APPROVAL SHEET

Title of Dissertation: Constrained Estimation and Approximation Using Control, Optimization, and Spline Theory

Name of Candidate: Teresa M. Lebair
Doctor of Philosophy, 2016

Dissertation and Abstract Approved: ____________________
Dr. Jinglai Shen
Associate Professor
Department of Mathematics and Statistics

Date Approved: 6/28/2016

ABSTRACT

Title of dissertation:	Constrained Estimation and Approximation Using Control, Optimization, and Spline Theory
	Teresa M. Lebair, Doctor of Philosophy, 2016
Dissertation directed by:	Professor Jinglai Shen Department of Mathematics and Statistics

There has been an increasing interest in shape constrained estimation and approximation in the fields of applied mathematics and statistics. Applications from various areas of research such as biology, engineering, and economics have fueled this soaring attention. Due to the natural constrained optimization and optimal control formulations achieved by inequality constrained estimation problems, optimization and optimal control play an invaluable part in resolving computational and statistical performance matters in shape constrained estimation. Additionally, the favorable statistical, numerical, and analytical properties of spline functions grant splines an influential place in resolving these issues. Hence, the purpose of this research is to develop numerical and analytical techniques for general shape constrained estimation problems using optimization, optimal control, spline theory, and statistical tools. A number of topics in shape constrained estimation are examined. We first consider the computation and numerical analysis of smoothing splines subject to general dynamics and control constraints. Optimal control formulations and nonsmooth algorithms for computing such splines are established; we then verify the convergence of these algorithms. Second, we consider the asymptotic analysis of the nonparametric estimation of functions subject to general nonnegative derivative constraints in the supremum norm. A nonnegative derivative constrained B-spline estimator is proposed, and we demonstrate that this estimator achieves a critical uniform Lipschitz property. This property is then exploited to establish asymptotic bounds on the B-spline estimator bias, stochastic error, and risk in the supremum norm. Minimax lower bounds are then established for a variety of nonnegative derivative constrained function classes, using the same norm. For the first, second, and third order derivative constraints, these asymptotic lower bounds match the upper bounds on the constrained B-spline estimator risk, demonstrating that the nonnegative derivative constrained B-spline estimator performs optimally over suitable constrained Hölder classes, with respect to the supremum norm.

Constrained Estimation and Approximation Using Control, Optimization, and Spline Theory

by

Teresa M. Lebair

Dissertation submitted to the Faculty of the Graduate School of the
University of Maryland, Baltimore County in partial fulfillment
of the requirements for the degree of Doctorate
of Philosophy in Applied Mathematics
2016

Advisory Committee:
Associate Professor Jinglai Shen, Chair/Advisor
Associate Professor Andrei Draganescu
Professor Muddappa Seetharama Gowda
Assistant Professor Seung-Jun Kim
Professor Anindya Roy

DEDICATION

For Mom and Dad.

ACKNOWLEDGEMENTS

I would first, and most importantly, like to thank my adviser, Dr. Jinglai Shen. He has been an outstanding mentor, as well as a very kind and patient person. It is an honor to have been his first Ph.D. student. Secondly, I would like to thank my committee members, Dr. Andrei Draganescu, Dr. Muddappa Seetharama Gowda, Dr. Seung-Jun Kim, and Dr. Anindya Roy, for their time spent reviewing my thesis, their helpful comments, and an enjoyable defense. Additionally, I would like to thank Dr. Xiao Wang from Purdue University for collaborating with Dr. Shen and me on our work. Finally, I would like to thank my family and friends for being encouraging and supportive of my studies. The research in this thesis was partially supported by the NSF grants CMMI-1030804 and DMS-1042916.

TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

CHAPTER I

Introduction

Constrained estimation and approximation garners increasing attention in applied mathematics and statistics, with applications in a wide variety of disciplines. Moreover, various functions in all sorts of practices are known to adhere to a number of shape constraints such as monotonicity or convexity. Examples include monotone regulatory functions in genetic networks [73] and a shape restricted function in an attitude control system [62]. Other applications are found in reliability engineering (e.g., survival/hazard functions), medicine (e.g., dose-response curves), finance (e.g., option/delivery price), and astronomy (e.g., galaxy mass functions). When estimating or approximating such functions, it is desirable to obtain an estimator or approximation that preserves the shape of the true/original constrained function. Additionally, incorporating the knowledge of shape constraints into a construction procedure improves estimation efficiency and accuracy [61]. This has led to a surging interest in the study of constrained estimation and approximation in applied mathematics, statistics, and other related fields [52, 70, 71, 72, 80].

Estimation and approximation problems subject to inequality shape constraints can be naturally formulated as constrained optimization or optimal control problems. For instance, constrained smoothing splines achieve certain optimal control formulations [67, 70], and constrained penalized polynomial spline estimators can be formulated as the solutions of quadratic programs with linear constraints [71, 72]. Hence, optimization and control play a critical role in the numerical resolution and statistical performance analysis of constrained estimators. Additionally, splines are an important tool in shape constrained estimation due to their advantageous statistical, numerical, and analytical properties. Therefore, the goal of this research is to develop numerical and analytical techniques for general shape constrained estimation problems using optimization, optimal control, spline theory, and statistical tools. Several related topics in shape constrained estimation are studied.

We first consider the analysis and computation of smoothing splines subject to general linear dynamics and control constraints. Moreover, we begin by demonstrating how constrained smoothing splines achieve certain optimal control formulations. A nonsmooth Newton's method for B(ouligand)-differentiable functions is then introduced [53, 67], and is used to compute such constrained smoothing splines. Finally, the convergence analysis of this method is carried out.

Second, we consider the asymptotic analysis of the nonparametric estimation of smooth functions subject to general nonnegative derivative constraints, where we use the supremum norm as the performance metric. In particular, we establish the consistency and convergence rate of a certain nonnegative derivative constrained B-spline estimator under the supremum norm. After establishing this convergence rate, minimax asymptotic lower bounds (in the supremum norm) are developed for a variety of nonnegative derivative constrained function classes. Combining all of these developments yields that, in certain instances, the nonnegative derivative constrained B-spline estimator is an asymptotically optimally performing estimator over certain constrained function classes, with respect to the supremum norm.

In what follows, we discuss each of these individual topics in more detail.

1.1 Analysis and Computation of Shape Constrained Smoothing Splines

We first consider the analysis and computation of smoothing splines subject to general linear dynamics and control constraints.

1.1.1 Background and Motivation

With numerous applications in various scientific and engineering disciplines, spline models are studied extensively in approximation theory, numerical analysis, and statistics. Informally speaking, a univariate spline model produces a piecewise polynomial curve that "best" fits a given set of data. Spline models enjoy a plethora of favorable analytical and statistical properties, and attain efficient numerical algorithms [14]. A number of variations and extensions of spline models have been developed, e.g., penalized polynomial splines [72] and smoothing splines [78]. Specifically, the smoothing spline model is a smooth function $f : [0, 1] \to \mathbb{R}$ in a suitable function space that minimizes the following objective functional:

$$\frac{1}{n} \sum_{i=1}^{n} \big(f(t_i) - y_i \big)^2 + \lambda \int_0^1 \Big(f^{(m)}(t) \Big)^2 dt, \tag{1.1}$$

where the y_i's are data points at $t_i \in [0, 1]$, $i = 1, \ldots, n$, $f^{(m)}$ denotes the mth derivative of f, and $\lambda > 0$ is a penalty parameter that characterizes the tradeoff between the data fidelity and the smoothness of f. We refer the reader to [78] and references therein for extensive information on the statistical properties of smoothing splines.

From a control systems point of view, the smoothing spline model (1.1) is closely related to the finite-horizon linear quadratic optimal control problem when $f^{(m)}$ is treated as a control input [22]. Moreover, we may think of a smoothing spline as the output of a linear control system, which depends on the initial state of the system and the system control (e.g., $f^{(m)}$ in view of (1.1)). This has led to a highly interesting spline model characterized by a linear control system called a *control theoretic spline* [22]. It is shown in [22] and the references therein, e.g., [36, 75, 82], that a number of smoothing, interpolation, and path planning problems can be incorporated into this paradigm and studied using control theory and optimization techniques on Hilbert spaces with efficient numerical schemes. Other relevant approaches include control theoretic wavelets [25].

Although many important results for *unconstrained* or *equality constrained* spline models are available, various biological, engineering, and economic systems contain functions whose shape and/or dynamics are governed by *inequality* constraints, e.g., the monotone and convex constraints. Even though many meaningful applications with inequality constraints exist, there are substantially fewer results available on spline models subject to inequality constraints than their unconstrained or equality constrained counterparts [22, 78]. In this thesis, we focus on spline models subject to such inequality constraints, with these applications in mind.

The first part of this thesis focuses on constrained smoothing splines formulated as constrained linear optimal control problems with unknown initial state and control. Hence, two types of constraints arise: (i) control constraints; and (ii) state constraints. While several effective numerical methods have been developed for state constrained optimal control problems in [24], we focus on control constraints, since a variety of shape constraints, which may be imposed on derivatives of a function, can be easily formulated as control constraints. It should be noted that a control constrained optimal control problem is inherently nonsmooth, and thus is considerably different from a classical (unconstrained) linear optimal control problem, such as LQR. Moreover, the goal of the shape constrained spline problem is to find an optimal initial condition and an open-loop like optimal control that "best" fit the sample data, rather than finding an optimal state feedback as in LQR, where the cost function is written in terms of the state function.

1.1.2 Literature Review

Most of the current literature on control constrained smoothing splines focuses on relatively simple linear dynamics and special control constraints, e.g., [19, 20, 22, 36, 52, 76]. Moreover, all of these sources consider problems in which the control is given by a certain derivative of the constrained smoothing spline, and is required to be nonnegative. This gives rise to a variety of nonnegative derivative constraints such as monotonicity and convexity. For instance, in [19, 20], the authors consider a cubic smoothing spline interpolation problem, where the nonnegative constrained control is given by the second derivative of the smoothing spline. This forces the smoothing spline interpolant to be convex. In [22, Chapter 7], more general nonnegative derivative constraints are considered.

In general, a widely used approach in the literature concentrates on shape constrained smoothing splines whose linear dynamics are defined by certain nilpotent matrices, and whose control is restricted to a cone in $\mathbb{R}$ [20, 22, 46]. Such dynamics and control constraints correspond to the previously mentioned nonnegative derivative constraints. In this case, the smoothing spline is a piecewise continuous polynomial with a known degree. Hence the computation of the smoothing spline boils down to determining the parameters of a polynomial on each interval, which can be further reduced to a quadratic or semidefinite program that attains efficient algorithms [19, 22]. However, this approach fails to handle general linear dynamics and control constraints, e.g., when the control is given by a linear combination of the constrained smoothing spline derivatives and is required to belong to some polyhedron, since the solution form of a general shape constrained smoothing spline is unknown *a priori*. Therefore, many critical questions remain open in smoothing spline analysis and computation when general dynamics and control constraints are taken into account; new tools are needed to handle more general dynamics and control constraint induced nonsmoothness.

1.2 Asymptotic Analysis of General Nonnegative Derivative Constrained Nonparametric Estimation

We now consider the second topic of this work, i.e., the the asymptotic statistical analysis of the nonparametric estimation of functions subject to general nonnegative derivative constraints in the supremum norm.

1.2.1 Background and Motivation

The nonparametric estimation of unknown functions plays a central role in estimation theory, system identification, and systems and control [34, 49, 75, 77]. There has been an increasing interest in the estimation of nonnegative derivative constrained functions (e.g., monotone or convex functions) [22, 52, 70, 73, 79], driven by a variety of applications. The goal of constrained estimation is to develop an estimator that preserves a pre-specified constraint of the underlying true function, e.g., the monotone or convex constraint.

Given a collection of functions Σ subject to a pre-specified constraint, several key questions arise when evaluating the asymptotic performance of constraint preserving nonparametric estimators over Σ:

(Q1) What rates of convergence are possible (in terms of sample size) for constrained estimators uniformly over Σ? Is there a "best" convergence rate, for which any constrained estimator cannot achieve a faster rate of convergence uniformly over Σ?

(Q2) Is it possible to construct a constraint preserving estimator that achieves such a "best" rate of convergence? How should we construct such an estimator?

These questions address critical research issues in minimax theory of constrained nonparametric estimation [33, 34, 49, 77]. In particular, the first question pertains to the minimax lower bound on Σ [48], while the second question is related to the minimax upper bound on Σ. We are interested in addressing these questions when Σ is a general nonnegative derivative constrained Hölder class, and the supremum norm is used as the performance metric.

A major challenge in the development of general nonnegative derivative constrained nonparametric estimation is induced by the estimator *inequality* shape constraints, which lead to nonsmooth conditions in estimator characterization and complicate the estimator asymptotic performance analysis. Additionally, further difficulties arise when the supremum norm is used as the performance metric. For instance, a critical constrained B-spline estimator *uniform Lipschitz property* (c.f. Section 1.2.1.1) is easily established in the L_2-norm, but is much more difficult to verify under the supremum norm (see Chapter III). Unlike the L_2-norm, the supremum norm characterizes the worst-case performance of an estimator. The supremum norm is a widely studied norm in estimation theory [77].

In what follows, we consider questions (Q1) and (Q2) in the context of general nonnegative derivative constrained nonparametric estimation under the supremum norm. In Sections 1.2.1.1-1.2.1.2, we provide background information on a nonnegative derivative constrained B-spline estimator and its performance over suitable Hölder classes, in association to (Q2). Similarly, in Section 1.2.1.3, we motivate the study of asymptotic minimax lower bounds over several general nonnegative derivative constrained Hölder and Sobolev classes, in connection to (Q1).

1.2.1.1 Constrained B-spline Estimator: Uniform Lipschitz Property

It is observed that the monotone (resp. convex) constraint on a univariate function roughly corresponds to the first (resp. second) order nonnegative derivative constraint, under suitable smoothness conditions on the underlying function. Despite extensive research on the asymptotic analysis of monotone and convex estimation, very few performance analysis results are available for higher-order nonnegative derivative constraints, although such constraints arise in applications [62]. Motivated by these applications and the lack of performance analysis of the associated constrained estimators, we consider the estimation of a univariate function subject to the mth order nonnegative derivative constraint via B-spline estimators, for arbitrary $m \in \mathbb{N}$. B-splines are a popular tool in approximation and estimation theory thanks to their numerical advantages [14, 17]. Nonnegative derivative constraints on a B-spline estimator can be easily imposed on spline coefficients, which can then be efficiently computed via quadratic programs. In spite of this numerical simplicity and effciency, the asymptotic analysis of constrained B-spline estimators is far from trivial, particularly when uniform convergence and the supremum-norm risk are considered.

The asymptotic analysis of constrained B-spline estimators requires a deep understanding of the mapping from a (weighted) sample data vector to the corresponding B-spline coefficient vector. For a fixed sample size, this mapping is given by a Lipschitz piecewise linear function due to the inequality shape constraints. As the sample size increases and tends to infinity, an infinite family of size-varying piecewise linear functions arise. A critical *uniform Lipschitz property* has been established for monotone P-splines (corresponding to $m = 1$) [72] and convex B-splines (corresponding to $m = 2$) [80]. This property states that the size-varying piecewise linear functions attain a uniform Lipschitz constant under the ℓ_∞-norm, independent of sample size and the number of knots. It leads to many important results in asymptotic analysis, e.g., uniform convergence, pointwise mean squared risk, and optimal rates of convergence [80]. It has been conjectured that this property can be extended to B-spline estimators subject to higher-order nonnegative derivative constraints [80]. However, the extension encounters a major difficulty: the proof of the uniform Lipschitz property for the monotone and convex cases heavily relies on the diagonal dominance of certain matrices that no longer holds in the higher-order cases. In addition, the results in [72, 80] are based on the restrictive assumption of evenly spaced design points and knots; the extension to the unevenly spaced case is nontrivial. To overcome these difficulties, we develop various new results for the proof of the uniform Lipschitz property for an arbitrary $m \in \mathbb{N}$.

1.2.1.2 Constrained B-spline Estimator: Consistency and Convergence Rate

Using the aforementioned uniform Lipschitz property, we develop a number of results concerning the asymptotic analysis of the constrained B-spline estimator in the supremum norm (c.f. Propostions 4.3.1-4.3.3 and Theorems 4.3.1-4.3.2). Moreover, the risk or error associated with a given estimator can be decomposed into the sum of two terms: (i) the bias, which stems from approximating a true function by another function (e.g., a spline), and (ii) the stochastic error, which arises from random errors or noise. Therefore, we provide asymptotic bounds on each of these quantities, with respect to the supremum norm, utilizing the previously described uniform Lipschitz property.

One difficulty that arises in bounding the constrained B-spline estimator bias involves demonstrating that each sufficiently smooth function subject to a given nonnegative derivative constraint attains a *Jackson type* spline approximation with the same nonnegative derivative constraint (c.f. statement **(J)** in Chapter IV) [14, pg. 149]. For the monotone and convex constraints, i.e., the first and second order nonnegative derivative constraints, such a Jackson type approximation is easily verified. For third order nonnegative derivative constraints, Jackson type approximations are given by [38, 58]. Hence, we are able to obtain the optimal rate of convergence for the constrained B-spline estimator bias, and thus the risk, for the first, second, and third order nonnegative derivative constraints (c.f. Theorem 4.3.1 and Theorem 5.2.1). Alternatively, under an additional assumption, in which the true function's mth order derivative is also bounded below by a constant (independent of the function) away from zero, the optimal bias and rate of convergence can be achieved by the constrained B-spline estimator for any order derivative constraint (c.f. Proposition 4.2.3). However, for forth and higher order derivative constraints, the optimal convergence rate may not be attained by the constrained B-spline estimator if no such assumption is made (c.f. Proposition 4.2.2) [39]; rather, a larger than desired lower bound on the estimator performance may be established (c.f. Remark 4.2.1).

1.2.1.3 Constrained Nonparametric Estimation Minimax Lower Bounds

For *unconstrained* estimation, question (Q1) (see above) has been satisfactorily addressed for both the Hölder and Sobolev classes under the L_2-norm and supremum norm. Moreover minimax lower bounds have been developed for a variety of unconstrained Hölder and Sobolev classes using a variety of norms; see [18, 33, 43, 48, 49, 77] and references therein for details. This has led to well known optimal rates of convergence over unconstrained function classes. However, if shape constraints, such as nonnegative derivative constraints, are imposed, then minimax asymptotic analysis becomes more complicated; fewer results have been reported, particularly when the supremum norm is considered. It is worth mentioning that a shape constraint does not improve the unconstrained optimal rate of convergence [37], and it is believed that the same optimal rate holds on a constrained function class, although no rigorous justification has been given for general nonnegative derivative constraints.

1.2.2 Literature Review

The current literature on nonnegative derivative constrained nonparametric estimation focuses mostly on monotone estimation, e.g., [10, 51, 52, 72, 79], and convex estimation, e.g., [8, 21, 27, 71, 80], i.e., estimation related to the first and second order nonnegative derivative constraints. All of these papers study the performance of certain constrained estimators, e.g., the least-squares, B-spline, and P-spline estimators, for sufficiently large sample size. Typical performance issues include consistency, convergence rates, and minimax risk [49, 77]. For instance, in [72], the consistency and uniform convergence of a monotone P-spline estimator is verified. In the realm of convex (or concave) estimation, the least squares convex estimator is studied in [27, 31, 45]. This estimator is shown to be consistent on the interior of the interval of interest [31]. The pointwise rate of convergence for this estimator is developed in [45]. Finally, the pointwise asymptotic distributions of this estimator are characterized in [27]. The minimax analysis of convex estimation in the L_2-norm has recently been carried out in [7, 28, 29]. In addition to monotone and convex estimation, results on k-monotone estimation are given in [2] for higher order nonnegative derivative constraints. Such results from [2] concern the consistency of a k-monotone maximum likelihood estimator, as well as minimax asymptotic lower bounds for k-monotone functions in the L_1-norm. However, all of the above results are either are (i) concerned only with lower order derivative constraints, or (ii) do not examine the estimator performance under the supremum norm, which is an important performance metric, as it is a critical tool in arguments used to establish estimator consistency and uniform convergence rates.

1.3 Summary of Research Contributions

We summarize the major results and contributions made in the areas of constrained estimation and approximation presented in this thesis as follows:

(1) We first develop the optimal control formulation and analytical properties of smoothing splines subject to general linear dynamics and control constraints using optimal control techniques. By using the Hilbert space method and variational techniques, optimality conditions are established for these constrained smoothing splines in the form of variational inequalities. These optimality conditions yield a nonsmooth equation of an optimal initial condition; it is shown that the unique solution of this equation completely determines an optimal control and thus the desired smoothing spline (c.f. Theorem 2.3.2 and Corollary 2.3.1).

(2) We utilize techniques from nonsmooth optimization to provide results on the numerical computation of constrained smoothing splines. Moreover, in order to solve the above mentioned equation, we verify its B-differentiability and other nonsmooth properties. A modified nonsmooth Newton's algorithm with line search [53] is invoked to solve the equation. This algorithm does not require knowing the solution form of a smoothing spline *a priori*. However, the convergence of the original nonsmooth Newton's method in [53] relies on several critical assumptions, including the boundedness of level sets and global existence of direction vectors for a related equation. The verification of these assumptions for constrained smoothing splines turns out to be rather nontrivial, due to the dynamics and constraint induced complexities. By using various techniques from nonsmooth analysis, polyhedral theory, and piecewise affine switching systems, we establish the global convergence of the proposed algorithm for a general polyhedral control constraint under mild technical conditions (c.f. Theorems 2.5.1–2.5.2).

(3) We establish the critical uniform Lipschitz property for the constrained B-spline estimator introduced in Section 1.2.1.1. A novel technique for the proof of the uniform Lipschitz property depends on a deep result in B-spline theory (dubbed de Boor's conjecture) first proved by A. Shardin [64]; see [26] for a recent, simpler proof. Informally speaking, this result says that the ℓ_∞-norm of the inverse of the Gramian formed by the normalized B-splines of order m is uniformly bounded, independent of the spline knot sequence and the number of B-splines (c.f. Theorem 3.2.2 in Section 3.2.3). Recall that the uniform Lipschitz property states that the size-varying piecewise linear functions that map the (weighted) sample data vector to the constrained B-spline estimator coefficients attain a uniform Lipschitz constant independent of the data sample size and the number of spline knots. Inspired by Shardin's result, we construct (nontrivial) coefficient matrices

for these piecewise linear functions, and use these constructions to approximate related matrices by suitable B-spline Gramians via analytic techniques. This yields the uniform bounds in the ℓ_∞-norm for arbitrary m and possibly unevenly spaced design points and knots; see Theorem 3.2.1.

(4) Using the uniform Lipschitz property, we show that for any spline order m, the constrained B-spline estimator achieves uniform convergence and consistency on the entire interval of interest, even when the design points and/or the knots are unevenly spaced (c.f. Theorem 4.3.1). Moreover, we develop several important results on constrained spline approximation (c.f. Propositions 4.2.1-4.2.3), which are used to the bound estimator bias. After bounding the bias, standard techniques and the uniform Lipschitz property are utilized to bound the constrained B-spline estimator stochastic error. Furthermore, these bounds allow us to develop a convergence rate for the B-spline estimator in the supremum norm (c.f. Theorem 4.3.1 and Remark 4.3.1); this rate sheds light on the optimal convergence and minimax risk analysis of the B-spline estimator under general nonnegative derivative constraints.

(5) Finally, we develop multiple minimax lower bounds under the supremum norm for a variety of nonnegative derivative constrained nonparametric regression problems over Hölder and Sobolev classes (c.f. Theorem 5.2.1). This is done by constructing a family of functions (or hypotheses) satisfying an appropriate supremum norm separation order and a small total L_2-distance order that also adhere to the specified nonnegative derivative constraint [77, Section 2]. This construction is the first of its kind for minimax general nonnegative derivative constrained estimation. Combining the minimax lower bounds with the previous results demonstrates that the nonnegative derivative constrained B-

spline estimator achieves the optimal asymptotic performance over a suitable Hölder class in the supremum norm, for certain order nonnegative derivative constraints.

1.4 Organization

This thesis is organized as follows. In Chapter II, we study both the analytical properties and computation of smoothing splines subject to general linear dynamics and control constraints. In Chapters III-V, we consider the nonparametric estimation of smooth functions subject to general nonnegative derivative constraints. Moreover, in Chapter III a nonnegative derivative constrained B-spline estimator is proposed, and the critical uniform Lipschitz property for this estimator is established. In Chapter IV several results on constrained spline approximation are verified and then combined with the previously established uniform Lipschitz property to develop the consistency and convergence rate of the Chapter III B-spline estimator in the supremum norm. Finally, in Chapter V, a number of minimax lower bounds are developed (in the supremum norm) for a variety of general nonnegative derivative constrained nonparametric regression problems. These lower bounds are combined with the results from Chapter IV in order to demonstrate that the Chapter III constrained B-spline estimator obtains the optimal rate of convergence (with respect to the supremum norm) over suitable Hölder classes, for certain nonnegative derivative constraints. Several conclusions and future research directions are discussed in Chapter VI.

CHAPTER II

Shape Constrained Smoothing Splines: Analysis and Computation

2.1 Introduction

Spline models are extensively studied in approximation theory, numerical analysis, and statistics with broad applications in science and engineering. In particular, smoothing splines are smooth functions with favorable statistical properties, whose smoothness attributes deter the overfitting of model data [78]. From a control systems point of view, the smoothing spline model is closely associated with certain finite-horizon linear quadratic optimal control problems [22]. In this chapter, we consider smoothing spline models subject to various control constraints. These splines achieve certain constrained linear optimal control formulations with unknown initial state and control. Attention is given to both the analysis and the computation of these shape constrained smoothing splines.

This chapter is organized as follows. In Section 2.2, we formulate a shape constrained smoothing spline as a constrained optimal control problem with optimality conditions developed in Section 2.3. In Section 2.4, critical analytical properties of constrained smoothing splines are formulated; such properties are relevant to the numerical computation of these splines. A nonsmooth Newton's method for computing constrained smoothing splines is given in Section 2.5; its convergence analysis and numerical results are presented in Section 2.5 and Section 2.6 respectively, for polyhedral control constraints. Finally, a summary is given in Section 2.7.

Notation. We introduce the following notation to be used throughout this chapter. Let $\langle \cdot, \cdot \rangle$ denote the inner product on the Euclidean space. Let $\mathbf{I}_S$ denote the indicator function for a set S. Let $\perp$ denote the orthogonality of two vectors in $\mathbb{R}^n$, i.e., $a \perp b$ implies $a^T b = 0$. For a closed convex set $\mathcal{K}$ in $\mathbb{R}^n$, $\Pi_{\mathcal{K}}(z)$ denotes the Euclidean projection of $z \in \mathbb{R}^n$ onto $\mathcal{K}$. It is known that $\Pi_{\mathcal{K}}(\cdot)$ is Lipschitz continuous on $\mathbb{R}^n$ with the Lipschitz constant $L = 1$ with respect to the Euclidean norm [23]. Throughout this chapter, let $\int$ be the Lebesgue integral. For a matrix M, $M_{j\bullet}$ denotes its jth row and $\mathrm{Ker}(M)$ denotes the null space of M. Finally, for a function $F : \mathbb{R}^n \to \mathbb{R}^n$ and a closed convex set $\mathcal{K}$ in $\mathbb{R}^n$, let $\mathrm{VI}(\mathcal{K}, F)$ be the variational inequality problem whose solution is $z_* \in \mathcal{K}$ if $\langle z - z_*, F(z_*) \rangle \geq 0$ for all $z \in \mathcal{K}$. We use $\mathrm{SOL}(\mathcal{K}, F)$ to denote the solution set of $\mathrm{VI}(\mathcal{K}, F)$.

2.2 Shape Constrained Smoothing Splines: Constrained Optimal Control Formulation

Consider the linear control system on $\mathbb{R}^\ell$ subject to control constraint:

$$\dot{x} = Ax + Bu, \qquad y = Cx, \tag{2.1}$$

where $A \in \mathbb{R}^{\ell \times \ell}$, $B \in \mathbb{R}^{\ell \times m}$, and $C \in \mathbb{R}^{p \times \ell}$. Let $\Omega \subseteq \mathbb{R}^m$ be a closed convex set. The control constraint is given by $u \in L_2([0,1]; \mathbb{R}^m)$ and $u(t) \in \Omega$ for almost all $t \in [0,1]$, where $L_2([0,1];\mathbb{R}^m)$ is the space of square $\mathbb{R}^m$-valued (Lebesgue) integrable functions. We denote this constrained linear control system by $\Sigma(A,B,C,\Omega)$. Define the set of permissible controls, which is clearly convex:

$$\mathcal{W} := \Big\{ u \in L_2([0,1];\mathbb{R}^m) \mid u(t) \in \Omega, \text{ a.e. } [0,1] \Big\}.$$

Let the underlying function $f : [0,1] \to \mathbb{R}^p$ be the output $f(t) := Cx(t)$ for an absolutely continuous trajectory $x(t)$ of $\Sigma(A,B,C,\Omega)$, which can be completely determined by its initial state and control. Consider the following (generalized) regression problem on the interval $[0,1]$:

$$y_i \ = \ f(t_i) + \varepsilon_i, \qquad i = 0,1,\ldots,n, \tag{2.2}$$

where t_i's are the pre-specified design points with $0 = t_0 < t_1 < \cdots < t_n = 1$, $y_i \in \mathbb{R}^p$ are samples, and $\varepsilon_i \in \mathbb{R}^p$ are noise or errors. Given the sample observation $(t_i, y_i)_{i=0}^n$, and $w_i > 0, i = 1,\ldots,n$ such that $\sum_{i=1}^n w_i = 1$ (e.g., $w_i = t_i - t_{i-1}$), define the cost functional

$$J := \sum_{i=1}^n w_i \big\| y_i - Cx(t_i) \big\|_2^2 + \lambda \int_0^1 \|u(t)\|_2^2 dt, \tag{2.3}$$

where $\lambda > 0$ is the penalty parameter. The goal of a shape constrained smoothing spline is to find an absolutely continuous trajectory $x(t)$ (which is determined by its initial state and control) that minimizes the cost functional J subject to the dynamics of the linear control system $\Sigma(A,B,C,\Omega)$ in (2.1) and the control constraint $u \in \mathcal{W}$.

Remark 2.2.1. Let $R \in \mathbb{R}^{m\times m}$ be a symmetric positive definite matrix. A more general cost functional

$$J := \sum_{i=1}^n w_i \big\| y_i - Cx(t_i) \big\|_2^2 + \lambda \int_0^1 u^T(t) R u(t) dt \tag{2.4}$$

may be considered. However, a suitable control transformation will yield an equivalent problem defined by the cost functional (2.3). In fact, let $R = P^T P$ for an invertible matrix P. Let $v(t) = Pu(t)$, $\Omega' = P\Omega$, and $\mathcal{W}' := \{ v \in L_2([0,1]; \mathbb{R}^m) \mid v(t) \in \Omega', \text{ a.e. } [0,1] \}$. Clearly, Ω' remains closed and convex, and likewise, $\mathcal{W}'$ remains convex. Therefore the constrained optimal control problem defined by (2.4) for the linear control system $\Sigma(A, B, C, \Omega)$ is equivalent to that defined by (2.3) with u replaced by v for the linear system $\Sigma(A, BP^{-1}, C, \Omega')$ subject to the constraint $(v, x_0) \in \mathcal{W}' \times \mathbb{R}^\ell$.

Example 2.2.1. The constrained linear control model (2.1) covers a wide range of estimation problems subject to shape and/or dynamical constraints. For instance, the standard monotone regression problem is a special case of the model (2.1) by letting the scalars $A = 0$, $B = C = 1$, and $\Omega = \mathbb{R}_+$. Another case is the convex regression, for which

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{2\times 2}, \quad B = \begin{bmatrix} 0 \\ 1 \end{bmatrix} \in \mathbb{R}^2, \quad C^T = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \in \mathbb{R}^2, \quad \Omega = \mathbb{R}_+.$$

2.3 Optimality Conditions of Shape Constrained Smoothing Splines

This section develops optimality conditions for the finite-horizon constrained optimal control problem (2.3) using Hilbert space techniques. We first introduce the following functions $P_i : [0,1] \to \mathbb{R}^{p\times m}$ inspired by [22]:

$$P_i(t) := \begin{cases} Ce^{A(t_i - t)}B, & \text{if } \ t \in [0, t_i] \\ 0, & \text{if } \ t > t_i \end{cases}, \quad i = 1, \ldots, n.$$

Hence,

$$f(t_i) = Cx(t_i) = Ce^{At_i}x_0 + \int_0^1 P_i(t)u(t)dt, \quad i = 1, \ldots, n,$$

where x_0 denotes the initial state of $x(t)$. Define the set $\mathcal{P} := \mathcal{W} \times \mathbb{R}^\ell$. It is easy to verify that $\mathcal{P}$ is convex. The constrained optimal control problem is formulated as

$$\inf_{(u,x_0)\in\mathcal{P}} J(u, x_0), \tag{2.5}$$

where $J : \mathcal{P} \to \mathbb{R}_+$ is given by

$$J(u, x_0) := \sum_{i=1}^{n} w_i \left\| Ce^{At_i} x_0 + \int_0^1 P_i(t)u(t)dt - y_i \right\|_2^2 + \lambda \int_0^1 \|u(t)\|_2^2 dt.$$

For given design points $\{t_i\}_{i=1}^n$ in $[0, 1]$, we introduce the following condition:

$$\mathbf{H.1}: \qquad \text{rank} \begin{pmatrix} Ce^{At_1} \\ Ce^{At_2} \\ \vdots \\ Ce^{At_n} \end{pmatrix} = \ell.$$

It is easy to see, via $t_i \in [0, 1]$ for all i, that if (C, A) is an observable pair, then the condition **H.1** holds for all sufficiently large n. Under this condition, the existence and uniqueness of an optimal solution can be shown via standard arguments in functional analysis, e.g., [3, 42, 44]. We present a proof in the following theorem for self-containment.

Theorem 2.3.1. *Suppose $\{(t_i, y_i)\}$, $\{w_i\}$, and $\lambda > 0$ are given. Under the condition* **H.1**, *the optimization problem (2.5) has a unique optimal solution $(u_*, x_0^*) \in \mathcal{P}$.*

Proof. Consider the Hilbert space $L_2([0, 1]; \mathbb{R}^m) \times \mathbb{R}^\ell$ endowed with the inner product $\langle (u, x), (v, z) \rangle := \int_0^1 u^T(t)v(t)dt + x^T z$ for any $(u, x), (v, z) \in L_2([0, 1]; \mathbb{R}^m) \times \mathbb{R}^\ell$. Its induced norm satisfies $\|(u, x)\|^2 := \|u\|_{L_2}^2 + \|x\|_2^2$, where $\|u\|_{L_2} := \left(\int_0^1 u^T(t)u(t)dt \right)^{1/2}$ for any $u \in L_2([0,1];\mathbb{R}^m)$ and $\|\cdot\|_2$ is the Euclidean norm on $\mathbb{R}^\ell$. The following properties of $J : L_2([0,1];\mathbb{R}^m) \times \mathbb{R}^\ell \to \mathbb{R}_+$ can be easily verified via the positive definiteness of the matrix $\sum_{i=1}^n w_i (Ce^{At_i})^T (Ce^{At_i}) \in \mathbb{R}^{\ell \times \ell}$ due to **H.1**:

(i) J is coercive, i.e., for any sequence $\{(u_k, x_k)\}$ with $\|(u_k, x_k)\| \to \infty$ as $k \to \infty$, $J(u_k, x_k) \to \infty$ as $k \to \infty$.

(ii) J is strictly convex, i.e., for any $(u,x),(v,z) \in L_2([0,1];\mathbb{R}^m) \times \mathbb{R}^\ell$, $J(\alpha(u,x) + (1-\alpha)(v,z)) < \alpha J(u,x) + (1-\alpha)J(v,z)$, $\forall\, \alpha \in (0,1)$.

Pick an arbitrary $(\widetilde{u}, \widetilde{x}) \in \mathcal{P}$ and define the level set $\mathcal{S} := \{(u,x) \in \mathcal{P} \,:\, J(u,x) \leq J(\widetilde{u}, \widetilde{x})\}$. Due to the convexity and the coercive property of J, $\mathcal{S}$ is a convex and (L_2-norm) bounded set in $L_2([0,1];\mathbb{R}^m) \times \mathbb{R}^\ell$. Since the Hilbert space $L_2([0,1];\mathbb{R}^m) \times \mathbb{R}^\ell$ is reflexive and self dual, it follows from Banach-Alaoglu Theorem [44] that an arbitrary sequence $\{(u_k, x_k)\}$ in $\mathcal{S}$ with $u_k \in \mathcal{W}$ and $x_k \in \mathbb{R}^\ell$ has a subsequence $\{(u'_k, x'_k)\}$ that attains a weak*, thus weak, limit $(u_*, x^*) \in L_2([0,1];\mathbb{R}^m) \times \mathbb{R}^\ell$. Clearly, $x^* \in \mathbb{R}^\ell$. Without loss of generality, we assume that for each u'_k, $u'_k(t) \in \Omega$ for all $t \in [0,1]$. Therefore, $Ce^{At_i}x'_k + \int_0^1 P_i(t) u'_k(t) dt$ converges to $Ce^{At_i}x^* + \int_0^1 P_i(t) u_*(t) dt$ for each i.

