,\, \mathbf{b} \in \mathcal{B},\\ (\mathbf{f},\mathbf{b}) \in C}}{\arg\min}\ \mathcal{L}(\mathbf{f}, \mathbf{b}) \ni \left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$$

by applying the same argument used to derive (64). Consequently if $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$ is unique, then $\left(\bar{\mathbf{f}}_{\text{app}}, \bar{\mathbf{b}}_{\text{app}}\right) = \left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$. Hence every weakly converging subsequence of $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ converges to $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$, so the whole sequence $\left(\mathbf{f}^{(k)}, \mathbf{b}^{(k)}\right)_{k\in\mathbb{N}}$ weakly converges to $\left(\bar{\mathbf{f}}, \bar{\mathbf{b}}\right)$.

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