Next we show that $u_* \in \mathcal{W}$ via the closedness and convexity of Ω. In view of the weak convergence of (u'_k) to u_*, it follows from Mazur's Lemma [60, Lemma 10.19] that there exists a sequence of convex combinations of (u'_k), denoted by (v_k), that converges to u_* strongly in $L_2([0,1];\mathbb{R}^m)$, i.e., for each k, there exist an integer $p_k \geq k$ and real numbers $\lambda_{k,j} \geq 0, k \leq j \leq p_k$ with $\sum_{j=k}^{p_k} \lambda_{k,j} = 1$ such that $v_k = \sum_{j=k}^{p_k} \lambda_{k,j} u_k$, and $\|v_k - u_*\|_{L_2} \to 0$ as $k \to \infty$. Since each $u_k(t) \in \Omega, \forall\, t \in [0,1]$, the same holds for each v_k via the convexity of Ω. Furthermore, due to the strong convergence of (v_k) to u_* (i.e., in the L_2-norm), (v_k) converges to u_* in measure [4, pp. 69], and hence has a subsequence that converges to u_*

pointwise almost everywhere on $[0,1]$ (cf. [4, Theorem 7.6] or [42, Theorem 5.2]). Since Ω is closed, $u_*(t) \in \Omega$ for almost all $t \in [0,1]$. This shows that $u_* \in \mathcal{W}$.

Furthermore, by using the (L_2-norm) boundedness of (u'_k) and the triangle inequality for the L_2-norm, it is easy to show that for any $\eta > 0$, there exists $K \in \mathbb{N}$ such that $\|u_*\|^2_{L_2} \leq \|u'_k\|^2_{L_2} + \eta, \forall\ k \geq K$. These results imply that for any $\varepsilon > 0$, $J(u_*, x^*) \leq J(u'_k, x'_k) + \varepsilon$ for all k sufficiently large. Consequently, $J(u_*, x^*) \leq J(\widetilde{u}, \widetilde{x})$ such that $(u_*, x^*) \in \mathcal{S}$. This thus shows that $\mathcal{S}$ is sequentially compact. In view of the (strong) continuity of J, we see that a global optimal solution exists on $\mathcal{S}$ [44, Section 5.10, Theorem 2], and thus on $\mathcal{P}$. Moreover, since J is strictly convex in (u, x_0) and the set $\mathcal{P}$ is convex, the optimal solution (u_*, x_0^*) must be unique. □

The next result provides the necessary and sufficient optimality conditions in terms of variational inequalities. In particular, the optimality conditions yield two equations: (2.6) and (2.7). It is shown in Corollary 2.3.1 that equation (2.6) implies that if x_0^* is known, then the smoothing spline can be determined inductively. Furthermore, the optimal initial state x_0^* can be solved from the (nonsmooth) equation (2.7), for which a nonsmooth Newton's method will be used (cf. Section 2.4).

Theorem 2.3.2. *The pair $(u_*, x_0^*) \in \mathcal{P}$ is an optimal solution to (2.5) if and only if the following two conditions hold:*

$$
\begin{aligned}
u_*(t) &= \Pi_\Omega\big(- G(t, u_*(t), x_0^*)/\lambda\big), \quad a.e. \quad [0,1], && (2.6)\\
L(u_*, x_0^*) &= 0, && (2.7)
\end{aligned}
$$

where

$$
G(t, u_*(t), x_0^*) := \sum_{i=1}^n w_i P_i^T(t)\Big(Ce^{At_i}x_0^* + \int_0^1 P_i(t)u_*(t)dt - y_i\Big), \qquad (2.8)
$$

and

$$L(u_*, x_0^*) := \sum_{i=1}^n w_i \big(Ce^{At_i}\big)^T \Big(Ce^{At_i} x_0^* + \int_0^1 P_i(t) u_*(t) dt - y_i\Big).$$

Proof. Let $(u', x') \in \mathcal{P}$ be arbitrary. Due to the convexity of $\mathcal{P}$, $(u_*, x_0^*) + \varepsilon[(u', x') - (u_*, x_0^*)] \in \mathcal{P}$ for all $\varepsilon \in [0, 1]$. Further, since (u_*, x_0^*) is a global optimizer, we have $J((u_*, x_0^*) + \varepsilon[(u', x') - (u_*, x_0^*)]) \geq J(u_*, x_0^*)$ for all $\varepsilon \in [0, 1]$. Therefore

$$\begin{aligned} 0 &\leq \lim_{\varepsilon \downarrow 0} \frac{J((u_*, x_0^*) + \varepsilon[(u', x') - (u_*, x_0^*)]) - J(u_*, x_0^*)}{\varepsilon} \\ &= 2\Bigg[\sum_{i=1}^n w_i \Big\langle Ce^{At_i} x_0^* + \int_0^1 P_i(t) u_*(t) dt - y_i\,,\; Ce^{At_i}(x' - x_0^*) \\ &\qquad + \int_0^1 P_i(t)\Big(u'(t) - u_*(t)\Big) dt \Big\rangle \;+\; \lambda \int_0^1 u_*(t)^T \Big(u'(t) - u_*(t)\Big) dt\Bigg]. \end{aligned}$$

This thus yields the necessary optimality condition: for all $(u', x') \in \mathcal{P}$,

$$\begin{aligned} &\sum_{i=1}^n w_i \Big\langle Ce^{At_i} x_0^* + \int_0^1 P_i(t) u_*(t) dt - y_i,\; Ce^{At_i}(x' - x_0^*) \\ &\qquad + \int_0^1 P_i(t)\Big(u'(t) - u_*(t)\Big) dt \Big\rangle \;+\; \lambda \int_0^1 u_*(t)^T \Big(u'(t) - u_*(t)\Big) dt \;\geq\; 0. \end{aligned} \tag{2.9}$$

This condition is also sufficient in light of the following inequality due to the convexity of J: for all $(u', x') \in \mathcal{P}$,

$$J(u', x') - J(u_*, x_0^*) \;\geq\; \lim_{\varepsilon \downarrow 0} \frac{J((u_*, x_0^*) + \varepsilon[(u', x') - (u_*, x_0^*)]) - J(u_*, x_0^*)}{\varepsilon}.$$

We now show that the optimality condition (2.9) is equivalent to

$$\Big\langle u'(t) - u_*(t),\; \lambda u_*(t) + G(t, u_*(t), x_0^*) \Big\rangle \;\geq\; 0, \text{ a.e. } [0, 1],\; \forall\, u' \in \mathcal{W}, \tag{2.10}$$

where $G(t, u_*(t), x_0^*)$ is given in (2.8), and

$$\Big\langle L(u_*, x_0^*),\ x' - x_0^* \Big\rangle \geq 0, \quad \forall\, x' \in \mathbb{R}^\ell. \tag{2.11}$$

Clearly, if (2.10) and (2.11) hold, then (2.9) holds. Conversely, by setting $u' = u_*$, we have from (2.9) that

$$\sum_{i=1}^{n} w_i \left\langle Ce^{At_i} x_0^* + \int_0^1 P_i(t) u_*(t) dt - y_i,\ Ce^{At_i}(x' - x_0^*) \right\rangle \geq 0, \quad \forall\ x' \in \mathbb{R}^\ell.$$

Since x' is arbitrary in $\mathbb{R}^\ell$, this yields (2.11) and thus (2.7). Furthermore, the condition (2.9) is reduced to

$$\int_0^1 \Big\langle u'(t) - u_*(t),\ \lambda u_*(t) + G(t, u_*(t), x_0^*) \Big\rangle dt \geq 0, \quad \forall\ u' \in \mathcal{W}.$$

Let $\widetilde{G}(t, u_*(t), x_0^*) := \lambda u_*(t) + G(t, u_*(t), x_0^*)$. Since Ω is closed and convex, $\widetilde{G} \in L_2([0,1]; \mathbb{R}^m)$, and $u' \in L_2([0,1]; \mathbb{R}^m)$, it follows from [55, Section 2.1] that the above integral inequality is equivalent to the variational inequality (2.10), which is further equivalent to $u_*(t) \in \mathrm{SOL}\big(\Omega, \widetilde{G}(t, \cdot, x_0^*)\big)$, a.e. $[0, 1]$. Hence, for almost all $t \in [0, 1]$,

$$\Big\langle w - u_*(t),\ u_*(t) + G(t, u_*(t), x_0^*)/\lambda \Big\rangle \geq 0, \quad \forall\ w \in \Omega.$$

This shows $u_*(t) = \Pi_\Omega(-G(t, u_*(t), x_0^*)/\lambda)$ a.e. $[0, 1]$. □

In what follows, we further develop the optimal control solution for the shape constrained smoothing spline. Let $\widehat{f}(t, x_0^*)$ denote the shape constrained smoothing spline for the given $\{y_i\}$, i.e.,

$$\widehat{f}(t, x_0^*) := Ce^{At}x_0^* + \int_0^t Ce^{A(t-s)}Bu_*(s, x_0^*)ds, \tag{2.12}$$

where u_* is the optimal control, and x_0^* is the optimal initial state.

Corollary 2.3.1. *The shape constrained smoothing spline* $\widehat{f}(t, x_0^*)$ *satisfies*

$$\sum_{i=1}^{n} w_i\big(Ce^{At_i}\big)^T\big(\widehat{f}(t_i, x_0^*) - y_i\big) = 0, \tag{2.13}$$

and $G(t, u_*(t), x_0^*)$ *in (2.8) is given by*

$$G(t, u_*(t), x_0^*) =$$
$$\begin{cases} 0, & \forall\ t \in [0, t_1) \\ -\sum_{i=1}^{k} w_i\big(Ce^{A(t_i-t)}B\big)^T\big(\widehat{f}(t_i, x_0^*) - y_i\big), & \forall\ t \in [t_k, t_{k+1}),\ k = 1, \ldots, n-1. \end{cases} \tag{2.14}$$

Note that since each $\widehat{f}(t_i, x_0^*)$ *depends on* u_* *via (2.12),* G *is a function of* t*,* u_**, and* x_0^**.*

Proof. Note that $\widehat{f}(t_i, x_0^*) = Ce^{At_i}x_0^* + \int_0^1 P_i(s)u_*(s, x_0^*)ds$ for $i = 1, \ldots, n$. In light of (2.7) and the definition of $L(u_*, x_0^*)$, we obtain (2.13). To establish (2.14), we see from (2.13) that

$$\sum_{i=1}^{n} w_i\Big(Ce^{At_i}\Big)^T\Big(\widehat{f}(t_i, x_0^*) - y_i\Big)\mathbf{I}_{[0,t_i]}$$
$$= \begin{cases} 0, & \forall\ t \in [0, t_1) \\ -\sum_{i=1}^{k} w_i\big(Ce^{At_i}\big)^T\big(\widehat{f}(t_i, x_0^*) - y_i\big), & \forall\ t \in [t_k, t_{k+1}),\ k = 1, \ldots, n-1. \end{cases} \tag{2.15}$$

Moreover, it follows from (2.8) and the definition of P_i that

$$\begin{aligned} G(t, u_*(t), x_0^*) &= \sum_{i=1}^{n} w_i \Big(C e^{A(t_i - t)} B \cdot \mathbf{I}_{[0,t_i]} \Big)^T \Big(\widehat{f}(t_i, x_0^*) - y_i \Big) \\ &= \sum_{i=1}^{n} w_i \Big(C e^{At_i} e^{-At} B \Big)^T \cdot \mathbf{I}_{[0,t_i]} \cdot \Big(\widehat{f}(t_i, x_0^*) - y_i \Big) \\ &= \Big(e^{-At} B \Big)^T \sum_{i=1}^{n} w_i \Big(C e^{At_i} \Big)^T \Big(\widehat{f}(t_i, x_0^*) - y_i \Big) \mathbf{I}_{[0,t_i]}. \end{aligned}$$

By virtue of this and (2.15), we obtain (2.14). □

This corollary shows that if the optimal initial condition x_0^* is known, then the constrained smoothing spline $\widehat{f}(t, x_0^*)$ can be determined inductively. Moreover, using (2.6) and (2.14), we may first compute $u_*(t)$ on $[0, t_1)$, and by extension, $\widehat{f}(t, x_0^*)$ on $[0, t_1]$ via (2.12). Once we have computed $\widehat{f}(t, x_0^*)$ on $[0, t_k]$, we may then compute $G(t, u_*(t), x_0^*)$, and thus $u_*(t)$ on $[t_k, t_{k+1})$, as each of these depend only on $\widehat{f}(t_i, x_0^*)$ when $i \le k$ (see (2.6) and (2.14)). From here, we may compute $\widehat{f}(t, x_0^*)$ on $[t_k, t_{k+1}]$, using (2.12). This inductive computation will be exploited to compute the constrained smoothing splines in Section 2.4.

We mention a few special cases of particular interest as follows. If $\mathcal{K}$ is a closed convex cone $\mathcal{C}$, then $z \in \mathrm{SOL}(\mathcal{K}, F)$ if and only if $\mathcal{C} \ni z \perp F(z) \in \mathcal{C}^*$, where $\mathcal{C}^*$ is the dual cone of $\mathcal{C}$. In particular, if $\mathcal{K}$ is the nonnegative orthant $\mathbb{R}^n_+$, then $z \in \mathrm{SOL}(\mathcal{K}, F)$ if and only if $0 \le z \perp F(z) \ge 0$, where the latter is called a *complementarity problem* (cf. [12, 23] for details). In the case where $F(z)$ is affine, i.e., $F(z) = Mz + q$ for a square matrix M and a vector q, then the complementarity problem becomes the linear complementarity problem (LCP). Another special case of significant interest is when $\mathcal{K}$ is a polyhedron, namely, $\mathcal{K} = \{ z \in \mathbb{R}^n \,|\, Dz \ge b, \ Ez = d \}$, where $D \in \mathbb{R}^{r \times n}$, $E \in \mathbb{R}^{q \times n}$, and $b \in \mathbb{R}^r$, $d \in \mathbb{R}^q$. In this case, it is well known that $z \in \mathrm{SOL}(\mathcal{K}, F)$ if and only if there exist multipliers

$\chi \in \mathbb{R}^r, \mu \in \mathbb{R}^q$ such that $F(z) - D^T\chi + E^T\mu = 0,\ 0 \le \chi \perp Dz - b \ge 0,\ Ez - d = 0$ [23, Proposition 1.2.1]. Along with these results, we obtain the following optimality condition for u_* in terms of a complementarity problem when Ω is polyhedral.

Proposition 2.3.1. *Let $\Omega = \{w \in \mathbb{R}^m \,|\, Dw \ge b\}$ be a (nonempty) polyhedron with $D \in \mathbb{R}^{r\times m}$ and $b \in \mathbb{R}^r$. Then*

$$u_*(t) \;=\; \Big[- G(t, u_*(t), x_0^*) + D^T\chi(G(t, u_*(t), x_0^*))\Big]/\lambda, \qquad a.e. \quad [0,1],$$

where $D^T\chi : \mathbb{R}^m \to \mathbb{R}^m$ is a continuous piecewise affine function defined by the solution of the linear complementarity problem: $0 \le \chi \perp \lambda^{-1}DD^T\chi - \lambda^{-1}Dz - b \ge 0$.

Proof. It follows from $u_* \in \mathrm{SOL}(\Omega, \widetilde{G}(t,\cdot,x_0^*))$ a.e. $[0,1]$, where $\widetilde{G}(t, u_*(t), x_0^*) = \lambda u_* + G(u_*(t), x^*)$, and the above discussions that u_* is the optimal control if and only if for almost all $t \in [0,1]$, there exists $\chi \in \mathbb{R}^r$ such that

$$\lambda u_*(t) + G(u_*(t), x_0^*) - D^T\chi = 0, \quad \text{ and } \quad 0 \le \chi \perp Du_*(t) - b \ge 0.$$

This is equivalent to the linear complementarity problem

$$0 \le \chi \perp \lambda^{-1}DD^T\chi - \lambda^{-1}z - b \ge 0, \tag{2.16}$$

where $z := G(u_*(t), x_0^*)$. Due to the positive semidefinite plus structure [69], it follows from complementarity theory [12] that for any $z \in \mathbb{R}^m$, the LCP (2.16) has a solution $\chi(z)$, and $D^T\chi(z)$ is unique. Furthermore, this implies that $D^T\chi(\cdot)$ is a continuous piecewise affine function [69]. □

2.4 Computation of Shape Constrained Smoothing Splines: Formulation and Analytic Properties

In this section, we discuss the numerical issues of the shape constrained smoothing splines. As indicated below Corollary 2.3.1, in order to determine $\widehat{f}(t, x_0^*)$, it suffices to find the optimal initial state x_0^*, since once x_0^* is known, u_* and $\widehat{f}$ can be computed recursively. In fact, it follows from Corollary 2.3.1 that $\widehat{f}(t, x_0^*)$ is given by

$$\widehat{f}(t, x_0^*) \;=\; Ce^{At}x_0^* + \int_0^t Ce^{A(t-s)}Bu_*(s, x_0^*)ds, \tag{2.17}$$

where

$$u_*(t, x_0^*) \;=\; \begin{cases} \Pi_\Omega(0), & \forall\; t \in [0, t_1) \\ \Pi_\Omega\Big(\lambda^{-1}\sum_{i=1}^{k} w_i\big(Ce^{A(t_i-t)}B\big)^T\big(\widehat{f}(t_i, x_0^*) - y_i\big)\Big), & \forall\; t \in [t_k, t_{k+1}),\; k = 1, \ldots, n-1, \end{cases}$$

and $\widehat{f}(t, x_0^*)$ satisfies

$$H_{y,n}(x_0^*) \;:=\; \sum_{i=1}^{n} w_i\Big(Ce^{At_i}\Big)^T\Big(\widehat{f}(t_i, x_0^*) - y_i\Big) \;=\; 0. \tag{2.18}$$

To compute the optimal initial state x_0^*, we consider the equation $H_{y,n}(z) = 0$, where $\widehat{f}(t, z)$ in $H_{y,n}(z)$ is defined by (2.17) when x_0^* is replaced by z. The following lemma is a direct consequence of Theorem 2.3.1 and the definition of $\widehat{f}$.

Lemma 2.4.1. *For any given* $\{(t_i, y_i)\}$, $\{w_i\}$, *and* $\lambda > 0$ *satisfying* **H.1**, *the equation* $H_{y,n}(z) = 0$ *has a unique solution, which corresponds to the optimal initial state* x_0^* *of the smoothing spline* $\widehat{f}(t, x_0^*)$.

It should be noted that the function $H_{y,n} : \mathbb{R}^\ell \to \mathbb{R}^\ell$ is nonsmooth in general, due to the constraint induced nonsmoothness of $u_*(t, x_0^*)$ in x_0^*. However, the following proposition shows the B(ouligand)-differentiability of $\widehat{f}(t, z)$ in z [23, Section 3.1]. Recall that a function $G : \mathbb{R}^\ell \to \mathbb{R}^\ell$ is B-differentiable if it is Lipschitz continuous and directionally differentiable on $\mathbb{R}^\ell$, namely, for any $z \in \mathbb{R}^\ell$ and any direction vector $d \in \mathbb{R}^\ell$, the following (one-sided) directional derivative exists

$$G'(z; d) := \lim_{\tau \downarrow 0} \frac{G(z + \tau d) - G(z)}{\tau}.$$

Proposition 2.4.1. *Assume that* $\Pi_\Omega : \mathbb{R}^m \to \mathbb{R}^m$ *is directionally differentiable on* $\mathbb{R}^m$. *For any given* $\{(t_i, y_i)\}$, $\{w_i\}$, $\lambda > 0$, *and* $z \in \mathbb{R}^\ell$, $\widehat{f}(t, z)$ *is B-differentiable in* z *for any fixed* $t \in [0, 1]$.

Proof. We prove the B-differentiability of $\widehat{f}(t, z)$ in z by induction on the intervals $[t_k, t_{k+1}]$, for $k = 0, 1, \ldots, n-1$. Consider $t \in [0, t_1]$ first. Since $u_*(t, z) = \Pi_\Omega(0), \forall\, t \in [0, t_1)$ and $\widehat{f}(t, z)$ is continuous in t, $\widehat{f}(t, z) = Ce^{At}z + \int_0^t Ce^{A(t-s)} B\, \Pi_\Omega(0) ds, \forall\, t \in [0, t_1]$, which is clearly Lipschitz continuous and directionally differentiable. Thus $\widehat{f}(t, \cdot)$ is B-differentiable in z for any fixed $t \in [0, t_1]$.

Now assume that $\widehat{f}(t, \cdot)$ is B-differentiable for all $t \in [0, t_1] \cup \cdots \cup [t_{k-1}, t_k]$, and consider the interval $[t_k, t_{k+1}]$. Note that for any $t \in [t_k, t_{k+1})$, the optimal control

$$u_*(t, z) \;=\; \Pi_\Omega \left(\lambda^{-1} \sum_{i=1}^{k} w_i \Big(Ce^{A(t_i - t)} B \Big)^T \Big(\widehat{f}(t_i, z) - y_i \Big) \right). \tag{2.19}$$

Since the functions $\Pi_\Omega(\cdot)$ and $\widehat{f}(t_i, \cdot), i = 1, \ldots, k$ are all B-differentiable, it follows from [23, Proposition 3.1.6] that the composition given in $u_*(t, z)$ remains B-differentiable in z for each fixed $t \in [t_k, t_{k+1})$. For a given direction vector $d \in \mathbb{R}^\ell$ and a given $\tau \geq 0$, $u_*(t, z + \tau d)$ is continuous in t on $[t_k, t_{k+1})$. Therefore, $u_*(t, z + \tau d)$ is (Borel) measurable on $[t_k, t_{k+1})$ for any fixed τ and d. Since

$$u'_*(t, z; d) \; = \; \lim_{\tau \downarrow 0} \frac{u_*(t, z + \tau d) - u_*(t, z)}{\tau},$$

the function $u'_*(t, z; d)$ is also (Borel) measurable on $[t_k, t_{k+1})$ for any fixed z and d [4, Corollary 2.10 or Corollary 5.9]. It follows from the non-expansive property of Π_Ω with respect to the Euclidean norm $\| \cdot \|_2$ [23] that for any given $\tau > 0$,

$$\frac{\|u_*(t, z + \tau d) - u_*(t, z)\|_2}{\tau} \leq \frac{1}{\lambda \cdot \tau} \sum_{i=1}^{k} w_i \left\| \left(Ce^{A(t_i - t)} B\right)^T \right\|_2 \cdot \left\| \widehat{f}(t_i, z + \tau d) - \widehat{f}(t_i, z) \right\|_2 .$$

This shows that for each $t \in [t_k, t_{k+1})$,

$$\frac{\|u_*(t, z + \tau d) - u_*(t, z)\|_2}{\tau} \leq \sum_{i=1}^{k} \frac{w_i L(t_i) \|d\|_2}{\lambda} \left\|(Ce^{A(t_i - t)} B)^T\right\|_2,$$

where $L(t_i) > 0$ is the Lipschitz constant of $\widehat{f}(t_i, \cdot)$. Hence, it is easy to see that $u'_*(t, z; d)$ is bounded on the interval $[t_k, t_{k+1})$, i.e., there exists $\varrho_k > 0$ such that $\|u'_*(t, z; d)\|_2 \leq \varrho_k$ for all $t \in [t_k, t_{k+1})$. This shows that $u'_*(t, z; d)$ is (Lebesgue) integrable in t on $[t_k, t_{k+1}]$. In view of the above results and the Lebesgue Dominated Convergence Theorem [4, Theorem 5.6 or Corollary 5.9], we have $\widehat{f}'(t, z; d) \; = \; Ce^{At} d + \int_0^t Ce^{A(t-s)} B u'_*(s, z; d) ds$ for all $t \in [t_k, t_{k+1}]$. This shows that $\widehat{f}(t, \cdot)$ is directionally differentiable for each $t \in [t_k, t_{k+1}]$. Furthermore, since $\|\Pi_\Omega(z) - \Pi_\Omega(z')\|_2 \leq \|z - z'\|_2$ for all $z, z' \in \mathbb{R}^\ell$, and $u_*(t, z)$ depends on finitely many $\widehat{f}(t_i, z)$ on the interval $[t_j, t_{j+1})$ with $j = 1, \ldots, k$ (cf. (2.19)), it can be shown that for each $j = 1, \ldots, k$, there exists a uniform Lipschitz constant $L_j > 0$ (independent of t) such that for any $t \in [t_j, t_{j+1})$, $\|u_*(t, z) - u_*(t, z')\|_2 \leq L_j \|z - z'\|_2$ for all $z, z' \in \mathbb{R}^\ell$. In view of $\widehat{f}(t, z) = Ce^{At}z + \int_0^t Ce^{A(t-s)}Bu_*(s, z)ds$, the continuity of $\widehat{f}$ in t, and the induction hypothesis, we deduce the Lipschitz continuity of $\widehat{f}(t, \cdot)$ for each fixed $t \in [t_k, t_{k+1}]$. Therefore, the proposition follows by the induction principle. □

Clearly, the assumption of global directional differentiability of the Euclidean projector Π_Ω is critical to Proposition 2.4.1. In what follows, we identify a few important cases where this assumption holds. One of the most important cases is when Ω is polyhedral. In this case, as shown in Proposition 2.3.1, $\Pi_\Omega(\cdot)$ is a continuous piecewise affine function, and its directional derivative is given by a piecewise linear function of a direction vector d (cf. [23, Section 4.1] or [63]). When Ω is non-polyhedral, we consider a finitely generated convex set, i.e., $\Omega = \{w \in \mathbb{R}^m \,|\, G(w) \leq 0\}$, where $G : \mathbb{R}^m \to \mathbb{R}^{p_1}$ is such that each component function G_i is twice continuously differentiable and convex for $i = 1, \ldots, p_1$. It is known that if, for each $w \in \mathbb{R}^m$, the set Ω satisfies either the sequentially bounded constraint qualification (SBCQ) or the constant rank constraint qualification (CRCQ) at $\Pi_\Omega(w)$, then Π_Ω is directionally differentiable; see [23, Sections 4.4-4.5] for details.

More differential properties can be obtained for $\widehat{f}(t, z)$. Motivated by [56, Theorem 8], we consider the semismoothness of $\widehat{f}$. A function $G : \mathbb{R}^n \to \mathbb{R}^m$ is said to be *semismooth* at $z_* \in \mathbb{R}^n$ [23] if G is B-differentiable at all points in a neighborhood of z_* and satisfies

$$\lim_{z_* \neq z \to z_*} \frac{G'(z; z - z_*) - G'(z_*; z - z_*)}{\|z - z_*\|} = 0.$$

Semismooth functions play an important role in nonsmooth analysis and optimization; see [23] and the references therein for details.

Lemma 2.4.2. *Assume that $\Pi_\Omega : \mathbb{R}^m \to \mathbb{R}^m$ is directionally differentiable on $\mathbb{R}^m$. For any given $\{(t_i, y_i)\}$, $\{w_i\}$, $\lambda > 0$, and $z \in \mathbb{R}^\ell$, if $u_*(t, \cdot)$ is semismooth at z for each fixed $t \in [0, 1]$, so is $\widehat{f}(t, \cdot)$.*

Proof. Fix $\{(t_i, y_i)\}$, $\{w_i\}$, $\lambda > 0$, and $z \in \mathbb{R}^\ell$. It suffices to prove that $\widehat{x}(t, \cdot)$ is semismooth at z for each fixed $t \in [0, 1]$, where $\widehat{x}(t, z)$ satisfies the ODE: $\dot{x}(t) = Ax(t) + Bu_*(t, z)$, $t \in [0, 1]$ with $x(0) = z$. It follows from the proof of Proposition 2.4.1 that $\widehat{x}(t, z)$ is B-differential in z on $[0, 1]$ and for a given $d \in \mathbb{R}^\ell$ and $t \in [0, 1]$,

$$\widehat{x}\,'(t, z; d) = e^{At}d + \int_0^t e^{A(t-s)} B u_*'(s, z; d) ds.$$

In view of this, it is easy to verify that for a fixed $t \in [0, 1]$ and any $\widetilde{z} \in \mathbb{R}^\ell$,

$$\widehat{x}\,'(t, \widetilde{z}; \widetilde{z} - z) - \widehat{x}\,'(t, z; \widetilde{z} - z) = \int_0^t e^{A(t-s)} B\Big(u_*'(s, \widetilde{z}; \widetilde{z} - z) - u_*'(s, z; z - \widetilde{z})\Big) ds.$$

By the semismoothness of $u_*(s, \cdot)$ at z, we have for each fixed $s \in [0, t]$,

$$\lim_{z \neq \widetilde{z} \to z} \frac{u_*'(s, \widetilde{z}; \widetilde{z} - z) - u_*'(s, z; \widetilde{z} - z)}{\|\widetilde{z} - z\|} = 0.$$

Furthermore, it is shown in the proof of Proposition 2.4.1 that $u_*'(s, \widetilde{z}; \widetilde{z} - z)$ and $u_*'(s, z; \widetilde{z} - z)$ are Lebesgue integrable and bounded on $[0, 1]$. Therefore, it follows from Lebesgue Dominated Convergence Theorem [4, Theorem 5.6 or Corollary 5.9] that

$$\lim_{z \neq \widetilde{z} \to z} \frac{\widehat{x}'(t, \widetilde{z}; \widetilde{z} - z) - \widehat{x}'(t, z; \widetilde{z} - z)}{\|\widetilde{z} - z\|} = 0.$$

This shows that $\widehat{x}(t, z)$ is semismooth at z for each $t \in [0, 1]$. □

Proposition 2.4.2. *If Π_Ω is semimsooth at any point in $\mathbb{R}^m$, then for any $z \in \mathbb{R}^\ell$, $\widehat{f}(t, \cdot)$ is semismooth at z for each $t \in [0, 1]$. In particular, this holds true if Ω is polyhedral.*

Proof. Note that semimsoothness implies B-differentiability. Furthermore, $\widehat{f}(t, \cdot)$ is clearly semismooth in z on $[0, t_1]$. Now assume that $\widehat{f}(t, z)$ is semismooth in z for all $t \in [0, t_k]$. By the induction hypothesis and (2.19), we see that for any fixed $t \in [t_k, t_{k+1}]$, $u_*(t, z)$ is a composition of Π_Ω and a semismooth function of z. It follows from [23, Proposition 7.4.4] that $u_*(t, \cdot)$ is semismooth at z for any $t \in [t_k, t_{k+1}]$. In light of Lemma 2.4.2, $\widehat{f}(t, \cdot)$ is semismooth at z on $[t_k, t_{k+1}]$ and on $[0, t_{k+1}]$. By the induction principle, $\widehat{f}(t, \cdot)$ is semismooth at z for each $t \in [0, 1]$. Finally, since Ω is polyhedral, Π_Ω is continuous piecewise affine and hence (strongly) semismooth [23, Proposition 7.4.7]. □

It follows from the above results that $H_{y,n}$ is a vector-valued B-differentiable function (provided that $\Pi_\Omega(\cdot)$ is directionally differentiable). To solve the equation $H_{y,n}(z) = 0$, we consider a nonsmooth Newton's method with line search in [53]; its (unique) solution is the optimal initial state x_0^* that completely determines the smoothing spline $\widehat{f}(t, x_0^*)$. It is worth pointing out that the original nonsmooth Newton's method in [53] assumes the existence of a direction vector d solving the equation $H_{y,n}(z) + H'_{y,n}(z; d) = 0$ for any z. While this assumption is shown to be true for almost all z in Theorem 2.5.1, it is highly difficult to show that this assumption holds for certain "degenerate" z; we refer the reader to Section 2.5 for the definition of a degenerate z. To overcome this difficulty, we show in Proposition 2.5.2 that a suitable small perturbation to a degenerate z yields a non-degenerate vector for which the assumption is satisfied. This leads to a modified nonsmooth Newton's method for the constrained smoothing spline; we postpone the presentation of this modified algorithm to Section 2.5 after all essential technical results are given. Moreover, it is noted that if $\widehat{f}$ is semismooth, other nonsmooth Newton's methods may be applied [23]. However, these methods require computing multiple limiting Jacobians, which is usually numerically expensive. Alternatively, the modified nonsmooth Newton's method only requires computing directional derivatives (and a single Jacobian) at a non-degenerate point.

Before ending this section, we show that for any given $z^* \in \mathbb{R}^\ell$, the level set $\mathcal{S}_{z^*} := \{z \in \mathbb{R}^\ell : \|H_{y,n}(z)\| \leq \|H_{y,n}(z^*)\|\}$ is bounded. This boundedness property will be critical in the convergence analysis of the modified nonsmooth Newton's method; see the proof of Theorem 2.5.2.

We introduce some technical preliminaries first. Recall that the recession cone of a closed convex set $\mathcal{K}$ in $\mathbb{R}^n$ is defined by $\mathcal{K}^\infty := \{d \in \mathbb{R}^n \,|\, x + \mu d \in \mathcal{K}, \forall\, \mu \geq 0\}$ for some $x \in \mathcal{K}$. It is known [1] that in a finite dimensional space such as $\mathbb{R}^n$, $\mathcal{K}^\infty$ is equivalent to the asymptotic cone of $\mathcal{K}$ defined by

$$\left\{ d \in \mathbb{R}^n \,|\, \text{ there exist } 0 < \mu_k \to \infty, x_k \in \mathcal{K} \text{ such that } \lim_{k\to\infty} \frac{x_k}{\mu_k} = d \right\}.$$

Furthermore, $\mathcal{K}^\infty$ is a closed convex cone, and $\mathcal{K}$ is bounded if and only if $\mathcal{K}^\infty = \{0\}$. More properties of recession cones can be found in [1, Proposition 2.1.5]. We provide a lemma pertaining to the Euclidean projection onto a recession cone as follows.

Lemma 2.4.3. *Let Ω be a closed convex set in $\mathbb{R}^m$, let (v_k) be a sequence in $\mathbb{R}^m$, and let (μ_k) be a positive real sequence such that $\lim_{k\to\infty} \mu_k = \infty$ and $\lim_{k\to\infty} \frac{v_k}{\mu_k} = d$ for some $d \in \mathbb{R}^m$. Then*

$$\lim_{k\to\infty} \frac{\Pi_\Omega(v_k)}{\mu_k} = \Pi_{\Omega^\infty}(d),$$

where Ω^∞ is the recession cone of Ω.

Proof. It follows from a similar argument as in [23, Lemma 6.3.13] that

$$\lim_{\mu\to\infty} \frac{\Pi_\Omega(\mu d)}{\mu} = \Pi_{\Omega^\infty}(d).$$

Therefore, it suffices to show $\lim_{k\to\infty} \frac{\Pi_\Omega(v_k)}{\mu_k} = \lim_{k\to\infty} \frac{\Pi_\Omega(\mu_k d)}{\mu_k}$. Without loss of generality, we let the vector norm $\|\cdot\|$ be the Euclidean norm. By virtue of the non-expansive property of the Euclidean projector with respect to the Euclidean norm, we have

$$\frac{\big\|\Pi_\Omega(v_k) - \Pi_\Omega(\mu_k d)\big\|}{\mu_k} \le \frac{\big\|v_k - \mu_k d\big\|}{\mu_k} = \left\|\frac{v_k}{\mu_k} - d\right\| \longrightarrow 0, \quad \text{as } k \to \infty.$$

This shows the equivalence of the two limits, and hence completes the proof. □

With the help of this lemma, we establish a boundedness result for level sets defined by $H_{y,n}$. Recall that for a given $z^* \in \mathbb{R}^\ell$, the level set $\mathcal{S}_{z^*} := \{z \in \mathbb{R}^\ell : \|H_{y,n}(z)\| \le \|H_{y,n}(z^*)\|\}$.

Proposition 2.4.3. *Let Ω be a closed convex set in $\mathbb{R}^m$. Given any $\{(t_i, y_i)\}$ satisfying the condition* **H.1***, $\{w_i\}$, $\lambda > 0$, and $z^* \in \mathbb{R}^\ell$, the level set $\mathcal{S}_{z^*}$ is bounded.*

Proof. We prove the boundedness of $\mathcal{S}_{z^*}$ by contradiction. Suppose not. Then there exists a sequence (z_k) in $\mathcal{S}_{z^*}$ such that $\|z_k\| \to \infty$ as $k \to \infty$. Without loss of generality, we may assume that $(z_k/\|z_k\|)$ converges to $v^* \in \mathbb{R}^\ell$ with $\|v^*\| = 1$ by taking a suitable subsequence of (z_k) if necessary. Define the functions $\widetilde{f} : [0,1] \times \mathbb{R}^\ell \to \mathbb{R}^p$ and $\widetilde{u}_* : [0,1] \times \mathbb{R}^\ell \to \mathbb{R}^m$ as:

$$\widetilde{f}(t,z) := Ce^{At}z + \int_0^t Ce^{A(t-s)}B\widetilde{u}_*(s,z)\,ds, \quad \text{and}$$

$$\widetilde{u}_*(t,z) :=$$
$$\begin{cases} \Pi_{\Omega^\infty}(0), & \forall\ t \in [0, t_1) \\ \Pi_{\Omega^\infty}\Big(\lambda^{-1} \sum_{i=1}^{k} w_i \big(Ce^{A(t_i - t)}B\big)^T \widetilde{f}(t_i, z)\Big), & \forall\ t \in [t_k, t_{k+1}),\ k = 1, \ldots, n-1, \end{cases}$$

where Ω^∞ is the recession cone of Ω. Note that $\widetilde{f}$ can be treated as the shape constrained smoothing spline obtained from the linear control system $\Sigma(A, B, C, \Omega^\infty)$ for the given $\widetilde{y} := (\widetilde{y}_i)_{i=1}^n = 0$, i.e., when the control constraint set Ω is replaced by its recession cone Ω^∞ and y by the zero vector.

We claim that for each fixed $t \in [0, 1]$,

$$\lim_{k\to\infty} \frac{\widehat{f}(t, z_k)}{\|z_k\|} = \widetilde{f}(t, v^*).$$

We prove this claim by induction on the intervals $[t_j, t_{j+1}]$ for $j = 0, 1, \ldots, n-1$.

Consider the interval $[0, t_1]$ first. Recall that $u_*(t, z_k) = \Pi_\Omega(0), \forall\, t \in [0, t_1)$ such that $\widehat{f}(t, z_k) = Ce^{At}z_k + \int_0^t Ce^{A(t-s)}B\Pi_\Omega(0)ds$ for all $t \in [0, t_1]$. Hence, in view of $\Pi_{\Omega^\infty}(0) = 0$ such that $\widetilde{u}_*(t, v^*) = 0$ and $\widetilde{f}(t, v^*) = Ce^{At}v^*$ for all $t \in [0, t_1]$, we have, for each fixed $t \in [0, t_1]$,

$$\lim_{k\to\infty} \frac{\widehat{f}(t, z_k)}{\|z_k\|} = \lim_{k\to\infty} Ce^{At} \frac{z_k}{\|z_k\|} = Ce^{At}v^* = \widetilde{f}(t, v^*).$$

Now suppose the claim holds true for all $t \in [0, t_j]$ with $j \in \{1, \ldots, n-2\}$, and consider $[t_j, t_{j+1}]$. Note that for each $t \in [t_j, t_{j+1})$,

$$u_*(t, z) = \Pi_\Omega\left(\lambda^{-1} \sum_{i=1}^{j} w_i \big(Ce^{A(t_i - t)}B\big)^T \big(\widehat{f}(t_i, z) - y_i\big)\right).$$

By the induction hypothesis and the boundedness of $Ce^{A(t_i-t)}B$ on $[t_j, t_{j+1}]$ for all $i = 1, \ldots, j$, we have, for each fixed $t \in [t_j, t_{j+1})$,

$$\lim_{k\to\infty} \frac{\lambda^{-1}\sum_{i=1}^{j} w_i \big(Ce^{A(t_i-t)}B\big)^T \big(\widehat{f}(t_i, z) - y_i\big)}{\|z_k\|} = \lambda^{-1}\sum_{i=1}^{j} w_i \big(Ce^{A(t_i-t)}B\big)^T \widetilde{f}(t_i, v^*).$$

By Lemma 2.4.3, we further have, for each fixed $t \in [t_s, t_{s+1})$ with $s \in \{1, \ldots, j\}$,

$$\begin{aligned}
\lim_{k\to\infty} \frac{u_*(t, z_k)}{\|z_k\|} &= \lim_{k\to\infty} \frac{\Pi_\Omega\left(\lambda^{-1}\sum_{i=1}^{s} w_i \big(Ce^{A(t_i-t)}B\big)^T \big(\widehat{f}(t_i, z) - y_i\big)\right)}{\|z_k\|} \\
&= \Pi_{\Omega^\infty}\left(\lambda^{-1}\sum_{i=1}^{s} w_i \big(Ce^{A(t_i-t)}B\big)^T \widetilde{f}(t_i, v^*)\right) \\
&= \widetilde{u}_*(t, v^*).
\end{aligned}$$

Clearly, $\widetilde{u}_*(\cdot, v^*)$ is Lebesgue integrable and uniformly bounded on $[t_j, t_{j+1}]$. Therefore, for each fixed $t \in [t_j, t_{j+1}]$,

$$\begin{aligned}
\lim_{k\to\infty} \frac{\widehat{f}(t, z_k)}{\|z_k\|} &= \lim_{k\to\infty} \frac{Ce^{At}z_k + \int_0^t Ce^{A(t-s)}Bu_*(s, z_k)\, ds}{\|z_k\|} \\
&= \lim_{k\to\infty} \frac{Ce^{At}z_k}{\|z_k\|} + \int_0^t Ce^{A(t-s)}B\left(\lim_{k\to\infty}\frac{u_*(s, z_k)}{\|z_k\|}\right) ds \\
&= Ce^{At}v^* + \int_0^t Ce^{A(t-s)}B\widetilde{u}_*(s, v^*)\, ds \\
&= \widetilde{f}(t, v^*),
\end{aligned}$$

where the second equality follows from the Lebesgue Dominated Convergence Theorem [4, Theorem 5.6]. This establishes the claim by the induction principle.

In light of the claim and the definition of $H_{y,n}$ in (2.18), we hence have

$$\lim_{k\to\infty} \frac{H_{y,n}(z_k)}{\|z_k\|} = \sum_{i=1}^{n} w_i \big(Ce^{At_i}\big)^T \widetilde{f}(t_i, v^*) = \widetilde{H}_{\widetilde{y},n}(v^*)\big|_{\widetilde{y}=0},$$

where $\widetilde{H}_{\widetilde{y},n} : \mathbb{R}^\ell \to \mathbb{R}^\ell$ (with $\widetilde{y} = (\widetilde{y}_i)_{i=1}^n$) is defined by

$$\widetilde{H}_{\widetilde{y},n}(z) := \sum_{i=1}^{n} w_i \big(Ce^{At_i}\big)^T \Big(\widetilde{f}(t_i, z) - \widetilde{y}_i\Big).$$

Since the smoothing spline $\widetilde{f}$ is obtained from the linear control system $\Sigma(A, B, C, \Omega^\infty)$, and the recession cone Ω^∞ contains the zero vector, it is easy to verify that when $\widetilde{y} = 0$, the optimal solution pair $(\widetilde{u}_*, \widetilde{x}_0^*)$ for $\widetilde{f}(t, \widetilde{x}_0^*)$ is $\widetilde{x}_0^* = 0$ and $\widetilde{u}_*(t, \widetilde{x}_0^*) \equiv 0$ on $[0, 1]$ (such that $\widetilde{f}(t, \widetilde{x}_0^*) \equiv 0$ on $[0, 1]$). Based on Lemma 2.4.1, we deduce that the equation $\widetilde{H}_{0,n}(z) = 0$ has a unique solution $z = 0$. Since $v^* \neq 0$, we must have $\widetilde{H}_{0,n}(v^*) \neq 0$. Consequently,

$$\lim_{k\to\infty} \frac{\|H_{y,n}(z_k)\|}{\|z_k\|} = \big\|\widetilde{H}_{0,n}(v^*)\big\| > 0.$$

This shows that $\|H_{y,n}(z)\|$ is unbounded on $\mathcal{S}_{z^*}$, which yields a contradiction. □

2.5 The Modified Nonsmooth Newton's Method: Algorithm and Convergence Analysis

In this section, we study the modified nonsmooth Newton's method and its global convergence. In particular, we focus on the case where the control constraint set Ω is polyhedral for the following reasons: (i) the class of polyhedral Ω is already very broad and includes a number of important applications; (ii) since any closed convex set is the intersection of all closed half-spaces containing it, such a set can be accurately approximated by a polyhedron; (iii) when Ω is polyhedral, Π_Ω is globally B-differentiable, while this is not the case for a non-polyhedral Ω, unless certain constraint qualifications are imposed *globally*. Furthermore, for a non-polyhedral Ω, the directional derivatives of Π_Ω are difficult to characterize and compute.

Let $\Omega = \{w \in \mathbb{R}^m \,|\, Dw \geq b\}$ be a polyhedron with $D \in \mathbb{R}^{r\times m}$ and $b \in \mathbb{R}^r$. Proposition 2.3.1 shows that $\Pi_\Omega : \mathbb{R}^m \to \mathbb{R}^m$ is a (Lipschitz) continuous and piecewise affine (PA) function. It follows from (2.19) that for $t \in [t_k, t_{k+1})$ with $k = 1, 2, \ldots, n-1$, $Bu_*(t,z) = B\Pi_\Omega\big(B^T e^{-A^T t} v_k(z)\big)$, where

$$v_k(z) := \lambda^{-1} \sum_{i=1}^{k} w_i \big(Ce^{At_i}\big)^T \Big(\widehat{f}(t_i, z) - y_i\Big) \in \mathbb{R}^\ell. \tag{2.20}$$

Define the function $F : \mathbb{R}^\ell \to \mathbb{R}^\ell$ as $F := B \circ \Pi_\Omega \circ B^T$, which is also Lipschitz continuous and piecewise affine. It follows from the theory of piecewise smooth functions (e.g., [63]) that such a function admits an appealing geometric structure for its domain, which provides an alternative representation of the function. Specifically, let Ξ be a finite family of polyhedra $\{\mathcal{X}_i\}_{i=1}^{m_*}$, where each $\mathcal{X}_i := \{\, v \in \mathbb{R}^\ell \mid G_i v \geq h_i \,\}$ for a matrix G_i and a vector h_i. We call Ξ a *polyhedral subdivision* of $\mathbb{R}^\ell$ [23, 63] if

(a) the union of all polyhedra in Ξ is equal to $\mathbb{R}^\ell$, i.e., $\bigcup_{i=1}^{m_*} \mathcal{X}_i = \mathbb{R}^\ell$,

(b) each polyhedron in Ξ has a nonempty interior (thus is of dimension ℓ), and

(c) the intersection of any two polyhedra in Ξ is either empty or a common proper face of both polyhedra, i.e., $\mathcal{X}_i \cap \mathcal{X}_j \neq \emptyset \implies \big[\, \mathcal{X}_i \cap \mathcal{X}_j = \mathcal{X}_i \cap \{v \,|\, (G_i v - h_i)_\alpha = 0\} = \mathcal{X}_j \cap \{v \,|\, (G_j v - h_j)_\beta = 0\}$ for nonempty index sets α and β with $\mathcal{X}_i \cap \{v \,|\, (G_i v - h_i)_\alpha = 0\} \neq \mathcal{X}_i$ and $\mathcal{X}_j \cap \{v \,|\, (G_j v - h_j)_\beta = 0\} \neq \mathcal{X}_j \,\big]$.

For a Lipschitz PA function F, one can always find a polyhedral subdivision of $\mathbb{R}^\ell$ and finitely many affine functions $g_i(v) \equiv E_i v + l_i$ such that F coincides with one of the g_i's on each polyhedron in Ξ [23, Proposition 4.2.1] or [63]. Therefore, an alternative representation of F is given by

$$F(v) \;=\; E_i v + l_i, \quad \forall\, v \in \mathcal{X}_i, \qquad i = 1, \ldots, m_*,$$

and $v \in \mathcal{X}_i \cap \mathcal{X}_j \Longrightarrow E_i v + l_i = E_j v + l_j$.

Given $v \in \mathbb{R}^\ell$, define the index set $\mathcal{I}(v) := \{ i \,|\, v \in \mathcal{X}_i \}$. Moreover, given a direction vector $\widetilde{d} \in \mathbb{R}^\ell$, there exists $j \in \mathcal{I}(v)$ (dependent on $\widetilde{d}$) such that $F'(v; \widetilde{d}) = E_j \widetilde{d}$. (A more precise characterization of the directional derivative of the Euclidean projection is defined by the critical cone [23, Theorem 4.1.1], which shows that for a fixed v, $F'(v; \widetilde{d})$ is continuous and piecewise linear (PL) in $\widetilde{d}$.) In view of this and (2.19), we have that, for each fixed $t \in [t_k, t_{k+1})$ with $k = 1, \ldots, n-1$, there exists $j \in \mathcal{I}(e^{-A^T t} v_k(z))$ (dependent on d) such that

$$Bu_*'(t, z; d) \;=\; E_j e^{-A^T t} v_k'(z; d), \qquad \text{where} \quad v_k'(z; d) = \lambda^{-1} \sum_{i=1}^{k} w_i \big(C e^{A t_i} \big)^T \widehat{f}'(t_i, z; d). \tag{2.21}$$

For each fixed t, the matrix E_j not only depends on z, which is usually known, but also depends on the direction vector d that is unknown *a priori* in a numerical algorithm. This leads to great complexity and difficulty in solving the equation $H_{y,n}(z) + H_{y,n}'(z; d) = 0$ for a given z, where d is the unknown. In what follows, we identify an important case where $e^{-A^T t} v_k(z)$ is in the interior of some polyhedron $\mathcal{X}_j$ such that the matrix E_j relies on z (and t) but is independent of d.

For notational convenience, define

$$q(t, v) \;:=\; e^{-A^T t} v, \quad v \in \mathbb{R}^\ell,$$

which satisfies the linear ODE: $\dot{q}(t,v) = -A^T q(t,v)$. For a polyhedron $\mathcal{X}_i = \{v \,|\, G_i v \geq h_i\}$ in Ξ, define

$$\mathcal{Y}_i := \{v \in \mathbb{R}^\ell \,|\, (G_i v - h_i, G_i(-A^T)v, G_i(-A^T)^2 v, \ldots, G_i(-A^T)^\ell v) \succcurlyeq 0\},$$

where $\succcurlyeq$ denotes the lexicographical nonnegative order. For a given $v \in \mathbb{R}^\ell$, let the index set $\mathcal{J}(v) := \{i \,|\, v \in \mathcal{Y}_i\}$. Clearly, $\mathcal{J}(v) \subseteq \mathcal{I}(v)$ for any v. Furthermore, given a t_*, $q(t,v) \in \mathcal{X}_i$ for all $t \in [t_*, t_* + \varepsilon]$ for some $\varepsilon > 0$ if and only if $q(t_*, v) \in \mathcal{Y}_i$. We introduce more concepts as follows.

Definition 2.5.1. Let $q(t,v)$ and a time t_* be given. If $\mathcal{J}(q(t_*,v)) \neq \mathcal{I}(q(t_*,v))$, then we call t_* *a critical time* along $q(t,v)$ and its corresponding state $q(t_*,v)$ a *critical state*. Furthermore, if there exist $\varepsilon > 0$ and a polyhedron $\mathcal{X}_i$ in Ξ such that $q(t,v) \in \mathcal{X}_i, \forall\, t \in [t_* - \varepsilon, t_* + \varepsilon]$, then we call t_* a *non-switching-time* along $q(t,v)$; otherwise, we call t_* a *switching time* along $q(t,v)$.

It is known that a switching time must be a critical time but not vice versa [65]. Furthermore, a critical state must be on the boundary of a polyhedron in Ξ. The following result, which is a direct consequence of [65, Proposition 7], presents an extension of the so-called *non-Zenoness* of piecewise affine or linear systems (e.g., [9, 54, 66, 68]).

Proposition 2.5.1. *Consider $q(t,v)$ and a compact time interval $[t_*, t_*+T]$ where $T > 0$. Then there are finitely many critical times on $[t_*, t_*+T]$ along $q(t,v)$. Particularly, there exists a partition $t_* = \widehat{t}_0 < \widehat{t}_1 < \cdots < \widehat{t}_{M-1} < \widehat{t}_M = t_* + T$ such that for each $i = 0, 1, \ldots, M-1$, $\mathcal{I}(q(t,v)) = \mathcal{J}(q(t,v)) = \mathcal{J}(q(t',v)), \forall\, t \in (\widehat{t}_i, \widehat{t}_{i+1})$ for any $t' \in (\widehat{t}_i, \widehat{t}_{i+1})$.*

It follows from the above proposition that for any given v, there are finitely many critical times on the compact time interval $[t_k, t_{k+1}]$ along $q(t,v)$, where $k \geq 1$. We call

$q(t,v)$ *non-degenerate* on $[t_k, t_{k+1}]$ if, for any two consecutive critical times $\widehat{t}_j$ and $\widehat{t}_{j+1}$ on $[t_k, t_{k+1}]$, there exists an index i_* (dependent on $(\widehat{t}_j, \widehat{t}_{j+1})$) such that $\mathcal{I}(q(t,v)) = \{i_*\}$ for all $t \in (\widehat{t}_j, \widehat{t}_{j+1})$. In other words, $q(t,v)$ is non-degenerate if it is in the interior of some polyhedron of Ξ on the entire $(\widehat{t}_j, \widehat{t}_{j+1})$.

We introduce more notation and assumptions. First, it is clear that there exist constants $\rho_1 > 0$ and $\rho_2 > 0$ such that $\|Ce^{A(t-s)}\|_\infty \le \rho_1$ for all $t, s \in [0,1]$ and $\max_{i \in \{1,\dots,m_*\}} \|E_i\|_\infty \le \rho_2$. In addition, we assume that

H.2 there exist constants $\rho_t > 0$ and $\mu \ge \nu > 0$ such that for all n,

$$\max_{0 \le i \le n-1} |t_{i+1} - t_i| \le \frac{\rho_t}{n}, \qquad \frac{\nu}{n} \le w_i \le \frac{\mu}{n}, \quad \forall\, i.$$

Theorem 2.5.1. *Let Ω be a polyhedron in $\mathbb{R}^m$. Assume that* **H.1** $-$ **H.2** *hold and $\lambda \ge \mu^2 \rho_1^2 \rho_2 \rho_t / (4\nu)$. Given $z \in \mathbb{R}^\ell$, let $v_k(z)$ be defined as in (2.20). Suppose that $q(t, v_k(z)) = e^{-A^T t} v_k(z)$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, 2 \dots, n-1$. Then there exists a unique direction vector $d \in \mathbb{R}^\ell$ satisfying $H_{y,n}(z) + H'_{y,n}(z; d) = 0$.*

Proof. It follows from the non-degeneracy of $q(t, v_k(z))$ and Proposition 2.5.1 that, for the given z and each $[t_k, t_{k+1}]$ with $k = 1, \dots, n-1$, there exists a partition $t_k = \widehat{t}_{k,0} < \widehat{t}_{k,1} < \cdots < \widehat{t}_{k,M_k-1} < \widehat{t}_{k,M_k} = t_{k+1}$ such that for each $j = 0, \dots, M_k - 1$, $q(t, v_k(z))$ is in the interior of some polyhedron of Ξ for all $t \in (\widehat{t}_{k,j}, \widehat{t}_{k,j+1})$. It is easy to show via the continuity of $\widehat{f}(t,z)$ in z that for each open interval $(\widehat{t}_{k,j}, \widehat{t}_{k,j+1})$, there exists a matrix $E_{k,j} \in \{E_1, \dots, E_q\}$ such that for all $t \in (\widehat{t}_{k,j}, \widehat{t}_{k,j+1})$, $Bu'_*(t,z;d) = E_{k,j} e^{-A^T t} v'_k(z;d)$. Letting $\widetilde{w}_i := w_i/\lambda, i = 1, \dots, n$ and by (2.21), we have, for $r \ge k+1$,

$$\int_{t_k}^{t_{k+1}} Ce^{A(t_r - s)} Bu'_*(s,z;d) ds$$

$$
\begin{aligned}
&= \int_{t_k}^{t_{k+1}} Ce^{A(t_r-s)} \left(\sum_{j=0}^{M_k-1} E_{k,j} \cdot \mathbf{I}_{[\widehat{t}_{k,j}, \widehat{t}_{k,j+1}]} \right) e^{-A^T s} v_k'(z;d) ds \\
&= \int_{t_k}^{t_{k+1}} Ce^{A(t_r-s)} \left(\sum_{j=0}^{M_k-1} E_{k,j} \cdot \mathbf{I}_{[\widehat{t}_{k,j}, \widehat{t}_{k,j+1}]} \right) e^{-A^T s} \sum_{i=1}^{k} \widetilde{w}_i \big(Ce^{At_i} \big)^T \widehat{f}'(t_i, z; d) ds \\
&= \sum_{i=1}^{k} \widetilde{w}_i \left\{ \int_{t_k}^{t_{k+1}} Ce^{A(t_r-s)} \left(\sum_{j=0}^{M_k-1} E_{k,j} \cdot \mathbf{I}_{[\widehat{t}_{k,j}, \widehat{t}_{k,j+1}]} \right) \big(Ce^{A(t_i-s)} \big)^T ds \right\} \widehat{f}'(t_i, z; d) \\
&= \sum_{i=1}^{k} \widetilde{w}_i \, V_{(r,k,i),z} \, \widehat{f}'(t_i, z; d),
\end{aligned}
$$

where, for each $i = 1, \ldots, k$,

$$
V_{(r,k,i),z} \; := \; \int_{t_k}^{t_{k+1}} Ce^{A(t_r-s)} \left(\sum_{j=0}^{M_k-1} E_{k,j} \cdot \mathbf{I}_{[\widehat{t}_{k,j}, \widehat{t}_{k,j+1}]} \right) \big(Ce^{A(t_i-s)} \big)^T ds \; \in \; \mathbb{R}^{p \times p}.
$$

Note that for a fixed triple (r, k, i), $V_{(r,k,i),z}$ depends on z only and $r > k \geq i \geq 1$. For $r > i \geq 1$, define $W_{(r,i),z} := \widetilde{w}_i \sum_{j=i}^{r-1} V_{(r,j,i),z}$. Therefore, for each $k = 1, \ldots, n-1$,

$$
\begin{aligned}
\widehat{f}'(t_{k+1}, z; d) &= Ce^{At_{k+1}} d + \sum_{j=1}^{k} \int_{t_j}^{t_{j+1}} Ce^{A(t_{k+1}-s)} B u_*'(s, z; d) ds \\
&= Ce^{At_{k+1}} d + \sum_{j=1}^{k} \sum_{i=1}^{j} \widetilde{w}_i \, V_{(k+1,j,i),z} \, \widehat{f}'(t_i, z; d) \\
&= Ce^{At_{k+1}} d + \sum_{i=1}^{k} W_{(k+1,i),z} \, \widehat{f}'(t_i, z; d).
\end{aligned}
$$

In what follows, we drop z in the subscript of W for notational simplicity. In view of $\widehat{f}'(t_1, z; d) = Ce^{At_1} d$, it can be shown via induction that for each $k = 2, \ldots, n$,

$$
\begin{aligned}
&\widehat{f}'(t_k, z; d) \\
&\quad = Ce^{At_k} d + W_{(k,k-1)} Ce^{At_{k-1}} d + \Big(W_{(k,k-2)} + W_{(k,k-1)} W_{(k-1,k-2)} \Big) Ce^{At_{k-2}} d \\
&\quad + \qquad \cdots \qquad \cdots \qquad + \quad \cdots \qquad\qquad \cdots
\end{aligned}
$$

$$
\begin{aligned}
&+ \quad \Bigg(W_{(k,1)} + W_{(k,s)} W_{(s,1)} + \sum_{s_1=3}^{k-1} \sum_{s_2=2}^{s_1-1} W_{(k,s_1)} W_{(s_1,s_2)} W_{(s_2,1)} + \cdots \\
&\qquad \cdots \quad \cdots \cdots \; + W_{(k,k-1)} W_{(k-1,k-2)} \cdots W_{(3,2)} W_{(2,1)} \Bigg) C e^{At_1} d \\
&= \sum_{j=1}^{k} \widetilde{W}_{(k,j)} \, C e^{At_j} d,
\end{aligned}
$$

where the matrices $\widetilde{W}_{(k,j)}$ of order p are defined in terms of $W_{(k,s)}$ as shown above.

For a given $r \in \{1, \ldots, n\}$, define

$$
\mathbf{C}_r := \begin{pmatrix} Ce^{At_1} \\ Ce^{At_2} \\ \vdots \\ Ce^{At_r} \end{pmatrix} \in \mathbb{R}^{rp \times \ell}, \qquad \text{and}
$$

$$
\mathbf{W}_r := \operatorname{diag}(w_1 I_p, \ldots, w_r I_p) \begin{bmatrix} I_p & & & & \\ \widetilde{W}_{(2,1)} & I_p & & & \\ \widetilde{W}_{(3,1)} & \widetilde{W}_{(3,2)} & I_p & & \\ \vdots & \vdots & \ddots & \ddots & \\ \widetilde{W}_{(r,1)} & \widetilde{W}_{(r,2)} & \cdots & \widetilde{W}_{(r,r-1)} & I_p \end{bmatrix} \in \mathbb{R}^{rp \times rp}, \tag{2.22}
$$

where I_p is the identity matrix of order p and $\mathbf{W}_r$ depends on z but is independent of d. Hence, the directional derivative of $\sum_{i=1}^{r} w_i (Ce^{At_i})^T \big(\widehat{f}(t_i, z) - y_i\big)$ along the direction vector d is given by

$$
\sum_{i=1}^{r} w_i \big(Ce^{At_i}\big)^T \widehat{f}'(t_i, z; d) \; = \; \mathbf{C}_r^T \, \mathbf{W}_r \, \mathbf{C}_r \, d.
$$

Clearly, $\mathbf{W}_r$ is invertible for any r, and it can be easily verified via the property of $\widetilde{W}_{(k,j)}$ that

$$\mathbf{W}_r^{-1} = \begin{bmatrix} I_p & & & & \\ -W_{(2,1)} & I_p & & & \\ -W_{(3,1)} & -W_{(3,2)} & I_p & & \\ \vdots & \vdots & \ddots & \ddots & \\ -W_{(r,1)} & -W_{(r,2)} & \cdots & -W_{(r,r-1)} & I_p \end{bmatrix} \operatorname{diag}(w_1^{-1} I_p, \ldots, w_r^{-1} I_p).$$

Moreover, define the symmetric matrix

$$\mathbf{V}_r := \frac{1}{2}\left(\mathbf{W}_r^{-1} + \left(\mathbf{W}_r^{-1}\right)^T\right) = \begin{bmatrix} \frac{I_p}{w_1} & -\frac{W_{(2,1)}}{2w_1} & -\frac{W_{(3,1)}}{2w_1} & \cdots & -\frac{W_{(r,1)}}{2w_1} \\ -\frac{W_{(2,1)}}{2w_1} & \frac{I_p}{w_2} & -\frac{W_{(3,2)}}{2w_2} & \cdots & -\frac{W_{(r,2)}}{2w_2} \\ -\frac{W_{(3,1)}}{2w_1} & -\frac{W_{(3,2)}}{2w_2} & \frac{I_p}{w_3} & \ddots & \vdots \\ \vdots & \vdots & \ddots & \ddots & -\frac{W_{(r,r-1)}}{2w_{r-1}} \\ -\frac{W_{(r,1)}}{2w_1} & -\frac{W_{(r,2)}}{2w_2} & \cdots & -\frac{W_{(r,r-1)}}{2w_{r-1}} & \frac{I_p}{w_r} \end{bmatrix}.$$

It follows from assumption **H.2** that $\max_i \widetilde{w}_i \le \mu/(\lambda n)$ and that for any $1 \le j < k$,

$$\|W_{(k,j)}\|_\infty \le \frac{\mu}{\lambda n}\int_{t_j}^{t_k} \rho_1^2 \rho_2 d\tau \le \frac{\mu \rho_1^2 \rho_2}{\lambda n} \cdot \frac{\rho_t (k-j)}{n}.$$

Furthermore, we deduce from **H.2** that $\max_{i,j} \frac{w_i}{w_j} \le \mu/\nu$. Therefore, for any fixed $k = 1, \ldots, n$,

$$w_k \left(\sum_{i=1}^{k-1} \left\| \frac{W_{(k,i)}}{2w_i} \right\|_\infty + \sum_{i=k+1}^{n} \left\| \frac{W_{(i,k)}}{2w_k} \right\|_\infty \right) \le \frac{\mu^2 \rho_1^2 \rho_2 \rho_t}{2\lambda\nu\, n^2} \left(\sum_{i=1}^{k-1} (k-i) + \sum_{i=k+1}^{n} (i-k) \right)$$
$$\le \frac{\mu^2 \rho_1^2 \rho_2 \rho_t}{2\lambda\nu\, n^2} \sum_{i=1}^{n-1} i \le \frac{\mu^2 \rho_1^2 \rho_2 \rho_t\, (n-1)}{4\lambda\nu\, n} < 1,$$

where the last inequality follows from the assumption on λ. This implies that the symmetric matrix $\mathbf{V}_r$ is strictly diagonally dominant for any r. Hence, for each r, $\mathbf{V}_r$ is positive definite, so are $\mathbf{W}_r^{-1}$ and $\mathbf{W}_r$ (although not symmetric).

Finally, note that $H'_{y,n}(z; d) = \mathbf{C}_n^T \mathbf{W}_n \mathbf{C}_n d$, and $\mathbf{C}_n$ has full column rank, in light of the assumption **H.1**. Consequently, $\mathbf{C}_n^T \mathbf{W}_n \mathbf{C}_n$ is positive definite such that the unique direction vector $d = -\big(\mathbf{C}_n^T \mathbf{W}_n \mathbf{C}_n\big)^{-1} H_{y,n}(z)$ solves the equation $H_{y,n}(z) + H'_{y,n}(z; d) = 0$. □

The above result relies on the critical non-degenerate property of $q(t, v_k(z))$. In what follows, we consider the case where $q(t, v_k(z))$ is degenerate on some sub-interval of $[t_k, t_{k+1}]$. Geometrically, this implies that the trajectory of $q(t, v_k(z))$ travels on a face of a polyhedron in Ξ for some time. It shall be shown that under mild assumptions, a suitable small perturbation of z will lead to a non-degenerate trajectory. Recall that each polyhedron $\mathcal{X}_i$ in the polyhedral subdivision Ξ is defined by the matrix $G_i \in \mathbb{R}^{m_i}$ and the vector $h_i \in \mathbb{R}^{m_i}$. Since each $\mathcal{X}_i$ has non-empty interior, we assume, without loss of generality, that for each $j = 1, \ldots, m_i$, the set $\{v \in \mathcal{X}_i \,|\, (G_i v - h_i)_j = 0\}$ represents a (unique) facet of $\mathcal{X}_i$ (i.e., a $(\ell - 1)$-dimensional face of $\mathcal{X}_i$) [63, Proposition 2.1.3], where $(G_i)_{j\bullet}$ denotes the jth row of G_i and satisfies $\|(G_i)_{j\bullet}^T\|_2 = 1$.

Proposition 2.5.2. *Let Ω be a polyhedron in $\mathbb{R}^m$. For a given $z \in \mathbb{R}^\ell$, suppose that $q(t, v_k(z))$ is degenerate on the interval $[t_k, t_{k+1}]$ for some $k \in \{1, \ldots, n-1\}$, where $v_k(z)$ is defined in (2.20). Assume that (C, A) is an observable pair,* **H.1** – **H.2** *hold, and $\lambda \geq \mu^2 \rho_1^2 \rho_2 \rho_t / (4\nu)$. Then for any $\varepsilon > 0$, there exists $d \in \mathbb{R}^\ell$ with $0 < \|d\| \leq \varepsilon$ such that $q(t, v_k(z + d))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, \ldots, n-1$.*

Proof. Fix $\varepsilon > 0$. Define the set of vector-scalar pairs that represent all the facets of the polyhedra in Ξ:

$$\mathcal{S} := \Big\{ \big((G_i)^T_{j\bullet}, (h_i)_j\big) \,|\, i = 1, \ldots, m_*, \; j = 1, \ldots, m_i \Big\}.$$

Note that if $q(t, v_k(z))$ is degenerate on $[t_k, t_{k+1}]$ for some k, then there exist a pair $(g, \alpha) \in \mathcal{S}$ and an open subinterval $\mathcal{T} \subset [t_k, t_{k+1}]$ such that $g^T q(t, v_k(z)) - \alpha = 0$ for all $t \in \mathcal{T}$, which is further equivalent to $g^T q(t, v_k(z)) - \alpha = 0$ for all $t \in [t_k, t_{k+1}]$ in view of $q(t, v_k(z)) = e^{-A^T t} v_k(z)$. Therefore, we define for each $k \in \{1, \ldots, n-1\}$, $\mathcal{S}_{z,k,D} := \{(g, \alpha) \in \mathcal{S} \,|\, g^T q(t, v_k(z)) = \alpha, \, \forall \, t \in [t_k, t_{k+1}]\}$.

Let k_1 be the smallest k such that $\mathcal{S}_{z,k,D}$ is nonempty (or equivalently $q(t, v_k(z))$ is degenerate on $[t_k, t_{k+1}]$). Clearly, $k \geq 1$. Since $q(t, v_k(z))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, \ldots, k_1 - 1$, it follows from a similar argument in the proof of Theorem 2.5.1 that $v'_{k_1}(z; d) = \lambda^{-1} \mathbf{C}^T_{k_1} \mathbf{W}_{k_1,z} \mathbf{C}_{k_1} d$, where we write $\mathbf{W}_{k_1}$ as $\mathbf{W}_{k_1,z}$ to emphasize its dependence on z (but independent of d). Consider the following two cases:

(i) $(g, \alpha) \in \mathcal{S}_{z,k_1,D}$. It follows from the B-differentiability of $v_{k_1}(\cdot)$ that $q(t, v_{k_1}(z+d)) = q(t, v_{k_1}(z)) + q\big(t, v'_{k_1}(z; d) + o(\|d\|)\big)$ for each $t \in [t_{k_1}, t_{k_1+1}]$ [23, Proposition 3.1.3]. Therefore, using the fact that $\|g\|_2 = 1$, we have for each $t \in [t_{k_1}, t_{k_1+1}]$,

$$\begin{aligned} g^T q(t, v_{k_1}(z+d)) - \alpha &= \big(g^T q(t, v_{k_1}(z)) - \alpha\big) + g^T q\big(t, v'_{k_1}(z; d) + o(\|d\|)\big) \\ &= g^T q\big(t, v'_{k_1}(z; d)\big) + o(\|d\|). \end{aligned}$$

Furthermore, under **H.2** and the assumption on λ, it is shown in Theorem 2.5.1 that $\mathbf{W}_{k_1,z}$ is positive definite. Let the observability matrix

$$V_g := \begin{pmatrix} g^T \\ g^T A^T \\ \vdots \\ g^T (A^T)^{\ell-1} \end{pmatrix} \in \mathbb{R}^{\ell \times \ell}.$$

Since $g^T q(t, v'_{k_1}(z; d)) = g^T e^{-A^T t} \mathbf{C}_{k_1}^T \mathbf{W}_{k_1,z} \mathbf{C}_{k_2} d$, we see that $g^T q(t, v'_{k_1}(z; d))$ is nonvanishing on $[t_{k_1}, t_{k_1+1}]$ if and only if $d \notin \mathrm{Ker}(V_g \mathbf{C}_{k_1}^T \mathbf{W}_{k_1,z} \mathbf{C}_{k_1})$. Since g is nonzero, $\mathbf{W}_{k_1,z}$ is positive definite, and (C, A) is an observable pair, it is easy to show that $V_g \mathbf{C}_{k_1}^T \mathbf{W}_{k_1,z} \mathbf{C}_{k_1} \neq 0$ such that $\mathrm{Ker}(V_g \mathbf{C}_{k_1}^T \mathbf{W}_{k_1,z} \mathbf{C}_{k_1})$ is a proper subspace of $\mathbb{R}^\ell$. Hence there exists a scalar $\tau > 0$ such that for any $d \notin \mathrm{Ker}(V_g \mathbf{C}_{k_1}^T \mathbf{W}_{k_1,z} \mathbf{C}_{k_1})$ with $0 < \|d\| \leq \tau$, $g^T q(t, v'_{k_1}(z; d))$, and thus $g^T q(t, v_{k_1}(z + d)) - \alpha$, is nonvanishing on $[t_{k_1}, t_{k_1+1}]$, which further implies that $g^T q(t, v_{k_1}(z + d)) - \alpha$ has at most finitely many zeros on $[t_{k_1}, t_{k_1+1}]$.

(ii) $(g, \alpha) \in \mathcal{S} \backslash \mathcal{S}_{z,k_1,D}$. This means that there exists $t_* \in [t_{k_1}, t_{k_1+1}]$ such that $g^T q(t_*, v_{k_1}(z + d)) - \alpha \neq 0$. Due to the continuity of $v_{k_1}(z)$, we see that there exists $\tau > 0$ such that if $\|d\| \leq \tau$, then $g^T q(t_*, v_{k_1}(z + d)) - \alpha \neq 0$, which also implies that $g^T q(t, v_{k_1}(z + d)) - \alpha$ has at most finitely many zeros on $[t_{k_1}, t_{k_1+1}]$. Similarly, we see that for each $k = 1, \ldots, k_1 - 1$ and each $(g, \alpha) \in \mathcal{S}$, $g^T q(t, v_k(z + d)) - \alpha$ has at most finitely many zeros on $[t_{k_1}, t_{k_1+1}]$.

By virtue of the finiteness of $\mathcal{S}$ and the above results, we obtain a finite union of proper subspaces of $\mathbb{R}^\ell$ denoted by S and a constant $\eta > 0$ such that for each $(g, \alpha) \in \mathcal{S}$

and any $d \notin S$ with $0 < \|d\| \le \eta$, $g^T q(t, v_k(z+d)) - \alpha$ has at most finitely many zeros on $[t_k, t_{k+1}]$ for each $k = 1, \dots, k_1$. Since $g^T q(t, v_k(z+d)) - \alpha \neq 0$ for all but finitely many times in $[t_k, t_{k+1}]$ with $k = 1, \dots, k_1$ for all $(g, \alpha) \in \mathcal{S}$, we conclude that except finitely many times in $[t_k, t_{k+1}]$, $q(t, v_k(z+d))$ must be in the interior of some polyhedron in Ξ at each $t \in [t_k, t_{k+1}]$, where $k = 1, \dots, k_1$. This shows that $q(t, v_k(z+d))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, \dots, k_1$. In particular, we can choose a nonzero vector d^1 with $\|d^1\| \le \varepsilon/n$ satisfying this condition.

Now define $\widetilde{z}^1 := z + d^1$, and let k_2 be the smallest k such that $\mathcal{S}_{\widetilde{z}^1,k,D}$ is nonempty. Clearly, $k_2 \ge k_1 + 1$. By replacing z with $\widetilde{z}^1$ in the preceding proof, we deduce via a similar argument that there exists a nonzero vector d^2 with $\|d^2\| \le \min(\varepsilon/n, \|d^1\|/4)$ such that $q(t, v_k(\widetilde{z}^1 + d^2))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, \dots, k_2$. Continuing this process and using induction, we obtain at most $(n-1)$ nonzero vectors d^j with $\|d^j\| \le \min(\varepsilon/n, \|d^1\|/2^j)$ for $j \ge 2$ and $d^* := \sum_j d^j$ such that $q(t, v_k(z + d^*))$ is non-degenerate on $[t_k, t_{k+1}]$ for each $k = 1, \dots, n-1$. Obviously $\|d^*\| \le \varepsilon$. Furthermore, by virue of $\| \sum_{j \ge 2} d^j \| \le \|d^1\|/2$, we conclude that $d^* \neq 0$. □

We are now ready to present the modified nonsmooth Newton's algorithm. Let the merit function $g : \mathbb{R}^\ell \to \mathbb{R}_+$ be given by $g(z) := \frac{1}{2} H_{y,n}^T(z) H_{y,n}(z)$. Then g is B-differentiable and $g'(z; d) = H_{y,n}^T(z) H'_{y,n}(z; d)$. The numerical procedure of this algorithm is described in Algorithm 1.

Finally, we establish the global convergence of Algorithm 1 under suitable assumptions.

Theorem 2.5.2. *Let Ω be a polyhedron in $\mathbb{R}^m$. If (C, A) is an observable pair, the assumptions in Theorem 2.5.1 hold, and $\liminf_k \beta^{m_k} > 0$, then the sequence (z^k) generated by Algorithm 1 has an accumulation point that is a solution to the equation $H_{y,n}(z) = 0$.*

Algorithm 1 Modified Nonsmooth Newton's Method with Line Search

Choose scalars $\beta \in (0,1)$ and $\gamma \in (0, \frac{1}{2})$;
Initialize $k = 0$ and choose an initial vector $z^0 \in \mathbb{R}^\ell$ such that $q(t, v_j(z^0))$ is nondegenerate on each $[t_j, t_{j+1}]$;
repeat
  $k \leftarrow k+1$;
  Find a direction vector d^k such that $H_{y,n}(z^{k-1}) + H'_{y,n}(z^{k-1}; d^k) = 0$;
  Let m_k be the first nonnegative integer m for which $g(z^{k-1}) - g(z^{k-1} + \beta_k^m d^k) \geq -\gamma \beta_k^m g'(z^{k-1}; d^k)$;
  $z^k \leftarrow z^{k-1} + \beta^{m_k} d^k$;
  if $q(t, v_j(z^k))$ is degenerate on some $[t_j, t_{j+1}]$ **then**
    Choose $d' \in \mathbb{R}^\ell$ with sufficiently small $\|d'\| > 0$ such that $q(t, v_j(z^k + d'))$ is nondegenerate on each $[t_j, t_{j+1}]$;
    $z^k \leftarrow z^k + d'$;
  end if
until $g(z^k)$ is sufficiently small
return z^k

Proof. Let (z^k) be a sequence generated by Algorithm 1 from an initial vector $z^0 \in \mathbb{R}^\ell$; the existence of (z^k) is due to Theorem 2.5.1 and Proposition 2.5.2. Without loss of generality, we assume that $H_{y,n}(z^k) \neq 0$ for each k. Letting d' be the perturbation vector in the algorithm in case of degeneracy, we have $g(z^{k-1}) - g(z^k - d') \geq \sigma \beta^{m_k} \|H_{y,n}(z^k - d')\|_2^2$. Since $\|d'\|$ can be arbitrarily small and $H_{y,n}$ and g are continuous, it follows from an argument similar to that in the proof of [53, Theorem 4] that $g(z^{k-1}) - g(z^k) \geq \sigma \beta^{m_k} \Big(\|H_{y,n}(z^k)\|_2^2 + o(\|H_{y,n}(z^k)\|_2^2) \Big)$. Hence, $\big(g(z^k)\big)$ is a nonnegative and strictly decreasing sequence. This also shows, in view of Proposition 2.4.3, that the sequence (z^k) is bounded and thus has an accumulation point. Furthermore, $\big(g(z^k)\big)$ converges and $\lim_{k\to\infty}(\beta^{m_k}\|H_{y,n}(z^k)\|_2^2 + \varepsilon_k) = 0$, where each $|\varepsilon_k|$ is arbitrarily small by choosing small $\|d'\|$. (For example, $|\varepsilon_k|$ can be of order $o(\|H_{y,n}(z^k)\|_2^2)$ by choosing a suitable d'.) Hence, if $\liminf_k \beta^{m_k} > 0$, then an accumulation point of (z^k) is the desired solution to the B-differentiable equation $H_{y,n}(z) = 0$. $\square$

2.6 Numerical Examples

In this section, three nontrivial numerical examples are given to demonstrate the performance of the shape constrained smoothing spline and the proposed nonsmooth Newton's method. Recall the inductive procedure for computing $u_*(t, x_0^*)$ and $\widehat{f}(t, x_0^*)$ from the discussion following Corollary 2.3.1. For a given $z \in \mathbb{R}^\ell$, we may compute $u_*(t, z)$ and $\widehat{f}(t, z)$ on $[t_k, t_{k+1})$ and $[t_k, t_{k+1}]$ respectively using the same process. Additionally, given $\widehat{f}(t_i, z)$ for $i = 1, \ldots, k$, we may numerically represent $u_*(t, z)$ on $[t_k, t_{k+1}]$ by (i) computing $u_*(t, z)$ at a discrete set of points between t_k and t_{k+1}, in order to determine where $u_*(t, z)$ crosses the boundary of Ω, and (ii) representing $u_*(t, z)$ analytically between the points at which we determine it crosses the boundary. We then compute $\widehat{f}(t_{k+1}, z)$ given this representation of $u_*(t, z)$ analytically using (2.17), where we replace x_0^* with z. This procedure is used to compute $u_*(t, z)$ and $\widehat{f}(t, z)$ when the nonsmooth Newton's method is implemented for each of these numerical examples.

In the following examples, the underlying true function $f : [0, 1] \to \mathbb{R}$ is defined by $A \in \mathbb{R}^{2\times2}$, $B = (0, 1)^T$, $C = (1, 0)$, a true initial state x_0, and a true control function $u \in L_2([0, 1], \mathbb{R})$ with the control constraint set $\Omega \subset \mathbb{R}$. The sample data (y_i) is generated by $y_i = f(t_i) + \varepsilon_i$, where (ε_i) is an iid zero mean random error with variance σ^2. The weights w_i are chosen as $w_i = 1/n$ for each $i = 1, \ldots, n$ in all cases. Furthermore, different choices of (possibly unevenly spaced) design points (t_i) are considered in order to illustrate flexibility of the proposed algorithm.

In what follows, the true underlying function f, the corresponding matrix A, the true control u, the design points t_i, the true initial state x_0, the guess of the initial condition z^0 in the algorithm, the variance σ, and the penalty parameter λ are given for each example.

It is easy to verify that (C, A) is an observable pair, and that the assumptions **H.1** and **H.2** hold in each example.

Example 2.6.1. The convex constraint with unevenly spaced design points:

$$f(t) = \left(\tfrac{4}{3}t^3 - t + 1\right) \cdot \mathbf{I}_{[0,\frac{1}{2})} + \left(-\tfrac{8}{3}t^3 + 6t^2 - 4t + \tfrac{3}{2}\right) \cdot \mathbf{I}_{[\frac{1}{2},\frac{3}{4})} + \left(\tfrac{1}{2}t + \tfrac{3}{8}\right) \cdot \mathbf{I}_{[\frac{3}{4},1]},$$

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \quad x_0 = (1, -1)^T, \quad u(t) = 8t \cdot \mathbf{I}_{[0,\frac{1}{2})} + (12 - 16t) \cdot \mathbf{I}_{[\frac{1}{2},\frac{3}{4})},$$

$\Omega = [0, \infty)$, $z^0 = (2, 3)^T$, $\sigma = 0.1$, $\lambda = 10^{-4}$, and the design points $\left(t_i\right)_{i=0}^n =$

$$\left\{0, \frac{1}{2n}, \ldots, \frac{1}{20}, \frac{1}{20} + \frac{4}{3n}, \ldots, \frac{9}{20}, \frac{9}{20} + \frac{1}{2n}, \ldots, \frac{11}{20}, \frac{11}{20} + \frac{1}{2n}, \ldots, \frac{19}{20}, \frac{19}{20} + \frac{1}{2n}, \ldots, 1\right\}.$$

Example 2.6.2. The unbounded control constraint with unevenly spaced designed points:

$$f(t) = \begin{cases} 11.610t(e^{-t} + e^{-2t}) - 27.219e^{-t} + 25.219e^{-2t} + 2 & \text{if } t \in [0, \frac{1}{4}) \\ -6.234e^{-t} + 3.257e^{-2t} + 3 & \text{if } t \in [\frac{1}{4}, \frac{1}{2}) \\ -11.610t(e^{-t} + e^{-2t}) + 18.222e^{-t} - 21.692e^{-2t} + 3 & \text{if } t \in [\frac{1}{2}, \frac{3}{4}) \\ -3.345e^{-t} + 1.306e^{-2t} + 2 & \text{if } t \in [\frac{3}{4}, 1] \end{cases}$$

$$A = \begin{bmatrix} 0 & 1 \\ -2 & -3 \end{bmatrix}, \; x_0 = (7/2, -7)^T, \; u(t) = \begin{cases} 23.219(e^{-t} - e^{-2t}) + 8 & \text{if } t \in [0, \frac{1}{4}) \\ 12 & \text{if } t \in [\frac{1}{4}, \frac{1}{2}) \\ -38.282e^{-t} + 63.117e^{-2t} + 6 & \text{if } t \in [\frac{1}{2}, \frac{3}{4}) \\ 8 & \text{if } t \in [\frac{3}{4}, 1] \end{cases}$$

$\Omega = [8, \infty)$, $z^0 = (0, 1/2)^T$, $\sigma = 0.2$, $\lambda = 10^{-4}$, and the design points

$$\left(t_i\right)_{i=0}^n = \left\{0, \frac{1}{2n}, \frac{2}{2n}, \ldots, \frac{1}{20}, \frac{1}{20} + \frac{9}{8n}, \ldots, \frac{19}{20}, \frac{19}{20} + \frac{1}{2n}, \ldots, 1\right\}.$$

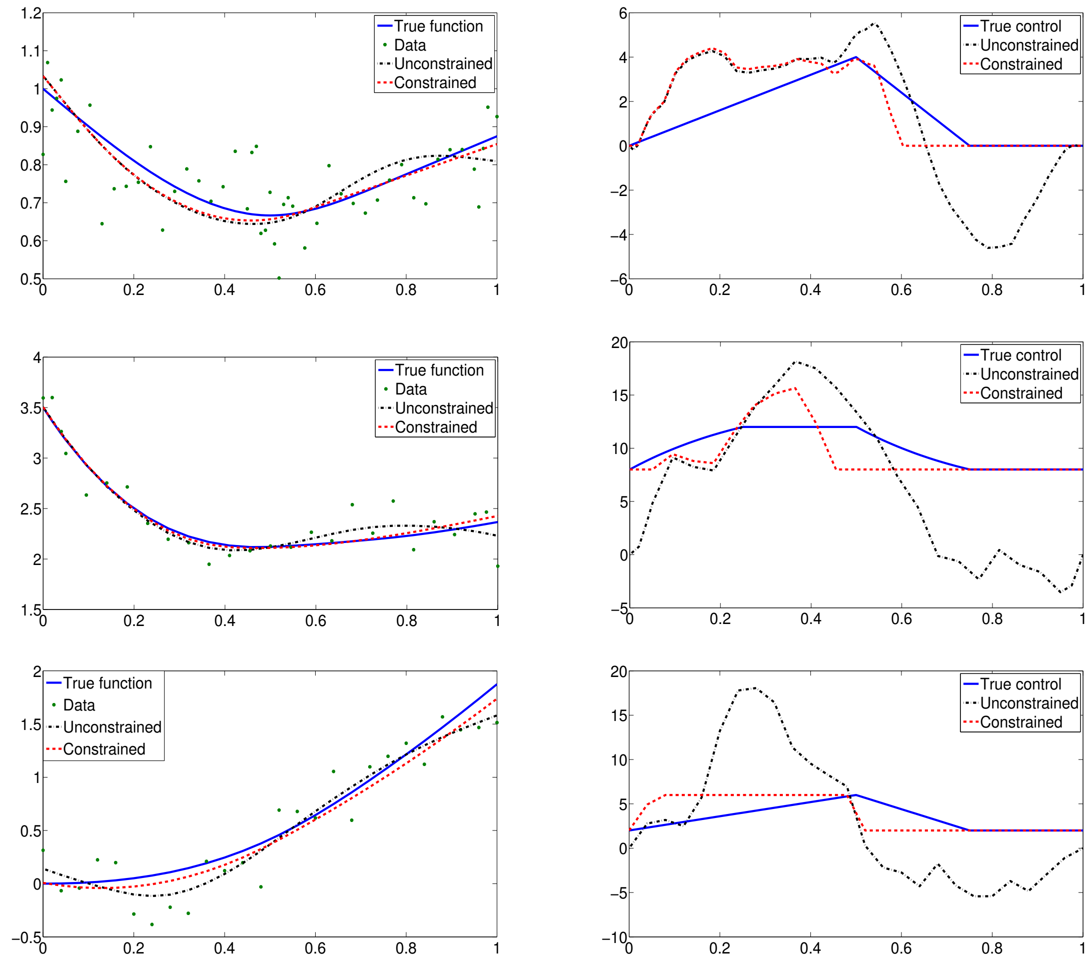


Figure 2.1: Left column: spline performance of Examples 2.6.1 (top), 2.6.2 (middle), and 2.6.3 (bottom); right column: the corresponding control performance of Examples 2.6.1–2.6.3.

Example 2.6.3. The bounded control constraint with evenly spaced designed points:

$$f(t) \;=\; \big(\tfrac{4}{3}t^3 + t^2\big)\cdot \mathbf{I}_{[0,\frac{1}{2})} + \big(-\tfrac{8}{3}t^3 + 7t^2 - 3t + \tfrac{1}{2}\big)\cdot \mathbf{I}_{[\frac{1}{2},\frac{3}{4})} + \big(t^2 + \tfrac{3}{2}t - \tfrac{5}{8}\big)\cdot \mathbf{I}_{[\frac{3}{4},1]},$$

$$A = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix}, \qquad x_0 = (0,0)^T, \qquad u(t) = (8t+2)\cdot \mathbf{I}_{[0,\frac{1}{2})} + (14-16t)\cdot \mathbf{I}_{[\frac{1}{2},\frac{3}{4})} + 2\cdot \mathbf{I}_{[\frac{3}{4},1]},$$

$$\Omega = [2,6], \quad z^0 = (2,3)^T, \quad \sigma = 0.3, \quad \lambda = 10^{-4}, \text{ and evenly spaced design points } t_i = \tfrac{i}{n}.$$

The proposed nonsmooth Newton's algorithm is used to compute the shape constrained smoothing splines for the three examples. In all cases, we choose $\beta = 0.25$ and $\gamma = 0.1$ in Algorithm 1 with the terminating tolerance as 10^{-6}. The numerical results for Example 2.6.1 with $n = 50$, Example 2.6.2 with $n = 25$, and Example 2.6.3 with $n = 25$

Table 2.1: Number of Iterations to Convergence for Nonsmooth Newton's Method

	sample size	min	max	mean	median
Example 1	$n = 25$	4	58	24.9	26
	$n = 50$	3	40	28.3	30
	$n = 100$	4	44	30.1	32
Example 2	$n = 25$	2	159	26.8	15
	$n = 50$	2	127	25.7	17
	$n = 100$	2	117	25.0	17
Example 3	$n = 25$	1	51	12.6	9
	$n = 50$	1	67	17.3	13
	$n = 100$	4	67	22.2	19

are displayed in Figure 2.1. For comparison, the unconstrained smoothing splines are also shown in Figure 2.1. The number of iterations for numerical convergence of the proposed nonsmooth Newton's algorithm ranges from a single digit to 160 with the median between 9 and 34 (depending on system parameters, sample data and size, and initial state guesses). A more detailed description for the number of iterations to convergence for 200 different numerical simulations is given in Table 2.1. It is observed that the proposed nonsmooth Newton's algorithm converges superlinearly overall.

To further compare the performance of constrained smoothing splines and unconstrained smoothing splines, simulations were run 200 times, and the average performance over these simulations was recorded in each case. Three performance metrics are considered, namely, the L_2-norm, the L_∞-norm, and the 2-norm of the difference between the true and computed initial conditions. Table 2.2 summarizes the spline performance of the two splines for different sample sizes, where $\widehat{f}$ denotes the computed smoothing splines and $\widehat{x}_0$ denotes the computed initial condition. It is seen in the above examples that the shape constrained smoothing spline usually outperforms its unconstrained counterpart. It should be pointed out that the performance of shape constrained smoothing splines criti-

Table 2.2: Performance of Constrained (constr.) Splines vs. Unconstrained Splines

		$\|f-\widehat{f}\|_{L_2}$		$\|f-\widehat{f}\|_{L_\infty}$		$\|x_0-\widehat{x}_0\|_2$	
Example	sample size	constr.	unconstr.	constr.	unconstr.	constr.	unconstr.
Ex. 2.6.1	$n=25$	0.00696	0.00723	0.06809	0.07216	0.25985	0.30825
	$n=50$	0.00351	0.00362	0.04971	0.05218	0.19141	0.22549
	$n=100$	0.00177	0.00180	0.03487	0.03588	0.14021	0.15958
Ex. 2.6.2	$n=25$	0.01302	0.01492	0.12639	0.15609	0.76778	1.45583
	$n=50$	0.00704	0.00791	0.09998	0.12474	0.70899	1.41832
	$n=100$	0.00387	0.00436	0.08048	0.10519	0.75410	1.54277
Ex. 2.6.3	$n=25$	0.01728	0.02138	0.16761	0.22974	0.44519	0.97093
	$n=50$	0.00912	0.01074	0.13525	0.16891	0.36184	0.67901
	$n=100$	0.00463	0.00531	0.09601	0.12063	0.31549	0.61803

cally depends on the penalty parameter λ, the weights w_i, the control constraint set Ω, and the function class that the true function belongs to. Detailed discussions of performance issues will be addressed in the future.

2.7 Summary

Smoothing splines subject to general linear dynamics and control constraints are studied. Such constrained smoothing splines are formulated as finite-horizon constrained optimal control problems with unknown initial state and control. Optimality conditions are derived using Hilbert space methods and variational techniques. To compute the constrained smoothing splines, the optimality conditions are converted to a nonsmooth B-differentiable equation, and a modified nonsmooth Newton's algorithm with line search is proposed to solve the equation. Detailed convergence analysis of this algorithm is given for a polyhedral control constraint, and numerical examples demonstrate the effectiveness of the algorithm.

CHAPTER III

Nonnegative Derivative Constrained B-spline Estimator: Uniform Lipschitz Property

The next three chapters, i.e., Chapters III–V, are devoted to the nonparametric estimation of functions subject to nonnegative derivative constraints. Moreover, attention is given to the asymptotic performance (measured using the supremum-norm) of a certain constrained B-spline estimator. In Chapter III, a critical *uniform Lipschitz* property is established for this estimator; this uniform Lipschitz property is crucial in the study of the constrained B-spline estimator performance analysis. Chapter IV provides asymptotic upper bounds on the estimator bias and stochastic error via the uniform Lipschitz property; asymptotic lower bounds on the estimator bias are also given for certain order derivative constraints. In Chapter V, a minimax asymptotic lower bound in the supremum norm is established for a family of nonparametric constrained estimation problems. The combination of the upper bounds on the estimator performance developed in Chapter IV together with the minimax lower bounds established in Chapter V demonstrate that under certain conditions, the asymptotic performance of the constrained B-spline estimator is optimal.

3.1 Introduction

B-splines are a popular tool in approximation and estimation theory [14, 17]. Nonnegative derivative constraints on a B-spline estimator can be easily imposed on spline coefficients, which can then be efficiently computed via quadratic programs. In spite of this numerical simplicity, the asymptotic analysis of constrained B-spline estimators is far from trivial, and requires a deep understanding of the mapping from a (weighted) sample data vector to the corresponding B-spline coefficient vector. As the sample size increases and tends to infinity, an infinite family of size-varying piecewise linear functions arises. A critical *uniform Lipschitz property* states that these size-varying piecewise linear mappings share a uniform Lipschitz constant under the ℓ_∞-norm, independent of the sample size and the number of knots; this property leads to many important results in asymptotic analysis [80]. In this chapter, we demonstrate that this uniform Lipschitz property holds for B-splines with nonnegative derivative constraints of arbitrary order.

The chapter is organized as follows. In Section 3.2, we introduce the constrained B-spline estimator and state the uniform Lipschitz property. Section 3.3 is devoted to the proof of the uniform Lipschitz property. A summary is given in Section 3.4.

Notation. We introduce some notation used in the chapter. Define the function δ_{ij} on $\mathbb{N} \times \mathbb{N}$ so that $\delta_{ij} = 1$ if $i = j$, and $\delta_{ij} = 0$ otherwise. Let $\mathbf{I}_S$ denote the indicator function for a set S. For an index set α, let $\overline{\alpha}$ denote its complement, and $|\alpha|$ denote its cardinality. In addition, for $k \in \mathbb{N}$, define the set $\alpha + k := \{i + k \,:\, i \in \alpha\}$. Let $\mathbf{1}_k \in \mathbb{R}^k$ denote the column vector of all ones and $\mathbf{1}_{k_1 \times k_2}$ denote the $k_1 \times k_2$ matrix of all ones. For a column vector $v \in \mathbb{R}^p$, let v_i denote its ith component. For a matrix $A \in \mathbb{R}^{k_1 \times k_2}$, let $[A]_{ij}$ or $[A]_{i,j}$ be its (i, j)-entry, let $(A)_{i\bullet}$ be its ith row, and $(A)_{\bullet j}$ be its jth column.

If $i_1 \le i_2$ and $j_1 \le j_2$, let $(A)_{i_1:i_2,\bullet}$ be the submatrix of A formed by its i_1th to i_2th rows, let $(A)_{\bullet,j_1:j_2}$ denote the submatrix of A formed by its j_1th to j_2th columns, and let $(A)_{i_1:i_2,j_1:j_2}$ denote the submatrix of A formed by its i_1th to i_2th rows and j_1th to j_2th columns. Given an index set α, let $v_\alpha \in \mathbb{R}^{|\alpha|}$ denote the vector formed by the components of v indexed by elements of α, and $(A)_{\alpha\bullet}$ denote the matrix formed by the rows of A indexed by elements of α.

3.2 Nonnegative Derivative Constrained B-splines: Uniform Lipschitz Property

Fix $m \in \mathbb{N}$. Consider the class of (generalized) shape constrained univariate functions on $[0, 1]$:

$$\mathcal{S}_m := \Big\{ f : [0,1] \to \mathbb{R} \ \Big| \ \text{the } (m-1)\text{th derivative } f^{(m-1)} \text{ exists a.e. on } [0,1], \text{ and} \\ \big(f^{(m-1)}(x_1) - f^{(m-1)}(x_2)\big) \cdot \big(x_1 - x_2\big) \ge 0 \ \text{ when } f^{(m-1)}(x_1), f^{(m-1)}(x_2) \text{ exist} \Big\}. \quad (3.1)$$

When $m = 1$, $\mathcal{S}_m$ represents the set of increasing functions on $[0, 1]$. Similarly, when $m = 2$, $\mathcal{S}_m$ denotes the set of continuous convex functions on $[0, 1]$.

This chapter focuses on the B-spline approximation of functions in $\mathcal{S}_m$. Toward this end, we provide a brief review of B-splines as follows; see [14] for more details. For a given $K \in \mathbb{N}$, let $T_\kappa := \{\kappa_0 < \kappa_1 < \cdots < \kappa_K\}$ be a sequence of $(K+1)$ knots in $\mathbb{R}$. Given $p \in \mathbb{N}$, let $\{B^{T_\kappa}_{p,k}\}_{k=1}^{K+p-1}$ denote the $(K+p-1)$ B-splines of order p (or equivalently degree $(p-1)$) with knots at $\kappa_0, \kappa_1, \ldots, \kappa_K$, and the usual extension $\kappa_{1-p} = \cdots = \kappa_{-1} = \kappa_0$ on the left and $\kappa_{K+1} = \cdots = \kappa_{K+p-1} = \kappa_K$ on the right, scaled such that $\sum_{k=1}^{K+p-1} B^{T_\kappa}_{p,k}(x) = 1$ for any $x \in [\kappa_0, \kappa_K]$. The support of $B^{T_\kappa}_{p,k}$ is given by (i) $[\kappa_{k-p}, \kappa_k)$ when $p = 1$ and

$1 \leq k \leq K-1$; (ii) $[\kappa_{k-p}, \kappa_k]$ when $p = 1$ and $k = K$ or for each $k = 1, \ldots, K+p-1$ when $p \geq 2$. We summarize some properties of the B-splines to be used in the subsequent development below:

(i) Nonnegativity, upper bound, and partition of unity: for each p, k, and T_κ, $0 \leq B^{T_\kappa}_{p,k}(x) \leq 1$ for any $x \in [\kappa_0, \kappa_K]$, and $\sum_{k=1}^{K+p-1} B^{T_\kappa}_{p,k}(x) = 1$ for any $x \in [\kappa_0, \kappa_K]$.

(ii) Continuity and differentiability: when $p = 1$, each $B^{T_\kappa}_{p,k}(x)$ is a (discontinuous) piecewise constant function given by $\mathbf{I}_{[\kappa_{k-1}, \kappa_k)}(x)$ for $1 \leq k \leq K-1$ or $\mathbf{I}_{[\kappa_{K-1}, \kappa_K]}(x)$ for $k = K$. Also, $B^{T_\kappa}_{p,k}(x) \cdot B^{T_\kappa}_{p,j}(x) = 0, \forall\ x$ if $k \neq j$. When $p = 2$, the $B^{T_\kappa}_{p,k}$'s are continuous piecewise linear splines, and there are at most three points in $\mathbb{R}$ where each $B^{T_\kappa}_{p,k}$ is not differentiable; when $p > 2$, each $B^{T_\kappa}_{p,k}$ is differentiable on $\mathbb{R}$. For $p \geq 2$, the derivative of $B^{T_\kappa}_{p,k}$ (when it exists) is

$$\left(B^{T_\kappa}_{p,k}(x)\right)' = \frac{p-1}{\kappa_{k-1} - \kappa_{k-p}} B^{T_\kappa}_{p-1,k-1}(x) - \frac{p-1}{\kappa_k - \kappa_{k-p+1}} B^{T_\kappa}_{p-1,k}(x), \tag{3.2}$$

where we define $\frac{p-1}{\kappa_k - \kappa_{k-p+1}} B^{T_\kappa}_{p-1,k}(x) := 0, \forall\, x \in [0,1]$ for $k = 0$ and $k = K+p-1$.

(iii) L_1-norm: for each k, the L_1-norm of $B^{T_\kappa}_{p,k}$ is known to be [14, Chapter IX, eqns.(5) and (7)]

$$\left\| B^{T_\kappa}_{p,k} \right\|_{L_1} := \int_{\mathbb{R}} \left| B^{T_\kappa}_{p,k}(x) \right| dx = \frac{\kappa_k - \kappa_{k-p}}{p}. \tag{3.3}$$

Let $T_\kappa := \{0 = \kappa_0 < \kappa_1 < \cdots < \kappa_{K_n} = 1\}$ be a given sequence of $(K_n + 1)$ knots in $[0,1]$, and let $g_{b,T_\kappa} : [0,1] \to \mathbb{R}$ be such that $g_{b,T_\kappa}(x) = \sum_{k=1}^{K_n+m-1} b_k B^{T_\kappa}_{m,k}(x)$, where the b_k's are real coefficients of B-splines and $b := (b_1, \ldots, b_{K_n+m-1})^T$ is the spline coefficient vector. Here the subscript n in K_n corresponds to the number of design points to be used in the subsequent sections.

To derive a necessary and sufficient condition for $g_{b,T_\kappa} \in \mathcal{S}_m$, we introduce the following matrices. Let $D^{(k)} \in \mathbb{R}^{k\times(k+1)}$ denote the first order difference matrix, i.e.,

$$D^{(k)} := \begin{bmatrix} -1 & 1 & & & \\ & -1 & 1 & & \\ & & \ddots & \ddots & \\ & & & -1 & 1 \end{bmatrix} \in \mathbb{R}^{k\times(k+1)}. \tag{3.4}$$

When $m = 1$, let $\widetilde{D}_{m,T_\kappa} := D^{(K_n-1)}$. In what follows, consider $m > 1$. For the given knot sequence T_κ with the usual extension $\kappa_k = 0$ for any $k < 0$ and $\kappa_k = 1$ for any $k > K_n$, define the following diagonal matrices: $\Delta_{0,T_\kappa} := I_{K_n-1}$, and for each $p = 1, \ldots, m-1$,

$$\Delta_{p,T_\kappa} := \frac{1}{p}\,\mathrm{diag}\Big(\kappa_1 - \kappa_{1-p},\ \kappa_2 - \kappa_{2-p},\ \ldots,\ \kappa_{K_n+p-1} - \kappa_{K_n-1}\Big) \in \mathbb{R}^{(K_n+p-1)\times(K_n+p-1)}. \tag{3.5}$$

Furthermore, define the matrices $\widetilde{D}_{p,T_\kappa} \in \mathbb{R}^{(K_n+m-1-p)\times(K_n+m-1)}$ inductively as:

$$\widetilde{D}_{0,T_\kappa} := I, \quad \text{and} \quad \widetilde{D}_{p,T_\kappa} := \Delta^{-1}_{m-p,T_\kappa} \cdot D^{(K_n+m-1-p)} \cdot \widetilde{D}_{p-1,T_\kappa}, \quad p = 1, \ldots, m. \tag{3.6}$$

Roughly speaking, $\widetilde{D}_{p,T_\kappa}$ denotes the pth order difference matrix weighted by the knots of T_κ. When the knots are equally spaced, $\widetilde{D}_{p,T_\kappa}$ is almost identical to a standard difference matrix (except on the boundary). Moreover, since $\Delta^{-1}_{m-p,T_\kappa}$ is invertible and $D^{(K_n+m-1-p)}$ has full row rank, it can be shown via induction that $\widetilde{D}_{p,T_\kappa}$ is of full row rank for any p and T_κ.

In what follows, define $N := K_n + m - 1$ for a fixed spline order $m \in \mathbb{N}$. Note that N depends on n, the number of design points.

Lemma 3.2.1. *Fix $m \in \mathbb{N}$. Let T_κ be a given sequence of (K_n+1) knots, and for each $p = 1, \ldots, m$, let $\{B_{p,k}^{T_\kappa}\}_{k=1}^{K_n+p-1}$ denote the B-splines of order p defined by T_κ. Then the following hold:*

(1) For any given $b \in \mathbb{R}^N$ and $j = 0, 1, \ldots, m-1$, the jth derivative of $g_{b,T_\kappa} := \sum_{k=1}^N b_k B_{m,k}^{T_\kappa}$ is $\sum_{k=1}^{N-j} (\widetilde{D}_{j,T_\kappa} b)_k B_{m-j,k}^{T_\kappa}$, except at (at most) finitely many points on $[0,1]$;

(2) $g_{b,T_\kappa} \in \mathcal{S}_m$ if and only if $\widetilde{D}_{m,T_\kappa} b \geq 0$.

Proof. For notational simplicity, we write g_{b,T_κ} as g and $\widetilde{D}_{j,T_\kappa}$ as $\widetilde{D}_j$ respectively in the proof.

(1) We prove statement (1) by induction on $j = 0, 1, \ldots, m-1$. Clearly, the statement holds for $j = 0$. Consider j with $1 \leq j \leq m-1$, and assume the statement holds for $(j-1)$. It follows from (3.2), the induction hypothesis, and the definitions of Δ_{j,T_κ} and $\widetilde{D}_j$ that

$$\begin{aligned}
g^{(j)} &= \left(g^{(j-1)}\right)' = \left(\sum_{k=1}^{N-j+1} \left(\widetilde{D}_{j-1} b\right)_k B_{m-j+1,k}^{T_\kappa}\right)' \\
&= (m-j) \sum_{k=1}^{N-j} \frac{(\widetilde{D}_{j-1} b)_{k+1} - (\widetilde{D}_{j-1} b)_k}{\kappa_k - \kappa_{k-m+j}} B_{m-j,k}^{T_\kappa} \\
&= \sum_{k=1}^{N-j} \left(\Delta_{m-j,T_\kappa}^{-1} D^{(N-j)} \widetilde{D}_{j-1} b\right)_k B_{m-j,k}^{T_\kappa} = \sum_{k=1}^{N-j} \left(\widetilde{D}_j b\right)_k B_{m-j,k}^{T_\kappa},
\end{aligned}$$

whenever $g^{(j)}$ and $g^{(j-1)}$ exist. Hence, statement (1) holds for j.

(2) It is easily seen that $g^{(m-1)}$ exists on $[0,1]$ except at (at most) finitely many points in $[0,1]$. It thus follows from statement (1) that $g^{(m-1)}$ is a piecewise constant function on $[0,1]$. Therefore, $g \in \mathcal{S}_m$ if and only if the spline coefficients of $g^{(m-1)}$ are increasing, i.e., $(\widetilde{D}_{m-1} b)_k \leq (\widetilde{D}_{m-1} b)_{k+1}$ for each $k = 1, \ldots, K_n - 1$. This is equivalent

to $D^{(K_n-1)}\widetilde{D}_{m-1}b \geq 0$, which is further equivalent to $\widetilde{D}_m\, b \geq 0$, in view of $\Delta_{0,T_\kappa} = I$ and $\widetilde{D}_m = D^{(K_n-1)}\widetilde{D}_{m-1}$. This gives rise to statement (2). $\square$

3.2.1 Nonnegative Derivative Constrained B-splines

Let $m \in \mathbb{N}$ be a fixed spline order throughout the rest of this chapter. Let $y := (y_0, y_1, \ldots, y_n)^T \in \mathbb{R}^{(n+1)}$ be a given sample sequence corresponding to a sequence of design points $P = (x_i)_{i=0}^n$ on $[0,1]$. For a given sequence T_κ of $(K_n + 1)$ knots on $[0,1]$, consider the following B-spline estimator that satisfies the shape constraint characterized by $\mathcal{S}_m$:

$$\widehat{f}^B_{P,T_\kappa}(x) := \sum_{k=1}^{K_n+m-1} \widehat{b}_k B^{T_\kappa}_{m,k}(x), \tag{3.7}$$

where the coefficient vector $\widehat{b}_{P,T_\kappa} := (\widehat{b}_k)$ is given by the constrained quadratic optimization problem:

$$\widehat{b}_{P,T_\kappa} := \operatorname*{arg\,min}_{\widetilde{D}_{m,T_\kappa} b \geq 0} \sum_{i=0}^{n} \left(x_{i+1} - x_i\right) \left(y_i - \sum_{k=1}^{N} b_k B^{T_\kappa}_{m,k}(x_i) \right)^2. \tag{3.8}$$

Here $x_{n+1} := 1$. It follows from Lemma 3.2.1 that $\widehat{f}^B_{P,T_\kappa} \in \mathcal{S}_m$. Note that $\widehat{f}^B_{P,T_\kappa}$ depends on P and T_κ.

Define the diagonal matrix $\Theta_n := \operatorname{diag}(x_1 - x_0,\, x_2 - x_1, \ldots, x_{n+1} - x_n) \in \mathbb{R}^{(n+1)\times(n+1)}$, the design matrix $\widehat{X} \in \mathbb{R}^{(n+1)\times N}$ with $[\widehat{X}]_{i,\,k} := B^{T_\kappa}_{m,k}(x_i)$ for each i and k, the matrix $\Lambda_{K_n,P,T_\kappa} := K_n \cdot \widehat{X}^T \Theta_n \widehat{X} \in \mathbb{R}^{N\times N}$, and the weighted sample vector $\overline{y} := K_n \cdot \widehat{X}^T \Theta_n y$. Therefore, the quadratic optimization problem in (3.8) for $\widehat{b}_{P,T_\kappa}$ can be written as:

$$\widehat{b}_{P,T_\kappa}(\bar{y}) := \operatorname*{arg\,min}_{\widetilde{D}_{m,T_\kappa}\, b \geq 0} \frac{1}{2} b^T \Lambda_{K_n,P,T_\kappa}\, b - b^T \overline{y}. \tag{3.9}$$

For the given P, T_κ and K_n, the matrix Λ_{K_n,P,T_κ} is positive definite, and the function $\widehat{b}_{P,T_\kappa} : \mathbb{R}^N \to \mathbb{R}^N$ is thus piecewise linear and globally Lipschitz continuous [63]. The piecewise linear formulation of $\widehat{b}_{P,T_\kappa}$ can be obtained from the KKT optimality conditions for (3.9):

$$\Lambda_{K_n,P,T_\kappa}\,\widehat{b}_{P,T_\kappa} - \overline{y} - \widetilde{D}^T_{m,T_\kappa}\,\chi \;=\; 0, \qquad 0 \;\leq\; \chi \;\perp\; \widetilde{D}_{m,T_\kappa}\,\widehat{b}_{P,T_\kappa} \;\geq\; 0, \tag{3.10}$$

where $\chi \in \mathbb{R}^{K_n-1}$ is the Lagrange multiplier, and $u \perp v$ means that the vectors u and v are orthogonal. It follows from an argument similar to those in [72, 71, 80] that each linear piece of $\widehat{b}_{P,T_\kappa}$ is characterized by index sets:

$$\alpha := \left\{ i \,:\, \big(\widetilde{D}_{m,T_\kappa}\,\widehat{b}_{P,T_\kappa}\big)_i = 0 \right\} \subseteq \{1, \ldots, K_n - 1\}. \tag{3.11}$$

Note that α may be the empty set. For each α, the KKT conditions (3.10) become

$$(\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}\,\widehat{b}_{P,T_\kappa} = 0, \qquad \chi_{\overline{\alpha}} = 0, \qquad \Lambda_{K_n,P,T_\kappa}\,\widehat{b}_{P,T_\kappa} - \overline{y} - \big((\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}\big)^T\,\chi_\alpha = 0.$$

Just as in [72, 71, 80], we may denote the linear piece of $\widehat{b}_{P,T_\kappa}$ for a given α as $\widehat{b}^{\alpha}_{P,T_\kappa}$, and let $F^T_\alpha \in \mathbb{R}^{N\times(|\overline{\alpha}|+m)}$ be a matrix whose columns form a basis for the null space of $(\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}$; if α is the empty set, then $N = (|\alpha| + m)$, and F^T_α will be the order N identity matrix. By [72, 71, 80],

$$\widehat{b}^{\alpha}_{P,T_\kappa}(\overline{y}) \;=\; F^T_\alpha\big(F_\alpha\Lambda_{K_n,P,T_\kappa}\,F^T_\alpha\big)^{-1}F_\alpha\,\overline{y}. \tag{3.12}$$

Note that for any invertible matrix $R \in \mathbb{R}^{(|\overline{\alpha}|+m)\times(|\overline{\alpha}|+m)}$,

$$(RF_\alpha)^T((RF_\alpha)\Lambda_{K_n,P,T_\kappa}(RF_\alpha)^T)^{-1}(RF_\alpha) = F^T_\alpha(F_\alpha\Lambda_{K_n,P,T_\kappa}F^T_\alpha)^{-1}F_\alpha.$$

Thus any choice of F_α leads to the same $\widehat{b}^{\alpha}_{P,T_\kappa}$, provided that the columns of F_α^T form a basis of the null space of $(\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}$.

3.2.2 Uniform Lipschitz Property of Constrained B-splines: Main Result

As indicated in the previous section, the piecewise linear function $\widehat{b}_{P,T_\kappa}(\cdot)$ is Lipschitz continuous for fixed K_n, P, T_κ. An important question is whether the Lipschitz constants of size-varying $\widehat{b}_{P,T_\kappa}$ are uniformly bounded with respect to the ℓ_∞-norm, independent of K_n, P, and T_κ, as long as the numbers of design points and knots are sufficiently large. If this is the case, we say that $\widehat{b}_{P,T_\kappa}$ satisfies the *uniform Lipschitz property*. Originally introduced and studied in [72, 71, 79, 80] for monotone P-splines and convex B-splines with equally spaced design points and knots, this property is shown to play a crucial role in the uniform convergence and asymptotic analysis of constrained B-spline estimators. In this section, we extend this property to constrained B-splines subject to general nonnegative derivative constraints under relaxed conditions on the design points and knots.

Fix $c_\omega \geq 1$, and for each $n \in \mathbb{N}$, define the following set of sequences of $(n+1)$ design points on $[0, 1]$:

$$\mathcal{P}_n := \left\{ (x_i)_{i=0}^n \;\middle|\; 0 = x_0 < x_1 < \cdots < x_n = 1, \quad \text{and} \quad x_i - x_{i-1} \leq \frac{c_\omega}{n}, \ \forall\, i = 1, \ldots, n \right\}. \tag{3.13}$$

Furthermore, let $c_{\kappa,1}$ and $c_{\kappa,2}$ with $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$ be given. For each $K_n \in \mathbb{N}$, define the following set of sequences of $(K_n + 1)$ knots on $[0, 1]$ with the usual extension on the left and right boundary:

$$\mathcal{T}_{K_n} \;:=\; \Big\{ (\kappa_i)_{i=0}^{K_n} \Big| \, 0 = \kappa_0 < \kappa_1 < \cdots < \kappa_{K_n} = 1,$$

$$\text{and } \frac{c_{\kappa,1}}{K_n} \le \kappa_i - \kappa_{i-1} \le \frac{c_{\kappa,2}}{K_n},\ \forall\, i = 1, \dots, K_n \Big\}. \tag{3.14}$$

For any $p, K_n \in \mathbb{N}$ and $T_\kappa \in \mathcal{T}_{K_n}$, it is noted that for any $\kappa_i \in T_\kappa$, we have, $\frac{\kappa_i - \kappa_{i-p}}{p} = \frac{1}{p}\sum_{s=i-p+1}^{i}(\kappa_s - \kappa_{s-1}) \le \frac{1}{p} \cdot p \cdot \frac{c_{\kappa,2}}{K_n} \le c_{\kappa,2}/K_n$. Moreover, in view of $\kappa_{i-p} = 0$ for any $i \le p$ and $\kappa_i = 1$ for any $i \ge K_n$, it can be shown that for each $1 \le i \le K_n + p - 1$, $\frac{\kappa_i - \kappa_{i-p}}{p} \ge c_{\kappa,1}/(p \cdot K_n)$ so that $\frac{p}{\kappa_i - \kappa_{i-p}} \le p \cdot K_n / c_{\kappa,1}$. In summary, we have, for each $i = 1, \dots, K_n + p - 1$,

$$\frac{c_{\kappa,1}}{p \cdot K_n} \le \frac{\kappa_i - \kappa_{i-p}}{p} \le \frac{c_{\kappa,2}}{K_n}, \qquad \text{and} \qquad \frac{K_n}{c_{\kappa,2}} \le \frac{p}{\kappa_i - \kappa_{i-p}} \le \frac{p \cdot K_n}{c_{\kappa,1}}. \tag{3.15}$$

Using the above notation, we state the main result of the paper, i.e., the uniform Lipschitz property of $\widehat{b}_{P,T_\kappa}$, as follows:

Theorem 3.2.1. *Let $m \in \mathbb{N}$ and constants $c_\omega, c_{\kappa,1}, c_{\kappa,2}$ be fixed, where $c_\omega \ge 1$ and $0 < c_{\kappa,1} \le 1 \le c_{\kappa,2}$. For any $n, K_n \in \mathbb{N}$, let $\widehat{b}_{P,T_\kappa} : \mathbb{R}^{K_n+m-1} \to \mathbb{R}^{K_n+m-1}$ be the piecewise linear function in (3.9) corresponding to the mth order B-spline defined by the design point sequence $P \in \mathcal{P}_n$ and the knot sequence $T_\kappa \in \mathcal{T}_{K_n}$. Then there exists a positive constant c_∞, depending on $m, c_{\kappa,1}$ only, such that for any increasing sequence (K_n) with $K_n \to \infty$ and $K_n/n \to 0$ as $n \to \infty$, there exists $n_* \in \mathbb{N}$, depending on (K_n) (and the fixed constants $m, c_\omega, c_{\kappa,1}, c_{\kappa,2}$) only, such that for any $P \in \mathcal{P}_n$ and $T_\kappa \in \mathcal{T}_{K_n}$ with all $n \ge n_*$,*

$$\Big\| \widehat{b}_{P,T_\kappa}(u) - \widehat{b}_{P,T_\kappa}(v) \Big\|_\infty \le c_\infty \, \| u - v \|_\infty, \quad \forall\, u, v \in \mathbb{R}^{K_n+m-1}.$$

The above result can be refined when we focus on a particular sequence P and T_κ.

Corollary 3.2.1. *Let (K_n) be an increasing sequence with $K_n \to \infty$ and $K_n/n \to 0$ as $n \to \infty$, and $\big((P_n, T_{K_n})\big)$ be a sequence in $\mathcal{P}_n \times \mathcal{T}_{K_n}$. Then there exists a positive constant*

c'_∞, *independent of* n, *such that for each* n,

$$\left\| \widehat{b}_{P_n, T_{K_n}}(u) - \widehat{b}_{P_n, T_{K_n}}(v) \right\|_\infty \leq c'_\infty \left\| u - v \right\|_\infty, \quad \forall\, u, v \in \mathbb{R}^{K_n + m - 1}.$$

This corollary recovers the past results on the uniform Lipschitz property for $m = 1, 2$ (e.g., [80]) when the design points and knots are equally spaced on $[0, 1]$.

3.2.3 Overview of the Proof

The proof of Theorem 3.2.1 is somewhat technical. To facilitate the reading, we outline its key ideas and provide a road map of the proof as follows. In view of the piecewise linear formulation of $\widehat{b}_{P,T_\kappa}$ in (3.12), it suffices to establish a uniform bound on $\|F_\alpha^T \left(F_\alpha \Lambda_{K_n,P,T_\kappa} F_\alpha^T\right)^{-1} F_\alpha\|_\infty$ for all large n, regardless of K_n, α, $P \in \mathcal{P}_n$, and $T_\kappa \in \mathcal{T}_{K_n}$.

Suppose that there exists a smooth function $f : [0, 1] \to \mathbb{R}$ satisfying $y_i = f(x_i)$ for each $x_i \in P$. The overarching idea of the proof is to think of the mapping from the unweighted data vector y to the spline $\widehat{f}^B_{P,T_\kappa}$ as an approximation of the L_2-projection of f onto the polyhedral cone of order m splines in $\mathcal{S}_m$ with knot sequence T_κ. Since the projection mapping from f to $\widehat{f}^B_{P,T_\kappa}$ is piecewise linear [63], each linear piece of this mapping is given by a projection onto a space of order m splines, whose knots lie in a subset (determined by α) of T_κ. A deep result in B-spline theory (dubbed de Boor's conjecture), proven by Shardin [64], states that the L_2-projection of functions onto a space of order m splines is bounded in the L_∞-norm, independent of the spline knot sequence. Hence, when n is sufficiently large, each linear piece of the mapping from y to $\widehat{f}^B_{P,T_\kappa}$ closely approximates such an L_2-projection, and is thus bounded in the L_∞-norm independent of K_n, α, $P \in \mathcal{P}_n$, and $T_\kappa \in \mathcal{T}_{K_n}$. Moreover, the matrix $F_\alpha^T \left(F_\alpha \Lambda_{K_n,P,T_\kappa} F_\alpha^T\right)^{-1} F_\alpha$ is intimately related to its corresponding linear piece of the mapping from y to $\widehat{f}^B_{P,T_\kappa}$. Consequently, results from [64] will prove invaluable in bounding $F^T_\alpha \big(F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1} F_\alpha$.

We may choose a diagonal matrix Ξ'_α to provide a positive scaling of the rows of F_α, so that $\|\Xi'_\alpha F_\alpha\|_\infty$ is uniformly bounded. We may then write that

$$F^T_\alpha \big(F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1} F_\alpha = F^T_\alpha \cdot \big(\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1} \cdot \Xi'_\alpha F_\alpha.$$

Hence,

$$\|F^T_\alpha \big(F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1} F_\alpha\|_\infty \leq \|F^T_\alpha\|_\infty \ \|\big(\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1}\|_\infty \ \|\Xi'_\alpha F_\alpha\|_\infty.$$

Therefore, our goal is to construct F^T_α, by choosing a suitable basis of $(\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}$, and select Ξ'_α so that $\|F^T_\alpha\|_\infty$ and $\|\big(\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1}\|_\infty$ are also uniformly bounded for sufficiently large n, independent of K_n, α, $P \in \mathcal{P}_n$ and $T_\kappa \in \mathcal{T}_{K_n}$. To this end, we will choose F^T_α and Ξ'_α so that $\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha$ approximates a certain B-spline Gramian matrix (cf. Theorem 3.2.2). A critical technique for establishing uniform bounds on $\|\big(\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1}\|_\infty$ and other related quantities relies on Theorem I of [64], which states that the ℓ_∞-norm of the inverse of the Gramian formed by the normalized B-splines of order m is uniformly bounded, independent of the knot sequence and the number of B-splines; the uniform boundedness of this B-spline Gramian is equivalent to the uniform boundedness of the aforementioned L_2-projection [15, Section 4]. To formally describe the result on the B-spline Gramian uniform boundedness, we introduce more notation. Let $\langle \cdot, \cdot \rangle$ denote the L_2-inner product of real-valued univariate functions on $\mathbb{R}$, i.e., $\langle f, g \rangle := \int_{\mathbb{R}} f(x) g(x)\, dx$, and $\| \cdot \|_{L_1}$ denote the L_1-norm of a real-valued univariate function on $\mathbb{R}$, i.e., $\|f\|_{L_1} := \int_{\mathbb{R}} |f(x)|\, dx$. The main result of [64] is stated in the following theorem.

Theorem 3.2.2. *[64, Theorem I] Fix a spline order $m \in \mathbb{N}$. Let $a, b \in \mathbb{R}$ with $a < b$, and $\{B^{T_\kappa}_{m,k}\}_{k=1}^{K+m-1}$ be the mth order B-splines on $[a, b]$ defined by a knot sequence $T_\kappa := \{a = t_0 < t_1 < \cdots < t_K = b\}$ for some $K \in \mathbb{N}$. Let $G \in \mathbb{R}^{(K+m-1)\times(K+m-1)}$ be the Gramian matrix given by*

$$\big[G\big]_{i,j} \ := \ \frac{\Big\langle B^{T_\kappa}_{m,i}, \ B^{T_\kappa}_{m,j} \Big\rangle}{\|B^{T_\kappa}_{m,i}\|_{L_1}}, \qquad \forall \ i, j \ = \ 1, \ldots, K + m - 1.$$

Then there exists a positive constant ρ_m, independent of a, b, T_κ and K, such that $\|G^{-1}\|_\infty \leq \rho_m$.

Inspired by this theorem, we intend to approximate $\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha$ and other relevant matrices by appropriate Gramian matrices of B-splines with uniform approximation error bounds. To achieve this goal, after establishing some preliminary technical results in Section 3.3.1, we construct a suitable matrix F_α (i.e., $F^{(m)}_{\alpha,T_\kappa}$) in Section 3.3.2 so that $\|F^T_\alpha\|_\infty$ is uniformly bounded via Corollary 3.3.1. In Section 3.3.3, we construct a B-spline collocation matrix approximation X_{m,T_κ,L_n} such that the product $F_\alpha \cdot X_{m,T_\kappa,L_n}$ may be computed via inductive principles at the conclusion of this section; this product allows us to then construct $\widetilde{\Lambda}_{T_\kappa,K_n,L_n}$, which will be used to approximate Λ_{K_n,P,T_κ}. We then show via analytical tools and Theorem 3.2.2 that these constructed matrices attain uniform bounds or uniform approximation error bounds in Section 3.3.4. With the help of these bounds, the uniform Lipschitz property is proven in Section 3.3.5.

3.3 Proof of the Uniform Lipschitz Property

In this section, we prove the uniform Lipschitz property stated in Theorem 3.2.1.

3.3.1 Technical Lemmas

We present two technical lemmas for the proof of Theorem 3.2.1. The first lemma characterizes the difference between an integral of a continuous function and its discrete approximation; it will be used multiple times through this section (cf. Propositions 3.3.2, 3.3.4, and 3.3.5).

Lemma 3.3.1. *Let $\widetilde{n} \in \mathbb{N}$, $v = (v_k) \in \mathbb{R}^{\widetilde{n}}$, $[a, b] \subset \mathbb{R}$ with $a < b$, and points $\{s_k\}_{k=0}^{\widetilde{n}}$ with $a = s_0 < s_1 < \cdots < s_{\widetilde{n}} = b$ such that $\max_{k=1,\ldots\widetilde{n}} |s_k - s_{k-1}| \le \varrho$ for some $\varrho > 0$. Let $f : [a, b] \to \mathbb{R}$ be a continuous function that is differentiable on $[a, b]$ except at finitely many points in $[a, b]$. Suppose there exist positive constants μ_1 and μ_2 such that $\max_{k=1,\ldots\widetilde{n}} |v_k - f(s_{k-1})| \le \mu_1$, and $|f'(x)| \le \mu_2$ for any $x \in [a, b]$ where $f'(x)$ exists. Then for each $i \in \{1, \ldots, \widetilde{n}\}$,*

$$\left| \sum_{k=1}^{i} v_k \left(s_k - s_{k-1}\right) - \int_{s_0}^{s_i} f(x)\, dx \right| \le \mu_1(b-a) + \frac{3}{2}\, \mu_2 \varrho (b-a).$$

Proof. Fix an arbitrary $k \in \{1, \ldots, \widetilde{n}\}$. Suppose that $\widetilde{s}_1, \ldots, \widetilde{s}_{\ell-1} \in (s_{k-1}, s_k)$ with $s_{k-1} := \widetilde{s}_0 < \widetilde{s}_1 < \widetilde{s}_2 < \cdots < \widetilde{s}_{\ell-1} < \widetilde{s}_\ell := s_k$ are the only points where f is non-differentiable on the interval (s_{k-1}, s_k). It follows from the continuity of f and the Mean-value Theorem that for each $j = 1, \ldots, \ell$, there exists $\xi_j \in (\widetilde{s}_{j-1}, \widetilde{s}_j)$ such that $f(\widetilde{s}_j) = f(\widetilde{s}_{j-1}) + f'(\xi_j)(\widetilde{s}_j - \widetilde{s}_{j-1}) = f(s_{k-1}) + \sum_{r=1}^{j} f'(\xi_r)(\widetilde{s}_r - \widetilde{s}_{r-1})$. Since f is continuous and piecewise differentiable, we have

$$\begin{aligned} &\left| \int_{s_{k-1}}^{s_k} f(x)\, dx - \big(s_k - s_{k-1}\big)\, f(s_{k-1}) \right| \\ = \; &\left| \sum_{j=1}^{\ell} \int_{\widetilde{s}_{j-1}}^{\widetilde{s}_j} \Big[f(\widetilde{s}_{j-1}) + f'(\xi_x)\big(x - \widetilde{s}_{j-1}\big) \Big] dx - \big(s_k - s_{k-1}\big)\, f(s_{k-1}) \right| \end{aligned}$$

$$
\begin{aligned}
&\leq \left|\sum_{j=1}^{\ell}\left[f(s_{k-1})+\sum_{r=1}^{j-1} f'(\xi_r)(\widetilde{s}_r-\widetilde{s}_{r-1})\right](\widetilde{s}_j-\widetilde{s}_{j-1})-\big(s_k-s_{k-1}\big)\,f(s_{k-1})\right| \\
&\quad + \left|\sum_{j=1}^{\ell}\int_{\widetilde{s}_{j-1}}^{\widetilde{s}_j} f'(\xi_x)\big(x-\widetilde{s}_{j-1}\big)dx\right| \\
&\leq \left|\sum_{j=1}^{\ell} f'(\xi_j)\big(\widetilde{s}_j-\widetilde{s}_{j-1}\big)\big(s_k-\widetilde{s}_j\big)\right| + \frac{\mu_2}{2}\sum_{j=1}^{\ell}\big(\widetilde{s}_j-\widetilde{s}_{j-1}\big)^2 \\
&\leq \frac{3\mu_2}{2}\Big(s_k-s_{k-1}\Big)^2 \ \leq\ \frac{3\mu_2\varrho}{2}\Big(s_k-s_{k-1}\Big).
\end{aligned}
$$

Consequently, for each $i \in \{1,\ldots,\widetilde{n}\}$,

$$
\begin{aligned}
&\left|\sum_{k=1}^{i} v_k\left(s_k-s_{k-1}\right)-\int_{s_0}^{s_i} f(x)\,dx\right| \ \leq\ \sum_{k=1}^{i}\left|v_k\left(s_k-s_{k-1}\right)-\int_{s_{k-1}}^{s_k} f(x)\,dx\right| \\
&\quad \leq\ \sum_{k=1}^{i}\big(s_k-s_{k-1}\big)\big|v_k-f(s_{k-1})\big| \ +\ \sum_{k=1}^{i}\left|\big(s_k-s_{k-1}\big)\,f(s_{k-1})-\int_{s_{k-1}}^{s_k} f(x)\,dx\right| \\
&\quad \leq\ \mu_1\sum_{k=1}^{i}\big(s_k-s_{k-1}\big) \ +\ \frac{3\mu_2\varrho}{2}\sum_{k=1}^{i}\big(s_k-s_{k-1}\big) \ \leq\ \mu_1(b-a)+\frac{3}{2}\,\mu_2\varrho(b-a).
\end{aligned}
$$

This completes the proof. □

The second lemma asserts that if corresponding matrices from two families of square matrices are sufficiently close, and that the matrices from one family are invertible with uniformly bounded inverses, then so are the matrices from the other family. This result is instrumental in establishing a uniform bound of the inverses of certain size-varying matrices (cf. Corollary 3.3.2).

Lemma 3.3.2. *Let $\{A_i \in \mathbb{R}^{n_i\times n_i} \,:\, i \in \mathcal{I}\}$ and $\{B_i \in \mathbb{R}^{n_i\times n_i} \,:\, i \in \mathcal{I}\}$ be two families of square matrices for a (possibly infinite) index set $\mathcal{I}$, where $n_i \in \mathbb{N}$ need not be the same for different $i \in \mathcal{I}$. Suppose that each A_i is invertible with $\mu := \sup_{i\in\mathcal{I}}\|A_i^{-1}\|_\infty < \infty$ and* *that for any $\varepsilon > 0$, there are only finitely many $i \in \mathcal{I}$ satisfying $\|A_i - B_i\|_\infty \geq \varepsilon$. Then for all but finitely many $i \in \mathcal{I}$, B_i is invertible with $\|B_i^{-1}\|_\infty \leq \frac{3}{2}\mu$.*

Proof. For the given positive constant $\mu := \sup_{i\in\mathcal{I}} \|A_i^{-1}\|_\infty < \infty$, define the positive constant $\varepsilon := 1/(3\mu)$. Let $\mathcal{I}_\varepsilon := \{i \in \mathcal{I} : \|A_i - B_i\|_\infty < \varepsilon\}$. Note that there exist only finitely many $i \in \mathcal{I}$ such that $\|A_i - B_i\|_\infty \geq \varepsilon$. Define $C_i := B_i - A_i$ so that $\|C_i\|_\infty < \varepsilon$ for each $i \in \mathcal{I}_\varepsilon$. Since $B_i = A_i + C_i$ and A_i is invertible, we have $A_i^{-1}B_i = I + A_i^{-1}C_i$. Hence, we obtain, via $\varepsilon = 1/(3\mu)$,

$$\left\|A_i^{-1}C_i\right\|_\infty \leq \|A_i^{-1}\|_\infty \cdot \|C_i\|_\infty \leq \mu \cdot \varepsilon = \frac{1}{3}, \qquad \forall\, i \in \mathcal{I}_\varepsilon.$$

This shows that $I + A_i^{-1}C_i$ is strictly diagonally dominant, and thus is invertible. Therefore, $A_i^{-1}B_i$ is invertible, and so is B_i for each $i \in \mathcal{I}_\varepsilon$. Hence all but finitely many $B_i, i \in \mathcal{I}$, are invertible.

By virtue of $\left\|A_i^{-1}C_i\right\|_\infty \leq 1/3$ for any $i \in \mathcal{I}_\varepsilon$, we deduce that

$$\left\|\left(I + A_i^{-1}C_i\right)^{-1}\right\|_\infty \leq \frac{1}{1 - \left\|A_i^{-1}C_i\right\|_\infty} \leq \frac{3}{2}, \qquad \forall\, i \in \mathcal{I}_\varepsilon.$$

Using $A_i^{-1}B_i = I + A_i^{-1}C_i$ again, we further have that

$$\|B_i^{-1}\|_\infty = \left\|\left(I + A_i^{-1}C_i\right)^{-1} \cdot A_i^{-1}\right\|_\infty \leq \left\|\left(I + A_i^{-1}C_i\right)^{-1}\right\|_\infty \cdot \|A_i^{-1}\|_\infty \leq \frac{3}{2}\mu,$$

for all $i \in \mathcal{I}_\varepsilon$. This yields the desired result. □

3.3.2 Construction of the Null Space Basis Matrix

In this subsection, we construct a suitable matrix F_α used in (3.12), whose rows form a basis for the null space of $(\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}$, such that $\|F_\alpha^T\|_\infty$ is uniformly bounded (cf. Corollary 3.3.1). For $K_n \in \mathbb{N}$, let $T_\kappa \in \mathcal{T}_{K_n}$ be a knot sequence, and $\alpha \subseteq \{1, \ldots, K_n - 1\}$ be an index set defined in (3.11). The complement of α is $\overline{\alpha} = \{i_1, \ldots, i_{|\overline{\alpha}|}\}$ with $1 \leq i_1 < \cdots < i_{|\overline{\alpha}|} \leq K_n - 1$. For notational simplicity, define $q_\alpha := |\overline{\alpha}| + m$.

We introduce the following two matrices, both of which have full row rank:

$$E_{\alpha,T_\kappa} := \begin{bmatrix} \mathbf{1}_{i_1}^T & & & \\ & \mathbf{1}_{i_2-i_1}^T & & \\ & & \ddots & \\ & & & \mathbf{1}_{K_n-i_{|\overline{\alpha}|}}^T \end{bmatrix} \in \mathbb{R}^{(|\overline{\alpha}|+1)\times K_n}, \ F_{\alpha,T_\kappa}^{(1)} := \begin{bmatrix} I_{m-1} & 0 \\ 0 & E_{\alpha,T_\kappa} \end{bmatrix} \in \mathbb{R}^{q_\alpha \times N}, \tag{3.16}$$

where we recall $N := K_n + m - 1$. Observe that when α is empty, then $F_{\alpha,K_n}^{(1)} := I_N$.

Note that each column of $F_{\alpha,T_\kappa}^{(1)}$ contains exactly one entry of 1, and all other entries are zero. The matrix $F_{\alpha,T_\kappa}^{(1)}$ characterizes the first order B-splines (i.e. the piecewise constant splines) with the knot sequence $\{\kappa_{i_k}\}$ defined by $\overline{\alpha}$. For the given α, define

$$\tau_{\alpha,T_\kappa,k} := \begin{cases} 0, & \text{for } k = 1-m, \ldots, 0 \\ \kappa_{i_k}, & \text{for } k = 1, \ldots, |\overline{\alpha}| \\ 1, & \text{for } k = |\overline{\alpha}|+1, \ldots, q_\alpha. \end{cases} \tag{3.17}$$

It is easy to verify that for each $k \in \{1, \ldots, |\overline{\alpha}| + 1\}$ and $\ell \in \{1, \ldots, K_n\}$,

$$\left(F^{(1)}_{\alpha,T_\kappa}\right)_{(k+m-1),(\ell+m-1)} = \left(E_{\alpha,T_\kappa}\right)_{k\ell} = \begin{cases} 1, & \text{if } \kappa_{\ell-1} \in [\tau_{\alpha,T_\kappa,k-1}, \tau_{\alpha,T_\kappa,k}) \\ 0, & \text{otherwise.} \end{cases} \tag{3.18}$$

For each $p = 1, \ldots, m$, we further introduce the following diagonal matrices

$$\begin{aligned} \Xi^{(p)}_{\alpha,T_\kappa} &:= \begin{bmatrix} I_{m-p} & 0 \\ 0 & \Sigma_{p,T_\kappa} \end{bmatrix} \\ &= \operatorname{diag}\left(\underbrace{1, \ldots, 1,}_{(m-p)-\text{copies}} \frac{p}{\tau_{\alpha,T_\kappa,1} - \tau_{\alpha,T_\kappa,1-p}}, \frac{p}{\tau_{\alpha,T_\kappa,2} - \tau_{\alpha,T_\kappa,2-p}}, \ldots, \frac{p}{\tau_{\alpha,T_\kappa,|\overline{\alpha}|+p} - \tau_{\alpha,T_\kappa,|\overline{\alpha}|}} \right), \end{aligned} \tag{3.19}$$

where $\Xi^{(p)}_{\alpha,T_\kappa}$ is of order q_α, and by using the definition of the matrix Δ_{p,T_κ} in (3.5),

$$\begin{aligned} \widehat{\Delta}_{p,T_\kappa} &:= \begin{bmatrix} I_{m-p} & 0 \\ 0 & \Delta_{p,T_\kappa} \end{bmatrix} \\ &= \operatorname{diag}\left(\underbrace{1, \ldots, 1,}_{(m-p)-\text{copies}} \frac{\kappa_1 - \kappa_{1-p}}{p}, \frac{\kappa_2 - \kappa_{2-p}}{p}, \ldots, \frac{\kappa_{K_n+p-1} - \kappa_{K_n-1}}{p} \right) \in \mathbb{R}^{N \times N}. \end{aligned} \tag{3.20}$$

In addition, define the following two matrices of order $r \in \mathbb{N}$:

$$\widehat{S}^{(r)} := \begin{bmatrix} 1 & 1 & 1 & \ldots & 1 \\ & 1 & 1 & \ldots & 1 \\ & & 1 & \ldots & 1 \\ & & & \ddots & \vdots \\ & & & & 1 \end{bmatrix}, \quad \text{and} \quad \widehat{D}^{(r)} := \left(\widehat{S}^{(r)}\right)^{-1} = \begin{bmatrix} 1 & -1 & & & \\ & 1 & -1 & & \\ & & \ddots & \ddots & \\ & & & 1 & -1 \\ & & & & 1 \end{bmatrix}. \tag{3.21}$$

Here multiplication by the matrix $\widehat{S}^{(r)}$ from right acts as discrete integration, while $\widehat{D}^{(r)}$ is similar to a difference matrix.

With the above notation, we define $F^{(p)}_{\alpha,T_\kappa}$ inductively: $F^{(1)}_{\alpha,T_\kappa}$ is defined in (3.16), and

$$F^{(p)}_{\alpha,T_\kappa} := \widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha,T_\kappa} \cdot F^{(p-1)}_{\alpha,T_\kappa} \cdot \widehat{\Delta}_{p-1,T_\kappa} \cdot \widehat{S}^{(N)} \in \mathbb{R}^{q_\alpha \times N}, \qquad p = 2, \ldots, m. \tag{3.22}$$

Since $\widehat{D}^{(q_\alpha)}$, $\Xi^{(p-1)}_{\alpha,T_\kappa}$, $\widehat{\Delta}_{p-1,T_\kappa}$, and $\widehat{S}^{(N)}$ are all invertible, each $F^{(p)}_{\alpha,T_\kappa}$ has full row rank by induction. Furthermore, it is easy to see that if α is the empty set, then $\overline{\alpha} = \{1, \ldots, K_n - 1\}$ so that $F^{(1)}_{\alpha,T_k}$ is the identity matrix I_N for any T_κ, which further shows via induction in (3.22) that $F^{(p)}_{\alpha,T_\kappa} = I_N$ for any $p = 2, \ldots, m$ and any T_κ.

It is shown below that $F^{(m)}_{\alpha,T_\kappa}$ constructed above is a suitable choice for F_α in the piecewise linear formulation of $\widehat{b}_{P,T_\kappa}$ in (3.12).

Proposition 3.3.1. *For any index set $\alpha \subseteq \{1, \ldots, K_n - 1\}$, the columns of $\big(F^{(m)}_{\alpha,T_\kappa}\big)^T$ form a basis of the null space of $(\widetilde{D}_{m,T_\kappa})_{\alpha\bullet}$.*

Proof. To simplify notation, we use $F_{\alpha,p}$ to denote $F^{(p)}_{\alpha,T_\kappa}$ and drop the subscript T_κ in $\widetilde{D}_{p,T_\kappa}$, Δ_{p,T_κ}, and $\widehat{\Delta}_{p,T_\kappa}$ for $p = 1, \ldots, m$; see (3.5)-(3.6) for the definitions of Δ_{p,T_κ} and $\widetilde{D}_{p,T_\kappa}$ respectively.

Suppose that α is empty. Then $F^{(1)}_{\alpha,K_n} := I_N$, and by induction, $F^{(m)}_{\alpha,K_n} := I_N$, whose columns form a basis of $\mathbb{R}^N$. Hence, the result holds for empty α. Therefore, consider nonempty α. We first show that the matrix product

$$\big(D^{(N-1)}\big)_{(\alpha+m-1)\bullet} F^T_{\alpha,1} = 0.$$

Since the first $(m-1)$ columns of $\left(D^{(N-1)}\right)_{(\alpha+m-1)\bullet}$ contain all zero entries and

$$\left(F_{\alpha,1}^T\right)_{\bullet,1:(m-1)} = \begin{bmatrix} I_{m-1} \\ \\ 0 \end{bmatrix} \in \mathbb{R}^{N\times(m-1)},$$

we see that the first $(m-1)$ columns of $\left(D^{(N-1)}\right)_{(\alpha+m-1)\bullet} F_{\alpha,1}^T$ have all zero entries. (If $m=1$, this result holds trivially.) Moreover, for each j with $m \le j \le q_\alpha := |\overline{\alpha}| + m$, we see, in light of (3.16) and (3.18), that

$$(F_{\alpha,1})_{j\bullet} = \Bigg(\underbrace{0,\ldots,0}_{i_{k-1}+m-1},\ \underbrace{1,\ldots,1}_{i_k-i_{k-1}},\ \underbrace{0,\ldots,0}_{K_n-i_k}\Bigg).$$

where $k = j-m+1$, $i_0 := 0$, and $i_{|\overline{\alpha}|+1} := K_n$. Note that for each $s \in \alpha$, the row $\left(D^{(N-1)}\right)_{(s+m-1)\bullet}$ is of the form $(\underbrace{0,\ldots,0}_{s+m-2},-1,1,\underbrace{0,\ldots,0}_{K_n-1-s})$. Using the fact that $i_{k-1}, i_k \in \overline{\alpha} \cup \{0, K_n\}$ for any $k = 1,\ldots,|\overline{\alpha}|+1$, we deduce that if $s \in \alpha$, then $s \notin \{i_{k-1}, i_k\}$ for $k = 1,\ldots,|\overline{\alpha}|+1$. This shows that $\left(D^{(N-1)}\right)_{(s+m-1)\bullet} \cdot \left(F_{\alpha,1}^T\right)_{\bullet j} = 0, \quad \forall\, s \in \alpha$. Hence the matrix product $\left(D^{(N-1)}\right)_{(\alpha+m-1)\bullet} F_{\alpha,1}^T = 0$.

It is easy to show via (3.6), (3.16), and the above result that the proposition holds when $m=1$. Consider $m \ge 2$ for the rest of the proof. Let $S_0 := I_N$, and $S_p := \widehat{\Delta}_{m-p} \cdot \widehat{S}^{(N)} \cdot S_{p-1}$ for $p = 1,\ldots,m-1$, where $\widehat{S}^{(N)}$ is defined in (3.21). It follows from the definition of S_p and (3.22) that $F_{\alpha,m} = Q \cdot F_{\alpha,1} \cdot S_{m-1}$ for a suitable matrix Q. We next show via induction on p that

$$\widetilde{D}_p \cdot S_p^T = \begin{bmatrix} 0_{(N-p)\times p} & I_{N-p} \end{bmatrix}, \qquad \forall\, p = 0,1,\ldots,m-1. \tag{3.23}$$

Clearly, this result holds for $p = 0$. Given $p \geq 1$ and assuming that (3.23) holds for $p-1$, it follows from (3.6), (3.22), and the induction hypothesis that

$$\begin{aligned}
\widetilde{D}_p \cdot S_p^T &= \left(\Delta_{m-p}^{-1} D^{(N-p)} \widetilde{D}_{p-1}\right) \cdot \left(S_{p-1}^T (\widehat{S}^{(N)})^T \widehat{\Delta}_{m-p}\right) \\
&= \Delta_{m-p}^{-1} D^{(N-p)} \begin{bmatrix} 0_{(N-(p-1))\times(p-1)} & I_{N-(p-1)} \end{bmatrix} \left(\widehat{S}^{(N)}\right)^T \widehat{\Delta}_{m-p} \\
&= \Delta_{m-p}^{-1} D^{(N-p)} \begin{bmatrix} \mathbf{1}_{(N-(p-1))\times(p-1)} & \left(\widehat{S}^{(N-(p-1))}\right)^T \end{bmatrix} \widehat{\Delta}_{m-p} \\
&= \Delta_{m-p}^{-1} \begin{bmatrix} 0_{(N-p)\times p} & I_{N-p} \end{bmatrix} \widehat{\Delta}_{m-p} \\
&= \Delta_{m-p}^{-1} \begin{bmatrix} 0_{(N-p)\times p} & \Delta_{m-p} \end{bmatrix} = \begin{bmatrix} 0_{(N-p)\times p} & I_{N-p} \end{bmatrix},
\end{aligned}$$

where the second to last equality is a consequence of (3.20). This gives rise to (3.23).

Combining the above results, we have

$$\begin{aligned}
(\widetilde{D}_m)_{\alpha\bullet} \cdot F_{\alpha,m}^T &= \left(\left(D^{(K_n-1)}\right)_{\alpha\bullet} \widetilde{D}_{m-1}\right) \cdot \left(Q\, F_{\alpha,1}\, S_{m-1}\right)^T \\
&= \left(D^{(K_n-1)}\right)_{\alpha\bullet} \cdot \widetilde{D}_{m-1} \cdot S_{m-1}^T \cdot F_{\alpha,1}^T \cdot Q^T \\
&= \left(D^{(K_n-1)}\right)_{\alpha\bullet} \begin{bmatrix} 0_{K_n\times(m-1)} & I_{K_n} \end{bmatrix} F_{\alpha,1}^T \cdot Q^T \\
&= \left(D^{(N-1)}\right)_{(\alpha+m-1)\bullet} \cdot F_{\alpha,1}^T \cdot Q^T = 0.
\end{aligned}$$

Recall that $F_{\alpha,m}$ has full row rank. Hence, the q_α columns of $F_{\alpha,m}^T$ are linearly independent. Additionally, since $\widetilde{D}_m$ is of full row rank as indicated after (3.6), so is $(\widetilde{D}_m)_{\alpha\bullet}$. Therefore, $\text{rank}[(\widetilde{D}_m)_{\alpha\bullet}] = |\alpha|$ and the null space of $(\widetilde{D}_m)_{\alpha\bullet}$ has dimension $(K_n + m - 1 - |\alpha|)$, which is equal to q_α in light of the fact that $|\alpha| + |\overline{\alpha}| = K_n - 1$. Therefore the columns of $F_{\alpha,m}^T$ form a basis for the null space of $(\widetilde{D}_m)_{\alpha\bullet}$. □

Before ending this section, we present a structural property of $F^{(p)}_{\alpha,T_\kappa}$ and a preliminary uniform bound for $\|F^{(m)}_{\alpha,T_\kappa}\|_\infty$, which will be useful later (cf. Corollary 3.3.1 and Proposition 3.3.3).

Lemma 3.3.3. *For any $m, K_n \in \mathbb{N}$, any knot sequence $T_\kappa \in \mathcal{T}_{K_n}$ and any index set α defined in (3.11), the following hold:*

(1) For each $p = 1, \ldots, m-1$, $F^{(p)}_{\alpha,T_\kappa} = \begin{bmatrix} I_{m-p} & 0 \\ 0 & W^{(p)}_{\alpha,T_\kappa} \end{bmatrix}$ for some matrix $W^{(p)}_{\alpha,T_\kappa} \in \mathbb{R}^{(|\overline{\alpha}|+p)\times(K_n+p-1)}$.

(2) $\|F^{(m)}_{\alpha,T_\kappa}\|_\infty \le \left(\frac{2m}{c_{\kappa,1}} \cdot \max\left(1, \frac{c_{\kappa,2}}{K_n}\right) \cdot N\right)^{m-1} \cdot \left(K_n\right)^m$, where $N = K_n + m - 1$.

Proof. (1) Fix m, K_n, $T_\kappa \in \mathcal{T}_{K_n}$, and α. We prove this result by induction on p. By the definition of $F^{(1)}_{\alpha,T_\kappa}$ in (3.16), we see that statement (1) holds for $p = 1$ with $W^{(p)}_{\alpha,T_\kappa} = E_{\alpha,T_\kappa}$. Now suppose statement (1) holds for $p = 1, \ldots, p'$ with $p' \le m-2$, and consider $p'+1$. In view of the recursive definition (3.22) and the definitions of $\widehat{D}^{(q_\alpha)}$, $\Xi^{(p)}_{\alpha,T_\kappa}$, $\widehat{\Delta}_{p,T_\kappa}$, and $\widehat{S}^{(N)}$ given in (3.19), (3.20), and (3.21), we deduce via the induction hypothesis that

$$
\begin{aligned}
F^{(p'+1)}_{\alpha,T_\kappa} &= \widehat{D}^{(q_\alpha)} \cdot \Xi^{(p')}_{\alpha,T_\kappa} \cdot F^{(p')}_{\alpha,T_\kappa} \cdot \widehat{\Delta}_{p',T_\kappa} \cdot \widehat{S}^{(N)} \\
&= \widehat{D}^{(q_\alpha)} \cdot \begin{bmatrix} I_{m-p'} & 0 \\ 0 & \Sigma_{p',T_\kappa} \end{bmatrix} \cdot \begin{bmatrix} I_{m-p'} & 0 \\ 0 & W^{(p')}_{\alpha,T_\kappa} \end{bmatrix} \cdot \begin{bmatrix} I_{m-p'} & 0 \\ 0 & \Delta_{p',T_\kappa} \end{bmatrix} \cdot \widehat{S}^{(N)} \\
&= \widehat{D}^{(q_\alpha)} \cdot \begin{bmatrix} \widehat{S}^{(m-p')} & \mathbf{1}_{(m-p')\times(K_n+p'-1)} \\ 0 & \star \end{bmatrix} = \begin{bmatrix} I_{(m-p'-1)} & 0 \\ 0 & \star' \end{bmatrix},
\end{aligned}
$$

where $\star$ and $\star'$ are suitable submatrices, and the last two equalities follow from the structure of $\widehat{S}^{(N)}$ and $\widehat{D}^{(q_\alpha)}$. Letting $W^{(p'+1)}_{\alpha,T_\kappa} := \star'$, we obtain the desired equality via induction.

(2) It follows from the definition of $F^{(1)}_{\alpha,T_\kappa}$ in (3.16) that $\|F^{(1)}_{\alpha,T_\kappa}\|_\infty \le K_n$. Furthermore, by (3.22) and the definitions of $\widehat{D}^{(q_\alpha)}$, $\Xi^{(p)}_{\alpha,T_\kappa}$, $\widehat{\Delta}_{p,T_\kappa}$, and $\widehat{S}^{(N)}$ given in (3.19), (3.20), and (3.21), we have, for each $p = 1, \ldots, m-1$,

$$\begin{aligned}
\|F^{(p+1)}_{\alpha,T_\kappa}\|_\infty &= \left\|\widehat{D}^{(q_\alpha)} \cdot \Xi^{(p)}_{\alpha,T_\kappa} \cdot F^{(p)}_{\alpha,T_\kappa} \cdot \widehat{\Delta}_{p,T_\kappa} \cdot \widehat{S}^{(N)}\right\|_\infty \\
&\le \|\widehat{D}^{(q_\alpha)}\|_\infty \cdot \|\Xi^{(p)}_{\alpha,T_\kappa}\|_\infty \cdot \|F^{(p)}_{\alpha,T_\kappa}\|_\infty \cdot \|\widehat{\Delta}_{p,T_\kappa}\|_\infty \cdot \|\widehat{S}^{(N)}\|_\infty \\
&\le 2 \cdot \frac{mK_n}{c_{\kappa,1}} \cdot \|F^{(p)}_{\alpha,T_\kappa}\|_\infty \cdot \max\left(1, \frac{c_{\kappa,2}}{K_n}\right) \cdot N,
\end{aligned}$$

where we use (3.15) to bound $\|\Xi^{(p)}_{\alpha,T_\kappa}\|_\infty$ and $\|\widehat{\Delta}_{p,T_\kappa}\|_\infty$ in the last inequality. In view of this result and $\|F^{(1)}_{\alpha,T_\kappa}\|_\infty \le K_n$, the desired inequality follows. □

More properties of $F^{(m)}_{\alpha,T_\kappa}$ will be shown in Proposition 3.3.3 and Corollary 3.3.1.

3.3.3 Approximation of the B-spline Collocation Matrix

This section is concerned with the construction of the matrix X_{m,T_κ,L_n}, which approximates a certain B-spline collocation matrix. Moreover, we may think of $(X_{m,T_\kappa,L_n})_{ij}$ as an approximation of $B^{T_\kappa}_{m,i}\left(\frac{j-1}{L_n}\right)$, for all $i = 1, \ldots, N$ and $j = 1, \ldots, L_n$. Consequently, we may use X_{m,T_κ,L_n} to construct $\widetilde{\Lambda}_{T_\kappa,K_n,L_n}$, which approximates Λ_{K_n,P,T_κ}. Additionally, X_{m,T_κ,L_n} is constructed in a way such that the product $F^{(m)}_{\alpha,T_\kappa} \cdot X_{m,T_\kappa,L_n}$ can be easily computed via inductive principles; this is the main motivation for constructing X_{m,T_κ,L_n}. For a given K_n, let $L_n \in \mathbb{N}$ with $L_n > K_n/c_{\kappa,1}$, which will be taken later to hold for all large n; see Property **H** in Section 3.3.4. For a given knot sequence $T_\kappa \in \mathcal{T}_{K_n}$ of (K_n+1) knots on $[0,1]$ with $T_\kappa = \{0 = \kappa_0 < \kappa_1 < \cdots < \kappa_{K_n} = 1\}$, define $\widetilde{E}_{T_\kappa,L_n} \in \mathbb{R}^{K_n \times L_n}$ as

$$\left[\widetilde{E}_{T_\kappa,L_n}\right]_{j\ell} := \mathbf{I}_{[\kappa_{j-1},\kappa_j)}\left(\frac{\ell-1}{L_n}\right), \qquad \forall\ j = 1, \ldots, K_n, \quad \ell = 1, \ldots, L_n, \tag{3.24}$$

where $\mathbf{I}_{[\kappa_{j-1},\kappa_j)}$ is the indicator function on the interval $[\kappa_{j-1},\kappa_j)$. For each $j = 1,\ldots,K_n$, let ℓ_j be the cardinality of the index set $\{\ell \in \mathbb{N} \,|\, L_n\kappa_{j-1}+1 \le \ell < L_n\kappa_j + 1\}$. Hence, we have

$$\widetilde{E}_{T_\kappa,L_n} = \begin{bmatrix} \mathbf{1}_{\ell_1}^T & & & \\ & \mathbf{1}_{\ell_2}^T & & \\ & & \ddots & \\ & & & \mathbf{1}_{\ell_{K_n}}^T \end{bmatrix} \in \mathbb{R}^{K_n \times L_n}.$$

Let $L'_n := L_n + m - 1$, and for each $p = 1,\ldots,m$, define

$$\Gamma_p := \begin{bmatrix} I_{(m-p)} & 0 \\ 0 & L_n^{-1}\cdot I_{(L_n+p-1)} \end{bmatrix} \in \mathbb{R}^{L'_n\times L'_n}, \quad \text{and} \quad \widetilde{S}^{(p)}_{L_n} := \Gamma_p \cdot \widehat{S}^{(L'_n)} \in \mathbb{R}^{L'_n\times L'_n},$$

where $\widehat{S}^{(r)}$ is defined in (3.21). We then define the matrices $X_{p,T_\kappa,L_n} \in \mathbb{R}^{N\times L'_n}$ for the given T_κ and L_n inductively as:

$$X_{1,T_\kappa,L_n} := \begin{bmatrix} I_{m-1} & 0 \\ 0 & \widetilde{E}_{T_\kappa,L_n} \end{bmatrix}, \quad \text{and} \quad X_{p,T_\kappa,L_n} := \widehat{D}^{(N)}\cdot\widehat{\Delta}^{-1}_{p-1,T_\kappa}\cdot X_{p-1,T_\kappa,L_n}\cdot\widetilde{S}^{(p-1)}_{L_n}, \tag{3.25}$$

for each $p = 2,\ldots,m$. Note that X_{1,T_κ,L_n} is of full row rank for any T_κ, L_n, and hence, so is X_{p,T_κ,L_n} for each $p = 2,\ldots,m$, since $\widehat{D}^{(N)}$, $\widehat{\Delta}^{-1}_{p-1,T_\kappa}$, $\widehat{S}^{(L'_n)}$, and Γ_{p-1} are all invertible. Finally, define the matrix

$$\widetilde{\Lambda}_{T_\kappa,K_n,L_n} := \frac{K_n}{L_n}\cdot\left(X_{m,T_\kappa,L_n}\right)_{1:N,1:L_n}\cdot\left[\left(X_{m,T_\kappa,L_n}\right)_{1:N,1:L_n}\right]^T \in \mathbb{R}^{N\times N}. \tag{3.26}$$

It will be shown later (cf. Proposition 3.3.5) that $\widetilde{\Lambda}_{T_\kappa,K_n,L_n}$ approximates Λ_{K_n,P,T_κ} for all large n when L_n is suitably chosen.

As discussed in Section 3.2.3, the proof of the uniform Lipschitz property boils down to establishing certain uniform bounds in the ℓ_∞-norm, including uniform bounds on $\|\big(\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F_\alpha^T\big)^{-1}\|_\infty$, where $\Xi'_\alpha := K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}$. Therefore it is essential to study $F_\alpha \widetilde{\Lambda}_{T_\kappa,K_n,L_n} F_\alpha^T$, which approximates $F_\alpha \Lambda_{K_n,P,T_\kappa} F_\alpha^T$. In view of the definition of $\widetilde{\Lambda}_{T_\kappa,K_n,L_n}$, we see that the former matrix product is closely related to $F^{(m)}_{\alpha,T_\kappa} X_{m,T_\kappa,L_n}$ for a given index set α, knot sequence T_κ, and $L_n \in \mathbb{N}$. In what follows, we demonstrate certain important properties of $F^{(m)}_{\alpha,T_\kappa} X_{m,T_\kappa,L_n}$ to be used in the subsequent development.

Lemma 3.3.4. *Fix $m \in \mathbb{N}$. For any given α, T_κ, and L_n, the following hold:*

(1) For each $p = 2, \ldots, m$, $F^{(p)}_{\alpha,T_\kappa} \cdot X_{p,T_\kappa,L_n} = \widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha,T_\kappa} \cdot F^{(p-1)}_{\alpha,T_\kappa} \cdot X_{p-1,T_\kappa,L_n} \cdot \widetilde{S}^{(p-1)}_{L_n}$.

(2) For each $p = 1, \ldots, m-1$, there exists a matrix $Z_{p,\alpha,T_\kappa,L_n} \in \mathbb{R}^{(q_\alpha - m+p)\times(L_n+p-1)}$ such that

$$F^{(p)}_{\alpha,T_\kappa} \cdot X_{p,T_\kappa,L_n} = \begin{bmatrix} I_{m-p} & 0 \\ 0 & Z_{p,\alpha,T_\kappa,L_n} \end{bmatrix} \in \mathbb{R}^{q_\alpha \times L'_n}.$$

Proof. (1) It follows from the definitions of $F^{(p)}_{\alpha,T_\kappa}$ in (3.22) and X_{p,T_κ,L_n} in (3.25) respectively and $\widehat{S}^{(N)} \cdot \widehat{D}^{(N)} = I$ that for each $p = 2, \ldots, m$,

$$\begin{aligned} F^{(p)}_{\alpha,T_\kappa} \cdot X_{p,T_\kappa,L_n} &= \Big(\widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha,T_\kappa} \cdot F^{(p-1)}_{\alpha,T_\kappa} \cdot \widehat{\Delta}_{p-1,T_\kappa} \cdot \widehat{S}^{(N)}\Big) \\ &\quad \cdot \Big(\widehat{D}^{(N)} \cdot \widehat{\Delta}^{-1}_{p-1,T_\kappa} \cdot X_{p-1,T_\kappa,L_n} \cdot \widetilde{S}^{(p-1)}_{L_n}\Big) \\ &= \widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha,T_\kappa} \cdot F^{(p-1)}_{\alpha,T_\kappa} \cdot X_{p-1,T_\kappa,L_n} \cdot \widetilde{S}^{(p-1)}_{L_n}. \end{aligned}$$

(2) When $p = 1$, it is easy to see that

$$F^{(1)}_{\alpha,T_\kappa} \cdot X_{1,T_\kappa,L_n} = \begin{bmatrix} I_{m-1} & 0 \\ 0 & E_{\alpha,T_\kappa} \end{bmatrix} \begin{bmatrix} I_{m-1} & 0 \\ 0 & \widetilde{E}_{T_\kappa,L_n} \end{bmatrix} = \begin{bmatrix} I_{m-1} & 0 \\ 0 & Z_{1,\alpha,T_\kappa,L_n} \end{bmatrix},$$

where $Z_{1,\alpha,T_\kappa,L_n} := E_{\alpha,T_\kappa} \cdot \widetilde{E}_{T_\kappa,L_n}$. Hence, statement (2) holds for $p = 1$. Suppose statement (2) holds for $p = 1, \ldots, p'$, and consider $p' + 1$. In view of statement (1), the definitions of $\Gamma_{p'}$ and $\widetilde{S}^{(p')}_{L_n}$, (3.19) for $\Xi^{(p')}_{\alpha,T_\kappa}$, and the induction hypothesis, we have

$$
\begin{aligned}
&F^{(p'+1)}_{\alpha,T_\kappa} \cdot X_{p'+1,T_\kappa,L_n} = \widehat{D}^{(q_\alpha)} \cdot \Xi^{(p')}_{\alpha,T_\kappa} \cdot F^{(p')}_{\alpha,T_\kappa} \cdot X_{p',T_\kappa,L_n} \cdot \widetilde{S}^{(p')}_{L_n} \\
&= \widehat{D}^{(q_\alpha)} \cdot \Xi^{(p')}_{\alpha,T_\kappa} \cdot F^{(p')}_{\alpha,T_\kappa} \cdot X_{p',T_\kappa,L_n} \cdot \Gamma_{p'} \cdot \widehat{S}^{L'_n} \\
&= \widehat{D}^{(q_\alpha)} \cdot \begin{bmatrix} I_{m-p'} & 0 \\ 0 & \Sigma_{p',T_\kappa} \end{bmatrix} \cdot \begin{bmatrix} I_{m-p'} & 0 \\ 0 & Z_{p',\alpha,T_\kappa,L_n} \end{bmatrix} \cdot \begin{bmatrix} I_{m-p'} & 0 \\ 0 & L_n^{-1} \cdot I_{L_n+p'-1} \end{bmatrix} \cdot \widehat{S}^{(L'_n)} \\
&= \widehat{D}^{(q_\alpha)} \cdot \begin{bmatrix} \widehat{S}^{(m-p')} & \mathbf{1}_{(m-p')\times(L_n+p'-1)} \\ 0 & \star \end{bmatrix} = \begin{bmatrix} I_{(m-p'-1)} & 0 \\ 0 & \star' \end{bmatrix},
\end{aligned}
$$

where $\star$ and $\star'$ are suitable submatrices, and the last two equalities follow from the structure of $\widehat{S}^{(L'_n)}$ and $\widehat{D}^{(q_\alpha)}$. Letting $Z_{p'+1,\alpha,T_\kappa,L_n} := \star'$, we arrive at the desired equality via induction. □

In what follows, we develop an inductive formula to compute $Z_{p,\alpha,T_\kappa,L_n}$. For notational simplicity, we use Z_p, Y_p, and τ_s in place of $Z_{p,\alpha,T_\kappa,L_n}$, $F^{(p)}_{\alpha,T_\kappa} \cdot X_{p,T_\kappa,L_n}$, and $\tau_{\alpha,T_\kappa,s}$ (cf. (3.17)) respectively for fixed α, T_κ, and L_n. For each $p = 2, \ldots, m$, it follows from statement (1) of Lemma 3.3.4 that for any $j = 1, \ldots, |\overline{\alpha}| + p$ and $k = 1, \ldots, L_n + p - 1$,

$$
\begin{aligned}
\big[Z_p\big]_{j,k} &= \Big[\widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha,T_\kappa} \cdot Y_{p-1} \cdot \widetilde{S}^{(p-1)}_{L_n}\Big]_{j+m-p,\, k+m-p} \\
&= \Big[\widehat{D}^{(q_\alpha)} \Xi^{(p-1)}_{\alpha,T_\kappa}\Big]_{(j+m-p)\bullet} \cdot \Big[Y_{p-1} \widetilde{S}^{(p-1)}_{L_n}\Big]_{\bullet(k+m-p)}.
\end{aligned}
$$

In light of (3.19), we have, for any $j = 1, \dots, |\overline{\alpha}| + p$,

$$\left(\widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha, T_\kappa}\right)_{(j+m-p)\bullet} = \begin{cases} \left(\underbrace{0, \dots, 0}_{m-p}, 1, -\frac{p-1}{\tau_1 - \tau_{2-p}}, \underbrace{0, \dots, 0}_{|\overline{\alpha}|+p-2}\right) & \text{if } \; j = 1 \\ \left(\underbrace{0, \dots, 0}_{j+m-p-1}, \frac{p-1}{\tau_{j-1} - \tau_{j-p}}, -\frac{p-1}{\tau_j - \tau_{j-p+1}}, \underbrace{0, \dots, 0}_{|\overline{\alpha}|-j+p-1}\right) & \text{if } \; 1 < j < |\overline{\alpha}| + p \\ \left(\underbrace{0, \dots, 0}_{|\overline{\alpha}|+m-1}, \frac{p-1}{\tau_{|\overline{\alpha}|+p-1} - \tau_{|\overline{\alpha}|}}\right) & \text{if } \; j = |\overline{\alpha}| + p. \end{cases}$$

Moreover, by virtue of Lemma 3.3.4, we have

$$\begin{aligned} Y_{p-1} \cdot \widetilde{S}^{(p-1)}_{L_n} &= Y_{p-1} \cdot \Gamma_{p-1} \cdot \widehat{S}^{(L'_n)} = \begin{bmatrix} I_{m-p+1} & 0 \\ 0 & \frac{Z_{p-1}}{L_n} \end{bmatrix} \cdot \widehat{S}^{(L'_n)} \\ &= \begin{bmatrix} I_{m-p} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \frac{Z_{p-1}}{L_n} \end{bmatrix} \cdot \widehat{S}^{(L'_n)} = \begin{bmatrix} \widehat{S}^{(m-p)} & \mathbf{1}_{m-p} & \mathbf{1}_{(m-p)\times(L_n+p-2)} \\ 0 & 1 & \mathbf{1}^T_{L_n+p-2} \\ 0 & 0 & \frac{Z_{p-1} \cdot \widehat{S}^{(L_n+p-2)}}{L_n} \end{bmatrix}. \end{aligned}$$

This shows in particular that for each $j = 2, \dots, |\overline{\alpha}| + p$ and $k = 2, \dots, L_n + p - 1$,

$$\left[Y_{p-1} \cdot \widetilde{S}^{(p-1)}_{L_n}\right]_{j+m-p,\, k+m-p} = L_n^{-1} \left[Z_{p-1} \cdot \widehat{S}^{(L_n+p-2)}\right]_{j-1,\, k-1} = L_n^{-1} \cdot \sum_{\ell=1}^{k-1} \left[Z_{p-1}\right]_{j-1,\, \ell}.$$

Combining the above results, we have, for any $p \geq 2$, $j = 1, \dots, |\overline{\alpha}| + p$, and $k = 1, \dots, L_n + p - 1$,

$$\left[Z_p\right]_{j,\, k} = \sum_{s=1}^{q_\alpha} \left[\widehat{D}^{(q_\alpha)} \cdot \Xi^{(p-1)}_{\alpha, T_\kappa}\right]_{j+m-p,\, s} \cdot \left[Y_{p-1} \cdot \widetilde{S}^{(p-1)}_{L_n}\right]_{s,\, k+m-p} \tag{3.27}$$

$$
= \begin{cases} \delta_{j,1} & \text{if } \ k=1 \\ 1-\frac{p-1}{L_n(\tau_1-\tau_{2-p})}\sum_{\ell=1}^{k-1}\left[Z_{p-1}\right]_{1,\ell} & \text{if } \ j=1, \text{ and } k>1 \\ \frac{p-1}{L_n(\tau_{j-1}-\tau_{j-p})}\sum_{\ell=1}^{k-1}\left[Z_{p-1}\right]_{j-1,\ell} & \\ \qquad -\frac{p-1}{L_n(\tau_j-\tau_{j-p+1})}\sum_{\ell=1}^{k-1}\left[Z_{p-1}\right]_{j,\ell} & \text{if } \ 1<j<|\overline{\alpha}|+p, \text{ and } k>1 \\ \frac{p-1}{L_n(\tau_{|\overline{\alpha}|+p-1}-\tau_{|\overline{\alpha}|})}\sum_{\ell=1}^{k-1}\left[Z_{p-1}\right]_{|\overline{\alpha}|+p-1,\ell} & \text{if } \ j=|\overline{\alpha}|+p, \text{ and } k>1. \end{cases}
$$

The above results on $Z_{p,\alpha,T_\kappa,L_n}$ will be exploited to establish uniform bounds for the uniform Lipschitz property in the next section (cf. Proposition 3.3.2).

3.3.4 Preliminary Uniform Bounds

This section establishes uniform bounds and uniform approximation error bounds on several of the constructed matrices. These results lay a solid foundation for the proof of Theorem 3.2.1.

The first result of this section (cf. Proposition 3.3.2) shows that the entries of each row of $Z_{p,\alpha,T_\kappa,L_n}$ introduced in Lemma 3.3.4 are sufficiently close to the corresponding values of a B-spline defined on a certain knot sequence for large L_n. Hence, each row of $Z_{p,\alpha,T_\kappa,L_n}$ can be approximated by an appropriate B-spline; more importantly, the approximation error is shown to be uniformly bounded, regardless of α and T_κ. This result forms a cornerstone for many critical uniform bounds in the proof of the uniform Lipschitz property.

Recall in Section 3.3.2 that for a given $K_n \in \mathbb{N}$, knot sequence $T_\kappa \in \mathcal{T}_{K_n}$, and index set $\alpha \subseteq \{1, \ldots, K_n - 1\}$ defined in (3.11), the complement of α is given by $\overline{\alpha} = \{i_1, \ldots, i_{|\overline{\alpha}|}\}$ with $1 \leq i_1 < \cdots < i_{|\overline{\alpha}|} \leq K_n - 1$. For the given $\overline{\alpha}$ and T_κ, define the following knot sequence with the usual extension $\kappa_{i_s} = 0$ for $s < 0$ and $\kappa_{i_s} = 1$ for $s > |\overline{\alpha}| + 1$:

$$V_{\alpha,T_\kappa} := \Big\{0 = \kappa_{i_0} < \kappa_{i_1} < \kappa_{i_2} < \cdots < \kappa_{i_{|\overline{\alpha}|}} < \kappa_{i_{|\overline{\alpha}|+1}} = 1\Big\}. \tag{3.28}$$

Let $\{B_{p,j}^{V_{\alpha,T_\kappa}}\}_{j=1}^{|\overline{\alpha}|+p}$ be the B-splines of order p on $[0,1]$ defined by V_{α,T_κ}. With this notation, we present the following proposition.

Proposition 3.3.2. *Given $K_n, L_n \in \mathbb{N}$, let $M_n \in \mathbb{N}$ with $M_n \geq m \cdot K_n/c_{\kappa,1}$. Then for each $p = 1, \ldots, m$, any $T_\kappa \in \mathcal{T}_{K_n}$, any index set α, any $j = 1, \ldots, |\overline{\alpha}| + p$, and any $k = 1, \ldots, L_n$,*

$$\left| \big[Z_{p,\alpha,T_\kappa,L_n}\big]_{j,\,k} - B_{p,j}^{V_{\alpha,T_\kappa}}\left(\frac{k-1}{L_n}\right) \right| \leq 6 \cdot \big(2^{p-1} - 1\big) \cdot \frac{\big(M_n\big)^{p-1}}{L_n}, \qquad \forall\ n \in \mathbb{N}.$$

Proof. We prove this result by induction on p. Given arbitrary $K_n, L_n \in \mathbb{N}$, $T_\kappa \in \mathcal{T}_{K_n}$, and α defined in (3.11), we use Z_p to denote $Z_{p,\alpha,T_\kappa,L_n}$ to simplify notation. Consider $p = 1$ first. It follows from the proof of statement (2) of Lemma 3.3.4 that $Z_1 = E_{\alpha,T_\kappa} \cdot \widetilde{E}_{T_\kappa,L_n}$. In view of the definitions of E_{α,T_κ} and $\widetilde{E}_{T_\kappa,L_n}$ in (3.16) and (3.24) respectively, we have, for any $j = 1, \ldots, |\overline{\alpha}| + 1$ and $k = 1, \ldots, L_n$,

$$\begin{aligned} \big[Z_1\big]_{j,\,k} &= \sum_{\ell=1}^{K_n} \big[E_{\alpha,T_\kappa}\big]_{j,\,\ell} \cdot \big[\widetilde{E}_{T_\kappa,L_n}\big]_{\ell,\,k} = \sum_{\ell=1}^{K_n} \mathbf{I}_{[\kappa_{i_{j-1}},\kappa_{i_j})}\left(\kappa_{\ell-1}\right) \cdot \mathbf{I}_{[\kappa_{\ell-1},\kappa_\ell)}\left(\frac{k-1}{L_n}\right) \\ &= \mathbf{I}_{[\kappa_{i_{j-1}},\kappa_{i_j})}\left(\frac{k-1}{L_n}\right) = B_{1,j}^{V_{\alpha,T_\kappa}}\left(\frac{k-1}{L_n}\right). \end{aligned} \tag{3.29}$$

This shows that the proposition holds for $p = 1$.

Suppose that the proposition holds for $p = 1, \ldots, \widehat{p}$ with $1 \le \widehat{p} \le m-1$. Consider $p = \widehat{p}+1$ now. Define

$$\theta_{\widehat{p},\alpha,T_\kappa,L_n} := 2M_n \max_{j=1,\ldots,|\overline{\alpha}|+\widehat{p}} \left(\max_{k=2,\ldots,L_n} \left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \big[Z_{\widehat{p}}\big]_{j,\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x)\,dx \right| \right). \quad (3.30)$$

We show below that $\big|[Z_{\widehat{p}+1}]_{j,k} - B_{\widehat{p}+1,j}^{V_\alpha,T_\kappa}(\frac{k-1}{L_n})\big| \le \theta_{\widehat{p},\alpha,T_\kappa,L_n}$ for any $j = 1, \ldots, |\overline{\alpha}| + \widehat{p}+1$ and $k = 1, \ldots, L_n$. To see this, consider the following cases via the entry formula of $Z_{\widehat{p}+1}$ in (3.27):

(i) $k = 1$ and $j = 1, \ldots, |\overline{\alpha}|+\widehat{p}+1$. In view of (3.27), we have $[Z_{\widehat{p}+1}]_{j,1} = \delta_{j,1} = B_{\widehat{p}+1,j}^{V_\alpha,T_\kappa}(0)$ for each j. This implies that $\big|[Z_{\widehat{p}+1}]_{j,1} - B_{\widehat{p}+1,j}^{V_\alpha,T_\kappa}(0)\big| = 0 \le \theta_{\widehat{p},\alpha,T_\kappa,L_n}$ for each j.

(ii) $j = 1$ and $k = 2, \ldots, L_n$. It follows from (3.2) that

$$\begin{aligned} B_{\widehat{p}+1,1}^{V_\alpha,T_\kappa}(x) &= B_{\widehat{p}+1,1}^{V_\alpha,T_\kappa}(0) - \frac{\widehat{p}}{\kappa_{i_1} - \kappa_{i_{1-\widehat{p}}}} \int_0^x B_{\widehat{p},1}^{V_\alpha,T_\kappa}(t)dt \\ &= 1 - \frac{\widehat{p}}{\kappa_{i_1} - \kappa_{i_{1-\widehat{p}}}} \int_0^x B_{\widehat{p},1}^{V_\alpha,T_\kappa}(t)dt. \end{aligned}$$

Since each τ_s in (3.27) is $\tau_{\alpha,T_\kappa,s}$ defined in (3.17), we have $\tau_1 = \kappa_{i_1}$ and $\tau_{2-\widehat{p}-1} = \kappa_{i_{1-\widehat{p}}}$. Hence,

$$\begin{aligned} \left| \big[Z_{\widehat{p}+1}\big]_{1,k} - B_{\widehat{p}+1,1}^{V_\alpha,T_\kappa}\Big(\frac{k-1}{L_n}\Big) \right| &= \frac{\widehat{p}}{\kappa_{i_1} - \kappa_{i_{1-\widehat{p}}}} \left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \big[Z_{\widehat{p}}\big]_{1,\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},1}^{V_\alpha,T_\kappa}(t)dt \right| \\ &\le \theta_{\widehat{p},\alpha,T_\kappa,L_n}, \end{aligned}$$

where the last inequality follows from (3.15) due to $\frac{\widehat{p}}{\kappa_{i_s} - \kappa_{i_{s-\widehat{p}}}} \le \widehat{p} \cdot K_n/c_{\kappa,1} \le M_n$ for any s.

(iii) $j = 2, \ldots, |\overline{\alpha}| + \widehat{p}$ and $k = 2, \ldots, L_n$. It follows from the integral form of (3.2) that

$$B_{\widehat{p}+1,j}^{V_\alpha,T_\kappa}(x) = \frac{\widehat{p}}{\kappa_{i_{j-1}} - \kappa_{i_{j-\widehat{p}-1}}} \int_0^x B_{\widehat{p},j-1}^{V_\alpha,T_\kappa}(t)dt - \frac{\widehat{p}}{\kappa_{i_j} - \kappa_{i_{j-\widehat{p}}}} \int_0^x B_{\widehat{p},j}^{V_\alpha,T_\kappa}(t)dt.$$

Using this equation, (3.27) and (3.30), and an argument similar to that of Case (ii), we have

$$\begin{aligned} &\left| \left[Z_{\widehat{p}+1}\right]_{j,k} - B_{\widehat{p}+1,j}^{V_\alpha,T_\kappa}\left(\frac{k-1}{L_n}\right) \right| \\ &\leq \frac{\widehat{p}}{\kappa_{i_{j-1}} - \kappa_{i_{j-\widehat{p}-1}}} \left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \left[Z_{\widehat{p}}\right]_{j-1,\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},j-1}^{V_\alpha,T_\kappa}(t)dt \right| \\ &\quad + \frac{\widehat{p}}{\kappa_{i_j} - \kappa_{i_{j-\widehat{p}}}} \left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \left[Z_{\widehat{p}}\right]_{j,\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},j}^{V_\alpha,T_\kappa}(t)dt \right| \leq \theta_{\widehat{p},\alpha,T_\kappa,L_n}. \end{aligned}$$

(iv) $j = |\overline{\alpha}| + \widehat{p} + 1$ and $k = 2, \ldots, L_n$. We have from (3.2) that

$$B_{\widehat{p}+1,|\overline{\alpha}|+\widehat{p}+1}^{V_\alpha,T_\kappa}(x) = \frac{\widehat{p}}{\kappa_{i_{|\overline{\alpha}|+\widehat{p}}} - \kappa_{i_{|\overline{\alpha}|}}} \int_0^x B_{\widehat{p},|\overline{\alpha}|+\widehat{p}}^{V_\alpha,T_\kappa}(t)dt.$$

This, along with (3.27) and an argument similar to that of Case (ii), leads to

$$\begin{aligned} &\left| \left[Z_{\widehat{p}+1}\right]_{|\overline{\alpha}|+\widehat{p}+1,k} - B_{\widehat{p}+1,|\overline{\alpha}|+\widehat{p}+1}^{V_\alpha,T_\kappa}\left(\frac{k-1}{L_n}\right) \right| \\ &= \frac{\widehat{p}}{\kappa_{i_{|\overline{\alpha}|+\widehat{p}}} - \kappa_{i_{|\overline{\alpha}|}}} \left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \left[Z_{\widehat{p}}\right]_{|\overline{\alpha}|+\widehat{p},\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},|\overline{\alpha}|+\widehat{p}}^{V_\alpha,T_\kappa}(t)dt \right| \leq \theta_{\widehat{p},\alpha,T_\kappa,L_n}. \end{aligned}$$

This shows that $\left|[Z_{\widehat{p}+1}]_{j,k} - B_{\widehat{p}+1,j}^{V_\alpha,T_\kappa}(\frac{k-1}{L_n})\right| \leq \theta_{\widehat{p},\alpha,T_\kappa,L_n}$ for any $j = 1, \ldots, |\overline{\alpha}| + \widehat{p} + 1$ and $k = 1, \ldots, L_n$.

Finally, we show that the upper bound $\theta_{\widehat{p},\alpha,T_\kappa,L_n}$ attains the specified uniform bound, regardless of α and T_κ. When $\widehat{p} = 1$, in light of (3.29) and $B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x) = \mathbf{I}_{[\kappa_{i_{j-1}},\kappa_{i_j})}(x)$ on

$[0,1)$, we derive via straightforward computation that for any $j = 1, \ldots, |\overline{\alpha}| + \widehat{p}$ and each $k = 2, \ldots, L_n$,

$$\left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \big[Z_{\widehat{p}}\big]_{j,\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x)\, dx \right| \le \frac{1}{L_n}. \tag{3.31}$$

This implies that $\theta_{\widehat{p},\alpha,T_\kappa,L_n} \le 2M_n/L_n \le 6 \cdot (2^{\widehat{p}} - 1) \cdot (M_n)^{\widehat{p}}/L_n$. In what follows, consider $2 \le \widehat{p} \le m-1$. Letting $C_{\widehat{p}} := 6 \cdot (2^{\widehat{p}-1} - 1)$, the induction hypothesis states that $\big|[Z_{\widehat{p}}]_{j,k} - B_{\widehat{p},j}^{V_\alpha,T_\kappa}(\frac{k-1}{L_n})\big| \le C_{\widehat{p}} \cdot (M_n)^{\widehat{p}-1}/L_n$ for any $j = 1, \ldots, |\overline{\alpha}| + \widehat{p}$ and $k = 1, \ldots, L_n$. Moreover, for each j, the B-spline $B_{\widehat{p},j}^{V_\alpha,T_\kappa}$ is continuous on $[0,1]$ and is differentiable except at (at most) finitely many points in $[0,1]$. By the derivative formula (3.2), we have, for any $x \in [0,1]$ where the derivative exists,

$$\begin{aligned} \left| \Big(B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x)\Big)' \right| &= \left| \frac{\widehat{p}-1}{\kappa_{i_{j-1}} - \kappa_{i_{j-\widehat{p}}}} B_{\widehat{p}-1,j-1}^{V_\alpha,T_\kappa}(x) - \frac{\widehat{p}-1}{\kappa_{i_j} - \kappa_{i_{j-\widehat{p}+1}}} B_{\widehat{p}-1,j}^{V_\alpha,T_\kappa}(x) \right| \\ &\le \frac{2(\widehat{p}-1)K_n}{c_{\kappa,1}}, \end{aligned} \tag{3.32}$$

where we use the upper bound on B-splines and the fact that $\frac{\widehat{p}-1}{\kappa_{i_s} - \kappa_{i_{s-\widehat{p}+1}}} \le (\widehat{p}-1)K_n/c_{\kappa,1}$ for any s. Since $M_n \ge m \cdot K_n/c_{\kappa,1}$, we have $(\widehat{p}-1)K_n/c_{\kappa,1} \le M_n$. This further implies via $\widehat{p} \ge 2$ that

$$\left| \Big(B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x)\Big)' \right| \le \frac{2(\widehat{p}-1)K_n}{c_{\kappa,1}} \le 2M_n \le 2(M_n)^{\widehat{p}-1}. \tag{3.33}$$

For each fixed $j = 1, \ldots, |\overline{\alpha}| + \widehat{p} + 1$, we apply Lemma 3.3.1 with $\widetilde{n} := L_n$, $a := 0$, $b := 1$, $s_k := k/L_n$, $\varrho := 1/L_n$, $f(x) := B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x)$, $v = (v_k) := \big([Z_{\widehat{p}}]_{j,k}\big)$, $\mu_1 := C_{\widehat{p}} \frac{(M_n)^{\widehat{p}-1}}{L_n}$, and $\mu_2 := 2(M_n)^{\widehat{p}-1}$ to obtain that for each $k = 2, \ldots, L_n$,

$$\left| \sum_{\ell=1}^{k-1} \frac{1}{L_n} \big[Z_{\widehat{p}}\big]_{j,\ell} - \int_0^{\frac{k-1}{L_n}} B_{\widehat{p},j}^{V_\alpha,T_\kappa}(x)\, dx \right| \le \frac{C_{\widehat{p}} \cdot (M_n)^{\widehat{p}-1}}{L_n} + \frac{3(M_n)^{\widehat{p}-1}}{L_n} = \big(C_{\widehat{p}} + 3\big) \frac{(M_n)^{\widehat{p}-1}}{L_n}.$$

Note that the above upper bound is independent of α, T_κ, j and k. By using this result, (3.30), and $C_{\widehat{p}} = 6 \cdot (2^{\widehat{p}-1} - 1)$, we deduce the following uniform bound for $\theta_{\widehat{p},\alpha,T_\kappa,L_n}$ independent of α and T_κ:

$$\theta_{\widehat{p},\alpha,T_\kappa,L_n} \leq 2M_n \cdot \big(C_{\widehat{p}} + 3\big) \frac{(M_n)^{\widehat{p}-1}}{L_n} = 6 \cdot (2^{\widehat{p}} - 1) \cdot \frac{(M_n)^{\widehat{p}}}{L_n}.$$

Therefore, the proposition holds by the induction principle. □

The uniform error bound established in Proposition 3.3.2 yields the following important result for the matrix $F^{(m)}_{\alpha,T_\kappa}$ constructed in Section 3.3.2.

Proposition 3.3.3. *For any given $m, K_n \in \mathbb{N}$, any knot sequence $T_\kappa \in \mathcal{T}_{K_n}$, and any index set α and its associated knot sequence V_{α,T_κ} defined in (3.28), the B-splines $\{B^{V_{\alpha,T_\kappa}}_{m,\ell}\}_{\ell=1}^{q_\alpha}$ and $\{B^{T_\kappa}_{m,j}\}_{j=1}^{N}$ satisfy for each $\ell = 1, \ldots, q_\alpha$,*

$$\sum_{j=1}^{N} \Big[F^{(m)}_{\alpha,T_\kappa}\Big]_{\ell,j} B^{T_\kappa}_{m,j}(x) = B^{V_{\alpha,T_\kappa}}_{m,\ell}(x), \qquad \forall\, x \in [0,1]. \tag{3.34}$$

Proof. Consider $m = 1$ first. Recall that $\kappa_{i_0} = 0$, $\kappa_{i_{|\overline{\alpha}|+1}} = \kappa_{i_{q_\alpha}} = 1$, and $F^{(1)}_{\alpha,T_\kappa} = E_{\alpha,T_\kappa}$ (cf. (3.16)). It follows from (3.17) and (3.18) that for each $\ell = 1, \ldots, q_\alpha$ and any $x \in [0,1]$,

$$\begin{aligned}
&\sum_{j=1}^{K_n} \Big[F^{(1)}_{\alpha,T_\kappa}\Big]_{\ell,j} B^{T_\kappa}_{1,j}(x) \\
&= \sum_{j=1}^{K_n-1} \mathbf{I}_{[\kappa_{i_{\ell-1}}, \kappa_{i_\ell})}(\kappa_{j-1}) \cdot \mathbf{I}_{[\kappa_{j-1}, \kappa_j)}(x) + \mathbf{I}_{[\kappa_{i_{\ell-1}}, \kappa_{i_\ell})}(\kappa_{K_n-1}) \cdot \mathbf{I}_{[\kappa_{K_n-1}, \kappa_{K_n}]}(x) \\
&= \begin{cases} \mathbf{I}_{[\kappa_{i_{\ell-1}}, \kappa_{i_\ell})}(x) & \text{if } \ \ell \in \{1, \ldots, q_\alpha - 1\} \\[2ex] \mathbf{I}_{[\kappa_{i_{q_\alpha-1}}, \kappa_{i_{q_\alpha}}]}(x) & \text{if } \ \ell = q_\alpha \end{cases} \\
&= B^{V_{\alpha,T_\kappa}}_{1,\ell}(x).
\end{aligned}$$

In what follows, consider $m \geq 2$. Recall that when α is the empty set, $q_\alpha = N = K_n + m - 1$, $F^{(m)}_{\alpha,T_\kappa} = I_N$, $B^{V_\emptyset,T_\kappa}_{m,\ell} = B^{T_\kappa}_{m,\ell}$ for each ℓ, and $Z_{m,\emptyset,T_\kappa,L_n} = X_{m,T_\kappa,L_n} \in \mathbb{R}^{q_\alpha \times (L_n+m-1)}$ (cf. Lemma 3.3.4). Motivated by these observations and $F^{(m)}_{\alpha,T_\kappa} \cdot X_{m,T_\kappa,L_n} = Z_{m,\alpha,T_\kappa,L_n}$ for any α and T_κ (cf. Lemma 3.3.4), a key idea for the subsequent proof is to approximate $B^{T_\kappa}_{m,j}$ and $B^{V_\alpha,T_\kappa}_{m,\ell}$ by X_{m,T_κ,L_n} and $Z_{m,\alpha,T_\kappa,L_n}$ respectively, where approximation errors can be made arbitrarily small by choosing a sufficiently large L_n in view of Proposition 3.3.2.

Fix m, K_n, α, and T_κ. Let $M_n := \lceil m \cdot K_n / c_{\kappa,1} \rceil$. Hence both M_n and $N := K_n + m - 1$ are fixed natural numbers. Since we shall choose a sequence of sufficiently large L_n independent of the above-mentioned fixed numbers, we write L_n as L_s below to avoid notational confusion. In order to apply Proposition 3.3.2, we first consider rational x in $[0, 1)$. Let $x_* \in [0, 1)$ be an arbitrary but fixed rational number, and let (L_s) be an increasing sequence of natural numbers (depending on x_*) such that $L_s \to \infty$ as $s \to \infty$ and for each s, $x_* = \frac{i^*_s - 1}{L_s}$ for some $i^*_s \in \{1, \ldots, L_s\}$. (Here i^*_s depends on x_* and L_s only.) In light of the observations $B^{V_\emptyset,T_\kappa}_{m,\ell} = B^{T_\kappa}_{m,\ell}$ and $Z_{m,\emptyset,T_\kappa,L_s} = X_{m,T_\kappa,L_s}$, it follows from Proposition 3.3.2 that for each $\ell = 1, \ldots, q_\alpha$ and each s,

$$\left| \big[X_{m,T_\kappa,L_s}\big]_{\ell,\, i^*_s} - B^{T_\kappa}_{m,\ell}(x_*) \right| = \left| \big[Z_{m,\emptyset,T_\kappa,L_s}\big]_{\ell,\, i^*_s} - B^{V_\emptyset,T_\kappa}_{m,\ell}\Big(\frac{i^*_s - 1}{L_s}\Big) \right| \leq \frac{6\,(2^m - 1)\, M_n^{m-1}}{L_s}. \tag{3.35}$$

By using $Z_{m,\alpha,T_\kappa,L_s} = F^{(m)}_{\alpha,T_\kappa} \cdot X_{m,T_\kappa,L_s}$ (cf. Lemma 3.3.4), we thus have, for each $\ell = 1, \ldots, q_\alpha$,

$$\left| \sum_{j=1}^{N} \big[F^{(m)}_{\alpha,T_\kappa}\big]_{\ell,j} \, B^{T_\kappa}_{m,j}(x_*) - B^{V_\alpha,T_\kappa}_{m,\ell}(x_*) \right|$$

$$
\begin{aligned}
&\leq \sum_{j=1}^{N} \left| \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} \cdot \Big(B_{m,j}^{T_\kappa}(x_*) - \big[X_{m,T_\kappa,L_s}\big]_{j,i_s^*} \Big) \right| \\
&\qquad + \left| \sum_{j=1}^{N} \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} \cdot \big[X_{m,T_\kappa,L_s}\big]_{j,i_s^*} - B_{m,\ell}^{V_{\alpha,T_\kappa}}(x_*) \right| \\
&\leq \sum_{j=1}^{N} \left| \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} \right| \cdot \left| B_{m,j}^{T_\kappa}(x_*) - \big[X_{m,T_\kappa,L_s}\big]_{j,i_s^*} \right| + \left| \big[Z_{m,\alpha,T_\kappa,L_s}\big]_{\ell,i_s^*} - B_{m,\ell}^{V_{\alpha,T_\kappa}}\Big(\frac{i_s^* - 1}{L_s}\Big) \right| \\
&\leq N \cdot \left[\Big(\frac{2m}{c_{\kappa,1}} \cdot \max\Big(1, \frac{c_{\kappa,2}}{K_n}\Big) \cdot N \Big)^{m-1} \cdot \big(K_n\big)^m \right] \cdot \frac{6(2^{m-1}-1)M_n^{m-1}}{L_s} \\
&\qquad + \frac{6\,(2^{m-1}-1)M_n^{m-1}}{L_s},
\end{aligned}
$$

where the last inequality follows from the bounds given in statement (2) of Lemma 3.3.3, (3.35), and Proposition 3.3.2. By virtue of the fact that $L_s^{-1} \to 0$ as $s \to \infty$, we have $\sum_{j=1}^{N} \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} B_{m,j}^{T_\kappa}(x_*) = B_{m,\ell}^{V_{\alpha,T_\kappa}}(x_*)$. This shows that (3.34) holds for all rational $x \in [0,1)$. Since $B_{m,j}^{T_\kappa}$ and $B_{m,\ell}^{V_{\alpha,T_\kappa}}$ are continuous on $[0,1]$ for any j, ℓ, T_κ, and α when $m \geq 2$, we conclude via the density of rational numbers in $[0,1)$ that (3.34) holds for all $x \in [0,1)$. Finally, the continuity of $B_{m,j}^{T_\kappa}$ and $B_{m,\ell}^{V_{\alpha,T_\kappa}}$ also shows that (3.34) holds at $x = 1$. □

Using Proposition 3.3.3, we derive tight uniform bounds for both $\big\|(F_{\alpha,T_\kappa}^{(m)})^T\big\|_\infty$ and $\big\|K_n^{-1}\,\Xi_{\alpha,T_\kappa}^{(m)}\,F_{\alpha,T_\kappa}^{(m)}\big\|_\infty$ in the next corollary; these bounds are crucial for the proof of Theorem 3.2.1 (cf. Section 3.3.5). We introduce more notation. Let $\mathbf{e}_\ell$ be the ℓth standard basis (column) vector in the Euclidean space, i.e., $\big[\mathbf{e}_\ell\big]_k = \delta_{\ell,k}$. Moreover, for a given vector $v = (v_1, \ldots, v_k) \in \mathbb{R}^k$, the number of sign changes of v is defined as the largest integer $r_v \in \mathbb{Z}_+$ such that for some $1 \leq j_1 < \cdots < j_{r_v} \leq k$, $v_{j_i} \cdot v_{j_{i+1}} < 0$ for each $i = 1, \ldots, r_v$ [14, page 138]. Clearly, $\mathbf{e}_\ell$ has zero sign changes for each ℓ.

Corollary 3.3.1. *For any $m \in \mathbb{N}$, any knot sequence $T_\kappa \in \mathcal{T}_{K_n}$, and any index set α defined in (3.11), the following hold:*

(1) $F^{(m)}_{\alpha,T_\kappa}$ *is a nonnegative matrix,* $\big\|(F^{(m)}_{\alpha,T_\kappa})^T\big\|_\infty = 1$*, and*

(2) $\big\|K_n^{-1}\,\Xi^{(m)}_{\alpha,T_\kappa}\,F^{(m)}_{\alpha,T_\kappa}\big\|_\infty \le \frac{m}{c_{\kappa,1}}$.

Proof. When α is the empty set, $F^{(m)}_{\alpha,T_\kappa}$ is the identity matrix and $\big\|K_n^{-1}\,\Xi^{(m)}_{\alpha,T_\kappa}\big\|_\infty \le \frac{m}{c_{\kappa,1}}$ (using (3.15)) so that the corollary holds. We thus consider nonempty α as follows.

(1) Observe that the knot sequence T_κ can be formed by inserting additional knots into the knot sequence V_{α,T_κ}. By Proposition 3.3.3, we see that for each $\ell = 1,\ldots,q_\alpha$, $\sum_{j=1}^{N}\big[F^{(m)}_{\alpha,T_\kappa}\big]_{\ell,j}B^{T_\kappa}_{m,j}(x) = B^{V_{\alpha,T_\kappa}}_{m,\ell}(x) = \sum_{i=1}^{q_\alpha}[\mathbf{e}_\ell]_i B^{V_{\alpha,T_\kappa}}_{m,i}(x)$ for all $x\in[0,1]$. Since $\mathbf{e}_\ell$ has zero sign changes, we deduce via [14, Lemma 27, Chapter XI] that $\big(F^{(m)}_{\alpha,T_\kappa}\big)_{\ell,\bullet}$ has zero sign changes for each $\ell = 1,\ldots,q_\alpha$. This shows that either $\big(F^{(m)}_{\alpha,T_\kappa}\big)_{\ell,\bullet}\ge 0$ or $\big(F^{(m)}_{\alpha,T_\kappa}\big)_{\ell,\bullet}\le 0$. In view of the nonnegativity of $B^{T_\kappa}_{m,j}$ and (3.34), the latter implies that $B^{V_{\alpha,T_\kappa}}_{m,\ell}(x)\le 0$ for all $x\in[0,1]$. But this contradicts the fact that $B^{V_{\alpha,T_\kappa}}_{m,\ell}(x) > 0$ when x is in the interior of the support of $B^{V_{\alpha,T_\kappa}}_{m,\ell}$. Therefore, $F^{(m)}_{\alpha,T_\kappa}$ is a nonnegative matrix.

When $m = 1$, it is clear that $\|(F^{(m)}_{\alpha,T_\kappa})^T\|_\infty = 1$. Consider $m\ge 2$ below. Thanks to the nonnegativity of $F^{(m)}_{\alpha,T_\kappa}$, we have $\|(F^{(m)}_{\alpha,T_\kappa})^T\|_\infty = \|(F^{(m)}_{\alpha,T_\kappa})^T\cdot\mathbf{1}_{q_\alpha}\|_\infty$. By the construction of $F^{(m)}_{\alpha,T_\kappa}$ in (3.22) and the structure of $\widehat{D}^{(q_\alpha)}$, $\Xi^{(m-1)}_{\alpha,T_\kappa}$, $F^{(m-1)}_{\alpha,T_\kappa}$, $\widehat{\Delta}_{m-1,T_\kappa}$, and $\widehat{S}^{(N)}$ given by (3.19), (3.20), (3.21), and statement (1) of Lemma 3.3.3, we have

$$
\begin{aligned}
\mathbf{1}^T_{q_\alpha}\cdot F^{(m)}_{\alpha,T_\kappa} &= \mathbf{1}^T_{q_\alpha}\cdot\widehat{D}^{(q_\alpha)}\cdot\Xi^{(m-1)}_{\alpha,T_\kappa}\cdot F^{(m-1)}_{\alpha,T_\kappa}\cdot\widehat{\Delta}_{m-1,T_\kappa}\cdot\widehat{S}^{(N)}\\
&= \mathbf{e}_1^T\cdot\Big(\Xi^{(m-1)}_{\alpha,T_\kappa}\cdot F^{(m-1)}_{\alpha,T_\kappa}\cdot\widehat{\Delta}_{m-1,T_\kappa}\Big)\cdot\widehat{S}^{(N)} = \mathbf{e}_1^T\cdot\begin{bmatrix}1 & 0\\ & \\ 0 & \star\end{bmatrix}\cdot\widehat{S}^{(N)}\\
&= \mathbf{e}_1^T\cdot\widehat{S}^{(N)} = \mathbf{1}_N^T.
\end{aligned}
$$

This shows that $\|(F^{(m)}_{\alpha,T_\kappa})^T\cdot\mathbf{1}_{q_\alpha}\|_\infty = 1$, completing the proof of statement (1).

(2) It follows from (3.34) that for each $\ell = 1, \ldots, q_\alpha$, $\sum_{j=1}^{N} \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} B_{m,j}^{T_\kappa}(x) = 0$ except on $[\kappa_{i_{\ell-m}}, \kappa_{i_\ell}]$, i.e., the support of $B_{m,\ell}^{V_{\alpha,T_\kappa}}$. Note that $i_s := s$ if $s < 0$, and $i_{|\overline{\alpha}|+p} := K_n + p - 1$ for any $p = 1, \ldots, m$; furthermore, $\kappa_i = 0$ if $i \le 0$ and $\kappa_i = 1$ for $i \ge |\overline{\alpha}| + 1$. Additionally, for any $r = 1, \ldots, K_n$, the B-splines $B_{m,j}^{T_\kappa}$ that are not identically zero on $[\kappa_{r-1}, \kappa_r]$ are linearly independent when restricted to $[\kappa_{r-1}, \kappa_r]$. Hence, if $\sum_{j=1}^{N} \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} B_{m,j}^{T_\kappa}(x) = B_{m,\ell}^{V_{\alpha,T_\kappa}}(x) = 0, \forall\, x \in [\kappa_{r-1}, \kappa_r]$ for some r, then $\big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} = 0$ for each $j = r, r+1, \ldots, r+m-1$. This, along with the fact that $B_{m,\ell}^{V_{\alpha,T_\kappa}}(x) = 0$ except on $[\kappa_{i_{\ell-m}}, \kappa_{i_\ell}]$, shows that $\big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} = 0$ for all $j = 1, 2, \ldots, i_{\ell-m} + m - 1$ and $j = i_\ell + 1, i_\ell + 2, \ldots, N$. Moreover, by the nonnegativity of $F_{\alpha,T_\kappa}^{(m)}$ and $\big\|(F_{\alpha,T_\kappa}^{(m)})^T\big\|_\infty = 1$, we see that all nonzero entries of $F_{\alpha,T_\kappa}^{(m)}$ are less than or equal to one. Therefore, for each $\ell = 1, \ldots, q_\alpha$,

$$
\begin{aligned}
\Big\| \Big(K_n^{-1} \Xi_{\alpha,T_\kappa}^{(m)} F_{\alpha,T_\kappa}^{(m)} \Big)_{\ell,\bullet} \Big\|_\infty &= K_n^{-1} \frac{m}{\kappa_{i_\ell} - \kappa_{i_{\ell-m}}} \sum_{j=i_{\ell-m}+m}^{i_\ell} \big[F_{\alpha,T_\kappa}^{(m)}\big]_{\ell,j} \\
&\le K_n^{-1} \cdot \frac{m}{\kappa_{i_\ell} - \kappa_{i_{\ell-m}}} \cdot \Big(i_\ell - i_{\ell-m} - m + 1 \Big).
\end{aligned}
$$

Since $\kappa_{i_\ell} - \kappa_{i_{\ell-m}} \ge \frac{c_{\kappa,1}}{K_n}\big(i_\ell - i_{\ell-m} - m + 1\big) > 0$ (see the discussions before (3.15)), we obtain, for each $\ell = 1, \ldots, q_\alpha$, $\big\|\big(K_n^{-1} \Xi_{\alpha,T_\kappa}^{(m)} F_{\alpha,T_\kappa}^{(m)}\big)_{\ell,\bullet}\big\|_\infty \le m/c_{\kappa,1}$. This completes the proof of statement (2). □

We exploit Proposition 3.3.2 to derive more uniform bounds and uniform error bounds. Many of these bounds require L_n to be sufficiently large and satisfy suitable order conditions with respect to K_n. We introduce these order conditions as follows. Let (K_n) be an increasing sequence of natural numbers with $K_n \to \infty$ as $n \to \infty$. We say that a sequence (L_n) of natural numbers satisfies

Property **H**: if there exist two increasing sequences (M_n) and (J_n) of natural numbers with $M_n \geq m \cdot K_n / c_{\kappa,1}$ for each n and $(J_n) \to \infty$ as $n \to \infty$ such that $L_n = J_n \cdot M_n^{m+1}$ for each n, where $c_{\kappa,1} > 0$ is used to define $\mathcal{T}_{K_n}$ in (3.14), and m is the fixed spline order.

Note that the sequence (L_n) implicitly depends on the sequence (K_n) through (M_n) in this property.

Define the truncated submatrix of $Z_{m,\alpha,T_\kappa,L_n} \in \mathbb{R}^{q_\alpha \times (L_n+m-1)}$:

$$H_{\alpha,T_\kappa,L_n} := \left(Z_{m,\alpha,T_\kappa,L_n}\right)_{1:q_\alpha,\, 1:L_n} \in \mathbb{R}^{q_\alpha \times L_n}. \tag{3.36}$$

The importance of H_{α,T_κ,L_n} is illustrated in the following facts for given α and $T_\kappa \in \mathcal{T}_{K_n}$:

(a) It follows from statement (2) of Lemma 3.3.4 that $F^{(m)}_{\alpha,T_\kappa} \cdot X_{m,T_\kappa,L_n} = Z_{m,\alpha,T_\kappa,L_n}$. Hence, by (3.36), we obtain

$$H_{\alpha,T_\kappa,L_n} = \left(Z_{m,\alpha,T_\kappa,L_n}\right)_{1:q_\alpha,1:L_n} = F^{(m)}_{\alpha,T_\kappa} \cdot \left(X_{m,T_\kappa,L_n}\right)_{1:N,1:L_n}.$$

(b) In light of the definition of $\widetilde{\Lambda}_{T_\kappa,K_n,L_n}$ (cf. (3.26)) and the result in (a), we have

$$\begin{aligned} & K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa} F^{(m)}_{\alpha,T_\kappa} \cdot \widetilde{\Lambda}_{T_\kappa,K_n,L_n} \left(F^{(m)}_{\alpha,T_\kappa}\right)^T \\ &= \frac{\Xi^{(m)}_{\alpha,T_\kappa}}{L_n} \cdot F^{(m)}_{\alpha,T_\kappa}\left(X_{m,T_\kappa,L_n}\right)_{1:N,1:L_n} \cdot \left(F^{(m)}_{\alpha,T_\kappa}\left(X_{m,T_\kappa,L_n}\right)_{1:N,1:L_n}\right)^T \\ &= \frac{1}{L_n} \cdot \Xi^{(m)}_{\alpha,T_\kappa} \cdot H_{\alpha,T_\kappa,L_n} \cdot \left(H_{\alpha,T_\kappa,L_n}\right)^T. \end{aligned} \tag{3.37}$$

This matrix will be used in Section 3.3.5 to approximate

$$K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa} F^{(m)}_{\alpha,T_\kappa} \Lambda_{K_n,P,T_\kappa} \left(F^{(m)}_{\alpha,T_\kappa}\right)^T$$

in the proof of Theorem 3.2.1.

(c) Note that $F^{(m)}_{\alpha,T_\kappa}$ is the identity matrix when α is the empty set; see the comments below (3.22). This observation, along with the result in (a), shows that if α is the empty set, then $\big(X_{m,T_\kappa,L_n}\big)_{1:N,1:L_n} = H_{\alpha,T_\kappa,L_n}$. Moreover, it follows from (3.37) that when α is the empty set, $\widetilde{\Lambda}_{T_\kappa,K_n,L_n} = \frac{K_n}{L_n} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T$. These results will be used in Proposition 3.3.5.

With the definition of H_{α,T_κ,L_n}, we establish a uniform error bound between a B-spline Gramian matrix and $(L_n)^{-1}\cdot \Xi^{(m)}_{\alpha,T_\kappa}\cdot H_{\alpha,T_\kappa,L_n}\cdot \big(H_{\alpha,T_\kappa,L_n}\big)^T$. In light of (3.37), this result is critical to obtaining a uniform bound of the ℓ_∞-norm of the matrix product $\big(\Xi'_\alpha F_\alpha \Lambda_{K_n,P,T_\kappa} F^T_\alpha\big)^{-1}$, a key step toward the uniform Lipschitz property. To this end, we first introduce a B-spline Gramian matrix. Consider the mth order B-splines $\big\{B^{V_{\alpha,T_\kappa}}_{m,j}\big\}_{j=1}^{|\overline{\alpha}|+m}$ corresponding to the knot sequence V_{α,T_κ} defined in (3.28) associated with any index set α and $T_\kappa\in\mathcal{T}_{K_n}$. Specifically, define the Gramian matrix $G_{\alpha,T_\kappa}\in\mathbb{R}^{q_\alpha\times q_\alpha}$ (where we recall $q_\alpha := |\overline{\alpha}|+m$) as

$$\big[G_{\alpha,T_\kappa}\big]_{i,j} := \frac{\Big\langle B^{V_{\alpha,T_\kappa}}_{m,i},\ B^{V_{\alpha,T_\kappa}}_{m,j}\Big\rangle}{\big\|B^{V_{\alpha,T_\kappa}}_{m,i}\big\|_{L_1}}, \qquad \forall\ i,j = 1,\ldots,q_\alpha. \tag{3.38}$$

Proposition 3.3.4. *Let (K_n) be an increasing sequence with $K_n\to\infty$ as $n\to\infty$, and (L_n) be of Property* **H** *defined by (J_n) and (M_n). Let G_{α,T_κ} and H_{α,T_κ,L_n} be defined for $T_\kappa\in\mathcal{T}_{K_n}$ and α. Then there exists $n_*\in\mathbb{N}$, which depends on (L_n) only and is independent of T_κ and α, such that for any $T_\kappa\in\mathcal{T}_{K_n}$ with $n\ge n_*$ and any index set α,*

$$\left\|G_{\alpha,T_\kappa} - \frac{1}{L_n}\cdot\Xi^{(m)}_{\alpha,T_\kappa}\cdot H_{\alpha,T_\kappa,L_n}\cdot\big(H_{\alpha,T_\kappa,L_n}\big)^T\right\|_\infty \le \frac{6\cdot c_{\kappa,1}\cdot(3\cdot 2^{m-1}-2)}{J_n}, \qquad \forall\ n\ge n_*,$$

where $\Xi^{(m)}_{\alpha,T_\kappa}$ *is defined in (3.19).*

Proof. Given arbitrary α, $T_\kappa \in \mathcal{T}_{K_n}$, and (L_n) of Property **H**, we use H and $\Xi^{(m)}$ to denote H_{α,T_κ,L_n} and $\Xi^{(m)}_{\alpha,T_\kappa}$ respectively to simplify notation. Also take $r_k := \frac{k-1}{L_n}$ for $k = 1,\ldots,L_n$. When $m = 1$, G_{α,T_κ} is diagonal (see the summary of B-splines at the beginning of Section 3.2 for the reason), and so is $H \cdot H^T$. Using $\left(\|B^{V_{\alpha,T_\kappa}}_{m,j}\|_{L_1}\right)^{-1} = \frac{m}{\kappa_{i_j}-\kappa_{i_{j-m}}} = \left[\Xi^{(m)}\right]_{j,j}$ and a result similar to (3.31), the desired result follows easily. We consider $m \geq 2$ next. It follows from the definition of $H \in \mathbb{R}^{q_\alpha \times L_n}$ and Proposition 3.3.2 that for each $j = 1,\ldots,q_\alpha$ and $k = 1,\ldots,L_n$,

$$\left|\left[H\right]_{j,k} - B^{V_{\alpha,T_\kappa}}_{m,j}(r_k)\right| = \left|\left[Z_{m,\alpha,T_\kappa,L_n}\right]_{j,k} - B^{V_{\alpha,T_\kappa}}_{m,j}(r_k)\right| \leq \frac{C_m(M_n)^{m-1}}{L_n} \leq \frac{C_m}{J_n(M_n)^2} \tag{3.39}$$

for any $n \in \mathbb{N}$, where $C_m := 6 \cdot (2^{m-1} - 1)$. Since $0 \leq B^{V_{\alpha,T_\kappa}}_{m,j}(x) \leq 1$ for each j, and

$$\begin{aligned}
&\left[H\right]_{j,\ell} \cdot \left[H\right]_{k,\ell} - B^{V_{\alpha,T_\kappa}}_{m,j}(r_\ell) \cdot B^{V_{\alpha,T_\kappa}}_{m,k}(r_\ell) \\
&= \Big(\left[H\right]_{j,\ell} - B^{V_{\alpha,T_\kappa}}_{m,j}(r_\ell)\Big) \cdot \Big(\left[H\right]_{k,\ell} - B^{V_{\alpha,T_\kappa}}_{m,k}(r_\ell)\Big) + B^{V_{\alpha,T_\kappa}}_{m,j}(r_\ell) \cdot \Big(\left[H\right]_{k,\ell} - B^{V_{\alpha,T_\kappa}}_{m,k}(r_\ell)\Big) \\
&\qquad + B^{V_{\alpha,T_\kappa}}_{m,k}(r_\ell) \cdot \Big(\left[H\right]_{j,\ell} - B^{V_{\alpha,T_\kappa}}_{m,j}(r_\ell)\Big),
\end{aligned}$$

we deduce, via (3.39), that for each $j, k = 1,\ldots,q_\alpha$ and $\ell = 1,\ldots,L_n$,

$$\left|\left[H\right]_{j,\ell} \cdot \left[H\right]_{k,\ell} - B^{V_{\alpha,T_\kappa}}_{m,j}(r_\ell) \cdot B^{V_{\alpha,T_\kappa}}_{m,k}(r_\ell)\right| \leq \left(\frac{C_m}{J_n(M_n)^2}\right)^2 + \frac{2C_m}{J_n(M_n)^2}, \quad \forall\, n \in \mathbb{N}.$$

Since $m \geq 2$, $\left(B^{V_{\alpha,T_\kappa}}_{m,j}(x) B^{V_{\alpha,T_\kappa}}_{m,k}(x)\right)$ is continuous and differentiable on $[0,1]$ except at (at most) finitely many points in $[0,1]$. In light of (3.33) we have, for any $x \in [0,1]$ where the derivative exists,

$$\left|\left(B_{m,j}^{V_\alpha,T_\kappa}(x)B_{m,k}^{V_\alpha,T_\kappa}(x)\right)'\right| = \left|\left(B_{m,j}^{V_\alpha,T_\kappa}\right)'(x)B_{m,k}^{V_\alpha,T_\kappa}(x) + B_{m,j}^{V_\alpha,T_\kappa}(x)\left(B_{m,k}^{V_\alpha,T_\kappa}\right)'(x)\right| \le 4M_n. \tag{3.40}$$

Combining these results with $\left(\|B_{m,j}^{V_\alpha,T_\kappa}\|_{L_1}\right)^{-1} = \frac{m}{\kappa_{i_j}-\kappa_{i_{j-m}}} = \left[\Xi^{(m)}\right]_{j,j}$, we apply Lemma 3.3.1 with $\widetilde{n} := L_n,\ a := 0,\ b := 1,\ s_k := k/L_n,\ \varrho := 1/L_n,\ f(x) := B_{m,j}^{V_\alpha,T_\kappa}(x) \cdot B_{m,k}^{V_\alpha,T_\kappa}(x)$, $v := (v_\ell) = \left([H]_{j,\ell} \cdot [H]_{k,\ell}\right)$, $\mu_1 := \left(\frac{C_m}{J_n(M_n)^2}\right)^2 + \frac{2C_m}{J_n(M_n)^2}$, and $\mu_2 := 4M_n$ to obtain $n_* \in \mathbb{N}$ depending on (L_n) only such that for any $j, k = 1, \ldots, q_\alpha$,

$$\begin{aligned}
\left|\frac{1}{L_n}\left[\Xi^{(m)} \cdot H \cdot H^T\right]_{j,k} - \left[G_{\alpha,T_\kappa}\right]_{j,k}\right| &= \left|\frac{1}{L_n}\left[\Xi^{(m)} \cdot H \cdot H^T\right]_{j,k} - \frac{\left\langle B_{m,j}^{V_\alpha,T_\kappa},\ B_{m,k}^{V_\alpha,T_\kappa}\right\rangle}{\left\|B_{m,j}^{V_\alpha,T_\kappa}\right\|_{L_1}}\right| \\
&= \frac{m}{\kappa_{i_j} - \kappa_{i_{j-m}}}\left|\sum_{\ell=1}^{L_n}\frac{v_\ell}{L_n} - \int_0^1 f(t)dt\right| \le M_n \cdot \left[\left(\frac{C_m}{J_n(M_n)^2}\right)^2 + \frac{2C_m}{J_n(M_n)^2} + \frac{6M_n}{L_n}\right] \\
&\le \frac{3C_m+6}{J_nM_n}, \qquad \forall\ n \ge n_*,
\end{aligned}$$

where we use $L_n = J_n \cdot (M_n)^{m+1}$. Since G_{α,T_κ} has q_α columns and $q_\alpha = |\overline{\alpha}| + m \le K_n + m - 1 \le m \cdot K_n \le c_{\kappa,1}M_n$, we may deduce that for any α and $T_\kappa \in \mathcal{T}_{K_n}$,

$$\left\|G_{\alpha,T_\kappa} - \frac{1}{L_n} \cdot \Xi^{(m)} \cdot H \cdot H^T\right\|_\infty \le q_\alpha \cdot \frac{3C_m+6}{J_nM_n} \le \frac{c_{\kappa,1} \cdot (3C_m+6)}{J_n}, \quad \forall\ n \ge n_*.$$

The proof is completed by noting that $3C_m + 6 = 6 \cdot (3 \cdot 2^{m-1} - 2)$. □

An immediate consequence of Proposition 3.3.4 is the invertibility of

$$\Xi_{\alpha,T_\kappa}^{(m)} H_{\alpha,T_\kappa,L_n}\left(H_{\alpha,T_\kappa,L_n}\right)^T / L_n$$

and the uniform bound of its inverse in the ℓ_∞-norm.

Corollary 3.3.2. *Let (K_n) be an increasing sequence with $K_n \to \infty$ as $n \to \infty$, and (L_n) be of Property* **H** *defined by (J_n) and (M_n). Then there exists $n'_* \in \mathbb{N}$, which depends on (L_n) only, such that for any $T_\kappa \in \mathcal{T}_{K_n}$ with $n \geq n'_*$, any index set α, and any $n \geq n'_*$, $\frac{1}{L_n}\Xi^{(m)}_{\alpha,T_\kappa} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T$ is invertible, and*

$$\Big\| \Big(\frac{1}{L_n}\Xi^{(m)}_{\alpha,T_\kappa} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T \Big)^{-1} \Big\|_\infty \leq \frac{3\rho_m}{2},$$

where ρ_m is a positive constant depending on m only.

Proof. Choose arbitrary α, $T_\kappa \in \mathcal{T}_{K_n}$, and (L_n) of Property **H**. It follows from [64, Theorem I] (cf. Theorem 3.2.2) that the Gramian matrix G_{α,T_κ} is invertible and there exists a positive constant ρ_m such that for any $T_\kappa \in \mathcal{T}_{K_n}$ and any index set α, $\|(G_{\alpha,T_\kappa})^{-1}\|_\infty \leq \rho_m$. Furthermore, it follows from Proposition 3.3.4 that for any $T_\kappa \in \mathcal{T}_{K_n}$ and any index set α, $\|G_{\alpha,T_\kappa} - \frac{1}{L_n}\Xi^{(m)}_{\alpha,T_\kappa} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T\|_\infty \leq 6c_{\kappa,1}(3\cdot 2^{m-1}-2)/J_n, \forall\, n \geq n_*$. Since $J_n \to \infty$ as $n \to \infty$, we deduce from Lemma 3.3.2 that there exists $n'_* \in \mathbb{N}$ with $n'_* \geq n_*$ such that for any $T_\kappa \in \mathcal{T}_{K_n}$ with $n \geq n'_*$, any index set α, and any $n \geq n'_*$, $\frac{1}{L_n}\Xi^{(m)}_{\alpha,T_\kappa} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T$ is invertible, and $\big\|\big(\frac{1}{L_n}\Xi^{(m)}_{\alpha,T_\kappa} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T\big)^{-1}\big\|_\infty \leq \frac{3}{2}\rho_m$. □

For any $K_n \in \mathbb{N}$ and $T_\kappa \in \mathcal{T}_{K_n}$, let $\{B^{T_\kappa}_{m,i}\}_{i=1}^N$ be the B-splines of order m defined by the knot sequence T_κ, where we recall that $N := K_n + m - 1$. Note that $B^{T_\kappa}_{m,i}$ is equal to $B^{V_{\alpha,T_\kappa}}_{m,i}$ when α is the empty set. For the given T_κ, define the $N \times N$ matrix $\widehat{\Lambda}_{K_n,T_\kappa}$ as

$$\big[\widehat{\Lambda}_{K_n,T_\kappa}\big]_{i,j} := K_n \cdot \Big\langle B^{T_\kappa}_{m,i}, B^{T_\kappa}_{m,j} \Big\rangle, \qquad \forall\, i,j = 1,\ldots,N. \tag{3.41}$$

Clearly, $\widehat{\Lambda}_{K_n,T_\kappa}$ is positive definite and invertible. The following result presents important properties of $\widehat{\Lambda}_{K_n,T_\kappa}$. In particular, it shows via $\widehat{\Lambda}_{K_n,T_\kappa}$ that $\widetilde{\Lambda}_{T_\kappa,K_n,L_n}$ approximates

Λ_{K_n,P,T_κ} with a uniform error bound, which is crucial to the proof of the uniform Lipschitz property. Note that the constant $\rho_m > 0$ used below is given in [64, Theorem I] (cf. Theorem 3.2.2) and depends on m only.

Proposition 3.3.5. *Let (K_n) be an increasing sequence with $K_n \to \infty$ as $n \to \infty$, and (L_n) be of Property* **H** *defined by (J_n) and (M_n). The following hold:*

(1) For any K_n and $T_\kappa \in \mathcal{T}_{K_n}$, $\|\big(\widehat{\Lambda}_{K_n,T_\kappa}\big)^{-1}\|_\infty \le m\rho_m/c_{\kappa,1}$;

(2) There exists $n_* \in \mathbb{N}$, depending on (L_n) only, such that for any $T_\kappa \in T_{K_n}$ with $n \ge n_*$,

$$\left\|\widetilde{\Lambda}_{T_\kappa,K_n,L_n} - \widehat{\Lambda}_{K_n,T_\kappa}\right\|_\infty \le \frac{6 \cdot c_{\kappa,2} \cdot c_{\kappa,1} \cdot (3 \cdot 2^{m-1} - 2)}{J_n}, \qquad \forall\, n \ge n_*;$$

(3) For any n, K_n, $P \in \mathcal{P}_n$, and $T_\kappa \in \mathcal{T}_{K_n}$,

$$\left\|\Lambda_{K_n,P,T_\kappa} - \widehat{\Lambda}_{K_n,T_\kappa}\right\|_\infty \le (2m-1)\left(\frac{6m^2 c_\omega c_{\kappa,2}}{c_{\kappa,1}} + 3c_\omega\right)\frac{K_n}{n}.$$

Proof. (1) For any $T_\kappa \in \mathcal{T}_{K_n}$, it follows from (3.38) and (3.41) that when α is the empty set, $G_{\emptyset,T_\kappa} = K_n^{-1} \cdot \Xi^{(m)}_{\emptyset,T_\kappa} \cdot \widehat{\Lambda}_{K_n,T_\kappa}$. Hence, in light of $\|\Xi^{(m)}_{\emptyset,T_\kappa}\|_\infty \le mK_n/c_{\kappa,1}$ and $\|\big(G_{\emptyset,T_\kappa}\big)^{-1}\|_\infty \le \rho_m$ for any $T_\kappa \in \mathcal{T}_{K_n}$, we have

$$\left\|\big(\widehat{\Lambda}_{K_n,T_\kappa}\big)^{-1}\right\|_\infty = K_n^{-1}\left\|\big(G_{\emptyset,T_\kappa}\big)^{-1} \cdot \Xi^{(m)}_{\emptyset,T_\kappa}\right\|_\infty \le K_n^{-1} \cdot \rho_m \cdot \frac{mK_n}{c_{\kappa,1}} = \frac{m\rho_m}{c_{\kappa,1}}, \quad \forall\, T_\kappa \in \mathcal{T}_{K_n}.$$

(2) Recall from the comment below (3.37) that $\widetilde{\Lambda}_{T_\kappa,K_n,L_n} = \frac{K_n}{L_n} H_{\alpha,T_\kappa,L_n}\big(H_{\alpha,T_\kappa,L_n}\big)^T$ when α is the empty set. Also, noting from the proof of statement (1) that $\widehat{\Lambda}_{K_n,T_\kappa} = K_n \cdot \big(\Xi^{(m)}_{\emptyset,T_\kappa}\big)^{-1} \cdot G_{\emptyset,T_\kappa}$, we obtain via Proposition 3.3.4 that there exists $n_* \in \mathbb{N}$, depending

on (L_n) only, such that for any $T_\kappa \in T_{K_n}$ with $n \geq n_*$,

$$
\begin{aligned}
\big\|\widetilde{\Lambda}_{T_\kappa,K_n,L_n} - \widehat{\Lambda}_{K_n,T_\kappa}\big\|_\infty &= K_n \cdot \left\| \big(\Xi^{(m)}_{\emptyset,T_\kappa}\big)^{-1} \cdot \Big(\frac{1}{L_n} \Xi^{(m)}_{\emptyset,T_\kappa} H_{\emptyset,T_\kappa,L_n} \big(H_{\emptyset,T_\kappa,L_n}\big)^T - G_{\emptyset,T_\kappa} \Big) \right\|_\infty \\
&\leq K_n \cdot \big\| \big(\Xi^{(m)}_{\emptyset,T_\kappa}\big)^{-1} \big\|_\infty \cdot \left\| \frac{1}{L_n} \Xi^{(m)}_{\emptyset,T_\kappa} H_{\emptyset,T_\kappa,L_n} \big(H_{\emptyset,T_\kappa,L_n}\big)^T - G_{\emptyset,T_\kappa} \right\|_\infty \\
&\leq K_n \cdot \frac{c_{\kappa,2}}{K_n} \cdot \frac{6 \cdot c_{\kappa,1} \cdot (3 \cdot 2^{m-1} - 2)}{J_n} \\
&= \frac{6 \cdot c_{\kappa,2} \cdot c_{\kappa,1} \cdot (3 \cdot 2^{m-1} - 2)}{J_n}, \qquad \forall\, n \geq n_*.
\end{aligned}
$$

(3) Consider an arbitrary knot sequence $T_\kappa \in \mathcal{T}_{K_n}$ given by $T_\kappa = \{0 = \kappa_0 < \kappa_1 < \cdots < \kappa_{K_n-1} < \kappa_{K_n} = 1\}$ with the usual extension. Furthermore, let $P \in \mathcal{P}_n$ be a design point sequence given by $P = \{0 = x_0 < x_1 < \cdots < x_n = 1\}$. Recall the design matrix $\widehat{X} \in \mathbb{R}^{(n+1)\times N}$ with $[\widehat{X}]_{\ell,i} = B^{T_\kappa}_{m,i}(x_\ell)$ for each ℓ and i, and $\Lambda_{K_n,P,T_\kappa} = K_n \cdot \widehat{X}^T \Theta_n \widehat{X} \in \mathbb{R}^{N\times N}$ with $\Theta_n = \text{diag}\big(x_1 - x_0, x_2 - x_1, \ldots, x_{n+1} - x_n\big)$. When $m = 1$, both $\widehat{\Lambda}_{K_n,T_\kappa}$ and Λ_{K_n,P,T_κ} are diagonal matrices, and the desired bound follows easily from an argument similar to that of Proposition 3.3.4. Hence, it suffices to consider $m \geq 2$ below. For any fixed $i, j = 1, \ldots, N$, we assume that there are $(\widetilde{n}_i + 1)$ design points in P on the support $[\kappa_{i-m}, \kappa_i]$ of $B^{T_\kappa}_{m,i}$. Specifically, there exists $r_i \in \mathbb{Z}_+$ such that: (i) $x_{r_i}, x_{r_i+1}, \ldots, x_{r_i+\widetilde{n}_i} \in [\kappa_{i-m}, \kappa_i]$; (ii) $x_{r_i} = 0$ or $x_{r_i-1} < \kappa_{i-m}$; and (iii) $x_{r_i+\widetilde{n}_i} = 1$ or $x_{r_i+\widetilde{n}_i+1} > \kappa_i$. Hence, letting $\omega_\ell := x_\ell - x_{\ell-1}$ for $\ell = 1, \ldots, n+1$, it follows from the definitions of Λ_{K_n,P,T_κ} and $\widehat{\Lambda}_{K_n,T_\kappa}$ that

$$
\begin{aligned}
&\Big| \Big[\Lambda_{K_n,P,T_\kappa} - \widehat{\Lambda}_{K_n,T_\kappa} \Big]_{i,j} \Big| \\
&= K_n \left| \sum_{\ell=r_i}^{r_i+\widetilde{n}_i} \omega_\ell \cdot B^{T_\kappa}_{m,i}(x_\ell) \cdot B^{T_\kappa}_{m,j}(x_\ell) - \int_{\kappa_{i-m}}^{\kappa_i} B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\, dx \right| \\
&\leq K_n \left| \sum_{\ell=r_i}^{r_i+\widetilde{n}_i-1} \omega_\ell \cdot B^{T_\kappa}_{m,i}(x_\ell) \cdot B^{T_\kappa}_{m,j}(x_\ell) - \int_{x_{r_i}}^{x_{r_i+\widetilde{n}_i}} B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\, dx \right|
\end{aligned}
$$

$$
\begin{aligned}
&+ K_n \int_{\kappa_{i-m}}^{x_{r_i}} B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\,dx \\
&+ K_n \int_{x_{r_i+\widetilde{n}_i}}^{\kappa_i} B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\,dx + K_n \cdot \omega_{r_i+\widetilde{n}_i} B^{T_\kappa}_{m,i}(x_{r_i+\widetilde{n}_i}) \cdot B^{T_\kappa}_{m,j}(x_{r_i+\widetilde{n}_i}) \\
\leq\ & K_n \left| \sum_{\ell=r_i+1}^{r_i+\widetilde{n}_i} \omega_{\ell-1} B^{T_\kappa}_{m,i}(x_{\ell-1}) B^{T_\kappa}_{m,j}(x_{\ell-1}) - \int_{x_{r_i}}^{x_{r_i+\widetilde{n}_i}} B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\,dx \right| + 3c_\omega \frac{K_n}{n},
\end{aligned}
$$

using the fact that for each i and $x \in [0,1]$, $0 \leq B^{T_\kappa}_{m,i}(x) \leq 1$ and $\max_\ell(x_{r_i} - \kappa_{i-m}, \kappa_i - x_{r_i+\widetilde{n}_i}, \omega_\ell) \leq c_\omega/n$.

By virtue of (3.32) and (3.40), it is easy to verify that $\left|\left(B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\right)'\right| \leq \frac{4mK_n}{c_{\kappa,1}}$ whenever the derivative exists on $[0,1]$. We apply Lemma 3.3.1 to the first term on the right hand side with $\widetilde{n} := \widetilde{n}_i$, $a := x_{r_i}$, $b := x_{r_i+\widetilde{n}_i}$, $s_k := x_{r_i+k}$, $\varrho := c_\omega/n$, $f(x) := B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)$, which is continuous on $[0,1]$ and is differentiable except at (at most) finitely many points, $v = (v_\ell) \in \mathbb{R}^{\tilde{n}_i}$ given by $v_\ell := B^{T_\kappa}_{m,i}(x_{r_i+\ell-1}) B^{T_\kappa}_{m,j}(x_{r_i+\ell-1})$, $\mu_1 := 0$, and $\mu_2 := 4mK_n/c_{\kappa,1}$, and we obtain

$$
\begin{aligned}
&K_n \left| \sum_{\ell=r_i+1}^{r_i+\widetilde{n}_i} \omega_{\ell-1} B^{T_\kappa}_{m,i}(x_{\ell-1}) B^{T_\kappa}_{m,j}(x_{\ell-1}) - \int_{x_{r_i}}^{x_{r_i+\widetilde{n}_i}} B^{T_\kappa}_{m,i}(x) B^{T_\kappa}_{m,j}(x)\,dx \right| \\
&\leq\ K_n \cdot \frac{3}{2} \cdot \frac{4mK_n}{c_{\kappa,1}} \cdot \frac{c_\omega}{n} \cdot \big(\kappa_i - \kappa_{i-m}\big) \ \leq\ \frac{6mK_n^2 c_\omega}{nc_{\kappa,1}} \cdot \frac{m\, c_{\kappa,2}}{K_n} \ =\ \frac{6m^2 c_\omega c_{\kappa,2}}{c_{\kappa,1}} \cdot \frac{K_n}{n}.
\end{aligned}
$$

Combining the above results yields $\left|[\Lambda_{K_n,P,T_\kappa} - \widehat{\Lambda}_{K_n,T_\kappa}]_{i,j}\right| \leq \big(\frac{6m^2 c_\omega c_{\kappa,2}}{c_{\kappa,1}} + 3c_\omega\big)\frac{K_n}{n}$ for any $i, j = 1, \ldots, N$. It is noted that $B^{T_\kappa}_{m,i} B^{T_\kappa}_{m,j} \equiv 0$ on $[0,1]$ whenever $|i-j| \geq m$. Hence both Λ_{K_n,P,T_κ} and $\widehat{\Lambda}_{K_n,T_\kappa}$ are banded matrices with bandwidth m. Thus, for any n, K_n, $P \in \mathcal{P}_n$, and $T_\kappa \in \mathcal{T}_{K_n}$,

$$
\left\| \Lambda_{K_n,P,T_\kappa} - \widehat{\Lambda}_{K_n,T_\kappa} \right\|_\infty \ \leq\ (2m-1) \left(\frac{6m^2 c_\omega c_{\kappa,2}}{c_{\kappa,1}} + 3c_\omega \right) \frac{K_n}{n}.
$$

This completes the proof of statement (3). □

3.3.5 Proof of the Main Result

In this section, we use the results established in the previous sections to show that the uniform Lipschitz property stated in Theorem 3.2.1 holds. Fix the B-spline order $m \in \mathbb{N}$. Let the strictly increasing sequence (K_n) be such that $K_n \to \infty$ and $K_n/n \to 0$ as $n \to \infty$. Consider the sequence (L_n):

$$L_n := K_n \cdot \left(\left\lceil \frac{mK_n}{c_{\kappa,1}} \right\rceil \right)^{m+1}, \qquad \forall\, n \in \mathbb{N}.$$

Clearly, (L_n) satisfies Property **H** as $J_n := K_n$, and $M_n := \lceil \frac{mK_n}{c_{\kappa,1}} \rceil$ depends on (K_n) only.

For any $P \in \mathcal{P}_n$, $T_\kappa \in \mathcal{T}_{K_n}$, and any index set α defined in (3.11), recall that $q_\alpha = |\overline{\alpha}| + m$, $N = K_n + m - 1$, and $\Lambda_{K_n,P,T_\kappa} \in \mathbb{R}^{N\times N}$. We construct the following matrices based on the development in the past subsections: $F^{(m)}_{\alpha,T_\kappa} \in \mathbb{R}^{q_\alpha \times N}$ (cf. (3.22)), $\Xi^{(m)}_{\alpha,T_\kappa} \in \mathbb{R}^{q_\alpha\times q_\alpha}$ (cf. (3.19)), $X_{m,T_\kappa,L_n} \in \mathbb{R}^{N\times(L_n+m-1)}$ (cf. (3.25)), $\widetilde{\Lambda}_{T_\kappa,K_n,L_n} \in \mathbb{R}^{N\times N}$ (cf. (3.26)), and $H_{\alpha,T_\kappa,L_n} \in \mathbb{R}^{q_\alpha\times L_n}$ (cf. (3.36)). In light of Proposition 3.3.1 and (3.12),

$$\widehat{b}^{\alpha}_{P,T_\kappa}(\bar{y}) \;=\; \big(F^{(m)}_{\alpha,T_\kappa}\big)^T \cdot\; \Big(F^{(m)}_{\alpha,T_\kappa}\Lambda_{K_n,P,T_\kappa}\big(F^{(m)}_{\alpha,T_\kappa}\big)^T\Big)^{-1} \cdot F^{(m)}_{\alpha,T_\kappa}\,\bar{y}.$$

Note that

$$\begin{aligned}
&\left\| \left(F^{(m)}_{\alpha,T_\kappa}\right)^T \cdot \left(F^{(m)}_{\alpha,T_\kappa} \cdot \Lambda_{K_n,P,T_\kappa}\left(F^{(m)}_{\alpha,T_\kappa}\right)^T\right)^{-1} \cdot F^{(m)}_{\alpha,T_\kappa}\right\|_\infty \\
&\le\; \left\|\left(F^{(m)}_{\alpha,T_\kappa}\right)^T\right\|_\infty \cdot \left\|K_n\left(\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \Lambda_{K_n,P,T_\kappa}\left(F^{(m)}_{\alpha,T_\kappa}\right)^T\right)^{-1}\right\|_\infty \cdot \left\|K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa}\right\|_\infty .
\end{aligned} \tag{3.42}$$

By Corollary 3.3.1, we have the uniform bounds $\|(F^{(m)}_{\alpha,T_\kappa})^T\|_\infty = 1$ and $\|K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa}\|_\infty \le m/c_{\kappa,1}$, regardless of $K_n, \alpha, T_\kappa \in \mathcal{T}_{K_n}$.

We now develop a uniform bound for $\|K_n(\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \Lambda_{K_n,P,T_\kappa} \cdot (F^{(m)}_{\alpha,T_\kappa})^T)^{-1}\|_\infty$ on the right hand side of (3.42). Recall from (3.37) that

$$K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \widetilde{\Lambda}_{T_\kappa,K_n,L_n}\left(F^{(m)}_{\alpha,T_\kappa}\right)^T = \frac{1}{L_n} \cdot \Xi^{(m)}_{\alpha,T_\kappa} \cdot H_{\alpha,T_\kappa,L_n} \cdot \left(H_{\alpha,T_\kappa,L_n}\right)^T.$$

By Corollary 3.3.2, we deduce the existence of $\widetilde{n}_\star \in \mathbb{N}$, which depends on (K_n) only, such that for any $T_\kappa \in \mathcal{T}_{K_n}$ with $n \ge \widetilde{n}_\star$, α, and $n \ge \widetilde{n}_\star$, $K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \widetilde{\Lambda}_{T_\kappa,K_n,L_n} \cdot (F^{(m)}_{\alpha,T_\kappa})^T$ is invertible and $\|K_n[\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \widetilde{\Lambda}_{T_\kappa,K_n,L_n} \cdot (F^{(m)}_{\alpha,T_\kappa})^T]^{-1}\|_\infty \le \frac{3\rho_m}{2}$. Moreover, noting that

$$\begin{aligned}&\left\|K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \widetilde{\Lambda}_{T_\kappa,K_n,L_n} \cdot \left(F^{(m)}_{\alpha,T_\kappa}\right)^T - K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \Lambda_{K_n,P,T_\kappa} \cdot \left(F^{(m)}_{\alpha,T_\kappa}\right)^T\right\|_\infty \\ \le\ &\left\|K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa}\right\|_\infty \cdot \left\|\widetilde{\Lambda}_{T_\kappa,K_n,L_n} - \Lambda_{K_n,P,T_\kappa}\right\|_\infty \cdot \left\|\left(F^{(m)}_{\alpha,T_\kappa}\right)^T\right\|_\infty\end{aligned}$$

and using Proposition 3.3.5 as well as the uniform bounds for both $\|(F^{(m)}_{\alpha,T_\kappa})^T\|_\infty$ and $\|K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa}\|_\infty$ from Corollary 3.3.1, we further deduce via Lemma 3.3.2 that there exists $n_* \in \mathbb{N}$ with $n_* \ge \widetilde{n}_\star$ such that for any α, $P \in \mathcal{P}_n$, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \ge n_*$, $K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \Lambda_{K_n,P,T_\kappa} \cdot (F^{(m)}_{\alpha,T_\kappa})^T$ is invertible and

$$\left\|\left(K_n^{-1}\Xi^{(m)}_{\alpha,T_\kappa}F^{(m)}_{\alpha,T_\kappa} \cdot \Lambda_{K_n,P,T_\kappa} \cdot \left(F^{(m)}_{\alpha,T_\kappa}\right)^T\right)^{-1}\right\|_\infty \le \frac{9\rho_m}{4}.$$

Finally, combining the above three uniform bounds, we conclude, in light of (3.42), that the theorem holds with the positive constant $c_\infty := 9m\rho_m/(4c_{\kappa,1})$ depending only on m and $c_{\kappa,1}$, and $n_* \in \mathbb{N}$ depending on (K_n) only (when $m, c_\omega, c_{\kappa,1}, c_{\kappa,2}$ are fixed).

3.4 Summary

This chapter establishes a critical uniform Lipschitz property for a B-spline estimator subject to general nonnegative derivative constraints with (possibly) unevenly spaced design points and/or knots. Subsequent chapters will consider the B-spline estimator rate of convergence for a variety of nonnegative derivative constraints.

CHAPTER IV

Nonnegative Derivative Constrained B-spline Estimator: Bias, Stochastic Error, and Convergence Rate in the Supremum Norm

In the previous chapter, we established a uniform Lipschitz property for a nonnegative derivative constrained B-spline estimator (c.f. Theorem 3.2.1). In this chapter, we will apply that result in order to bound the estimator risk (or error) in the supremum norm. Moreover, the risk associated with a given estimator can be decomposed into the sum of two terms: (i) the bias, which stems from approximating a true function by another function (e.g., a spline), and (ii) the stochastic error, which arises from random error or noise. The goal of this chapter is to bound both of these quantities in the supremum norm for the nonnegative derivative constrained B-spline estimator of Chapter III. We will then use the results from this chapter to demonstrate that this estimator achieves the optimal asymptotic performance with respect to the supremum norm over a suitable Hölder class in Chapter V, for certain nonnegative derivative constraints.

4.1 Introduction

Measuring the performance of an estimator boils down to bounding the estimator bias and stochastic error. For an unconstrained B-spline estimator, standard techniques are often used to bound both of these quantities [40, 77]. However, the nonnegative derivative constraints on the B-spline estimator from Chapter III complicate the analysis of this estimator's bias, even though the uniform Lipschitz property of the previous chapter has already been established. Specifically, the remaining difficulty in bounding the bias in the supremum norm arises in showing that each smooth nonnegative derivative constrained function f can be accurately approximated by a spline f_B with the same nonnegative derivative constraint. Once the existence of such a spline is verified for each f, the uniform Lipschitz property of Chapter III may then be applied to produce a bound on the estimator bias with the same order of magnitude as the approximation error, $\|f - f_B\|_\infty$. Standard techniques and the uniform Lipschitz property may then be used to bound the constrained B-spline estimator stochastic error, establish the estimator consistency, and provide the estimator convergence rate.

This chapter is organized as follows. In Section 4.2, we demonstrate that, under certain conditions, each nonnegative derivative constrained function in a suitable Hölder class may be accurately approximated by a spline with the same nonnegative derivative constraint. This result is then used in Section 4.3, along with the uniform Lipschitz property, to bound the Chapter III nonnegative derivative constrained B-spline estimator bias and stochastic error in the supremum norm. The consistency and convergence rate of this estimator are also established in this section. A summary is given in Section 4.4.

Notation: Given a function $g : [a,b] \to \mathbb{R}$, denote its supremum-norm (or simply sup-norm) by $\|g\|_\infty := \sup_{x\in[a,b]} |g(x)|$. Also, let $\mathbb{E}$ denote the expectation operator, let $\mathbb{P}(A)$ denote the probability of an event A, and let $f^{(\ell)}$ denote the ℓth derivative of the function f. Finally, we write $Y \sim \mathcal{N}(0,\sigma^2)$ if Y is a mean zero, normal random variable with variance σ^2.

4.2 Nonnegative Derivative Constrained Spline Approximations

In this section, we consider the problem of approximating a nonnegative derivative constrained function in an appropriate Hölder class by a spline with the same constraint, for a suitable fixed spline knot sequence. Moreover, we will explore the accuracy and limitations of such spline approximations. The results from this section will prove invaluable in measuring the performance of the Chapter III nonnegative derivative constrained B-spline estimator $\widehat{f}^B_{P,T_\kappa}$ (c.f. (3.7)-(3.8)) in Section 4.3.

For fixed $m \in \mathbb{N}$, recall the set of constrained functions $\mathcal{S}_m$ given by (3.1) in Chapter III. Fix $r \in (m-1, m]$ and $L > 0$. Define $\gamma := r - (m-1)$ and the Hölder class

$$H^r_L := \left\{ f : [0,1] \to \mathbb{R} \,\middle|\, |f^{(m-1)}(x_1) - f^{(m-1)}(x_2)| \le L|x_1 - x_2|^\gamma, \forall x_1, x_2 \in [0,1] \right\}, \quad (4.1)$$

so we may then construct the family of functions $\mathcal{S}_{m,H}(r,L) := \mathcal{S}_m \cap H^r_L$. Fix constants $c_{\kappa,1}, c_{\kappa,2} > 0$ such that $0 < c_{\kappa,1} \le 1 \le c_{\kappa,2}$. For each $K_n \in \mathbb{N}$, define the family of knot sequences $\mathcal{T}_{K_n}$ just as in (3.14). Finally, for each $T_\kappa \in \mathcal{T}_{K_n}$, define the set of constrained splines

$$\mathbb{S}^{T_\kappa}_{+,m} := \left\{ f_B : [0,1] \to \mathbb{R} \,\middle|\, f_B \text{ is an order } m \text{ spline with knots in } T_\kappa \text{ and } f_B \in \mathcal{S}_m \right\}. \quad (4.2)$$

It is known that for each $K_n \in \mathbb{N}$, $T_\kappa \in \mathcal{T}_{K_n}$, and $f \in H^r_L$, there exists an order m spline f_B with knot sequence T_κ such that $\|f - f_B\|_\infty \leq cK_n^{-r}$, where $c > 0$ is a constant independent of f, depending only on m, r, L, and $c_{\kappa,2}$. Such an accurate approximation of f is called a *Jackson type* approximation [14, pg. 149]. In our work, we are interested in finding Jackson type approximations of functions $f \in \mathcal{S}_{m,H}(r, L)$ that preserve the nonnegative derivative constraint of $f \in \mathcal{S}_m$; such a constraint preserving Jackson type approximation is critical in the performance analysis of the Chapter III constrained B-spline estimator. To this end, we wish to determine whether or not the following statement **(J)** holds for each $m \in \mathbb{N}$.

(J) There exists a constant $c_{\infty,m} > 0$ depending only on m, r, L, and $c_{\kappa,2}$ such that for each $K_n \in \mathbb{N}$, $T_\kappa \in \mathcal{T}_{K_n}$, and $f \in \mathcal{S}_{m,H}(r, L)$, there exists an order m spline $f_B \in \mathbb{S}^{T_\kappa}_{+,m}$ satisfying $\|f - f_B\|_\infty \leq c_{\infty,m}K_n^{-r}$.

By [6, 16], **(J)** holds for $m = 1$, with $c_{\infty,1} := Lc^r_{\kappa,2}$ (take f_B to be the piecewise constant least squares approximation or interpolant of f). Similarly, when $m = 2$, **(J)** holds, with $c_{\infty,2} := Lc^r_{\kappa,2}$ [5, 6, 80] (take f_B to be the piecewise linear interpolant of f at the knots in T_κ). In what follows, we examine statement **(J)** for higher order derivative constraints.

In Section 4.2.1, we will see that **(J)** holds for $m = 3$ (c.f. Proposition 4.2.1). However, in Section 4.2.2, we will show that **(J)** does not hold for $m > 3$ (c.f. Proposition 4.2.2). In spite of this, we will still be able to demonstrate that a weaker version of **(J)** holds for $m > 3$ in Proposition 4.2.3. Moreover, if we restrict f to an appropriate subclass of $\mathcal{S}_{m,H}(r, L)$ (c.f. (4.3)), then we can show that statement **(J)** holds when $\mathcal{S}_{m,H}(r, L)$ in **(J)** is replaced by that subclass.

4.2.1 Third Order Spline Approximation with Increasing Second Derivative

In this section, we will see that **(J)** holds for $m = 3$. Moreover, suppose that $m = 3$, so that $r \in (2, 3]$. We have the following proposition.

Proposition 4.2.1. *Statement* **(J)** *holds for* $m = 3$*, with* $c_{\infty,3} := \frac{3Lc_{\kappa,2}^r}{2}$.

A proof of this result for evenly spaced knots is given in [38]. Moreover, if $c_{\kappa,1} = c_{\kappa,2} = 1$, so that $T_\kappa := T := \{0 < K_n^{-1} < 2K_n^{-1} < \cdots < 1\}$, then for each $f \in \mathcal{S}_{3,H}(r, L)$, there exists $f_B \in \mathbb{S}_{+,3}^T$ such that

$$\|f - f_B\|_\infty \leq \frac{3}{2}K_n^{-2} \sup_{|x-y| \leq K_n^{-1}} |f''(x) - f''(y)| \leq \frac{3}{2}LK_n^{-r},$$

since $f \in H_L^r$. If instead $c_{\kappa,1}$ and $c_{\kappa,2}$ are any fixed constants with $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$, then it follows from an argument similar to that of [38] that **(J)** holds for $m = 3$ with $c_{\infty,3} := \frac{3L}{2}c_{\kappa,2}^r$.

Alternatively, fix $f \in \mathcal{S}_{3,H}(r, L)$. If we let $L(x, f', \kappa_{i-1}, \kappa_i)$ denote the linear interpolant of the convex function f' on $[\kappa_{i-1}, \kappa_i]$ for $i = 1, \ldots, K_n$, and

$$M := \max_i \int_{\kappa_{i-1}}^{\kappa_i} \left(L(x, f', \kappa_{i-1}, \kappa_i) - f'(x)\right) dx,$$

then by [58], which permits unevenly spaced knots, there exists $f_B \in \mathbb{S}_{+,3}^{T_\kappa}$ such that $\|f - f_B\|_\infty \leq 10M$. Furthermore, by the discussion following the statement of **(J)**,

$$\|f - f_B\|_\infty \leq 10M \leq 10 \max_i \int_{\kappa_{i-1}}^{\kappa_i} L\left(\frac{c_{\kappa,2}}{K_n}\right)^{1+\gamma} dx \leq 10L\ \left(\frac{c_{\kappa,2}}{K_n}\right)^r,$$

where $\gamma := r - (m - 1)$.

An additional proof of Proposition 4.2.1 independently constructed by the thesis author is given in Appendix A.

4.2.2 Lower Bound for Higher Order Derivative Constraints

By Section 4.2.1, we now have that **(J)** holds when $m = 1, 2, 3$. In this section, we show that **(J)** does not hold when $m > 3$ in the following proposition. This result is an application of the main theorem in [39].

Proposition 4.2.2. *Fix $m > 3$, $r \in (m-1, m]$, $L > 0$, and $T_\kappa := \{0 = \kappa_0 < \kappa_1 < \cdots < \kappa_{K_n} = 1\}$. (We need not have $T_\kappa \in \mathcal{T}_{K_n}$.) Then there exists $\widetilde{c}_m > 0$ depending only on m and L, as well as a function $f \in \mathcal{S}_{m,H}(r, L)$ such that for all $f_B \in \mathbb{S}^{T_\kappa}_{+,m}$, $\|f - f_B\|_\infty \geq \frac{\widetilde{c}_m}{K_n^3}$.*

Proof. Suppose that $L = 1$ first. As in [39], let AC_{loc} be the family of functions defined on $[0, 1]$ that are absolutely continuous on each closed subinterval of $(0, 1)$. Define

$$\triangle^m_+ W^m_\infty := \{f : [0, 1] \to \mathbb{R} \mid f^{(m-1)} \in \mathrm{AC}_{loc},\ \|f^{(m)}\|_\infty \leq 1,\ f \in \mathcal{S}_m\},$$

so that $\triangle^m_+ W^m_\infty$ is a constrained Sobolev class. Note that if $f \in \triangle^m_+ W^m_\infty$, then by the Mean Value Theorem,

$$|f^{(m-1)}(x_1) - f^{(m-1)}(x_2)| \leq |x_1 - x_2| \max_{x \in (x_1, x_2)} |f^{(m)}(x)| \leq |x_1 - x_2| \leq |x_1 - x_2|^\gamma.$$

Hence each $f \in \triangle^m_+ W^m_\infty$ is also in $\mathcal{S}_{m,H}(r, 1)$ when $r \in (m-1, m]$, so $\triangle^m_+ W^m_\infty \subseteq \mathcal{S}_{m,H}(r, 1)$.

Also let $L_\infty([0, 1])$ denote the set of all bounded (Lebesgue) measurable functions defined on $[0, 1]$, and define

$$\triangle^m_+ L_\infty := \{f : [0, 1] \to \mathbb{R} \mid f \in L_\infty([0, 1]),\ f \in \mathcal{S}_m\}.$$

Now let $M_* := M_*^{K_n+m-1}$ be the space of order m splines with knots in T_κ, and note that M_* has dimension (K_n+m-1). Let $\mathcal{M} := \mathcal{M}^{K_n+m-1} \subseteq L_\infty([0,1])$ be the collection of all linear manifolds (i.e., affine spaces) M of dimension (K_n+m-1) such that $M \cap \triangle_+^m L_\infty \neq \emptyset$. Note that $M_* \cap \triangle_+^m L_\infty = \mathbb{S}_{+,m}^{T_\kappa}$. By applying the main theorem in [39] (with $n = K_n+m-1$, $p = q = \infty$, and $s = r = m$), we have that there exists a constant $c > 0$ depending only on m such that

$$\sup_{f \in \triangle_+^m W_\infty^m} \inf_{f_B \in \mathbb{S}_{+,m}^{T_\kappa}} \|f - f_B\|_\infty = \sup_{f \in \triangle_+^m W_\infty^m} \inf_{f_B \in M_* \cap \triangle_+^m L_\infty} \|f - f_B\|_\infty$$
$$\geq \inf_{M \in \mathcal{M}} \sup_{f \in \triangle_+^m W_\infty^m} \inf_{f_B \in M \cap \triangle_+^m L_\infty} \|f - f_B\|_\infty = \frac{c}{(K_n + m - 1)^3} \geq \frac{c}{m^3 K_n^3}.$$

Hence, there exists $f \in \triangle_+^m W_\infty^m \subseteq \mathcal{S}_{m,H}(r,1)$ such that $\|f - f_B\|_\infty \geq \frac{c}{2m^3 K_n^3}$ for all $f_B \in \mathbb{S}_{+,m}^{T_\kappa}$. Taking $\widetilde{c}_m := \frac{c}{2m^3}$ completes the proof when $L = 1$.

Suppose now that $0 < L \neq 1$. By the previous argument, there exists $f \in \mathcal{S}_{m,H}(r,1)$ such that $\|f - f_B\|_\infty \geq \frac{\widetilde{c}_m}{K_n^3}$ for all $f_B \in \mathbb{S}_{+,m}^{T_\kappa}$. Hence, $\grave{f} := Lf \in \mathcal{S}_{m,H}(r,L)$, and

$$\|\grave{f} - f_B\|_\infty = \|Lf - f_B\|_\infty = L\|f - L^{-1} f_B\|_\infty \geq \frac{L\widetilde{c}_m}{K_n^3}$$

for all $g_B := L^{-1} f_B \in \mathbb{S}_{+,m}^{T_\kappa}$. Replacing $\widetilde{c}_m$ with $L\widetilde{c}_m$ completes the proof. □

Remark 4.2.1. By Proposition 4.2.2, there exists a function $f \in \mathcal{S}_{m,H}(r,L)$ such that $\|f - f_B\|_\infty \geq \frac{\widetilde{c}_m}{K_n^3}$ for all $f_B \in \mathbb{S}_{+,m}^{T_\kappa}$ when $m > 3$. Since the constrained B-spline estimator $\widehat{f}_{P,T_\kappa}^B$ from Chapter III belongs to $\mathbb{S}_{+,m}^{T_\kappa}$, the above result provides an asymptotic lower bound on the performance of this estimator over $\mathcal{S}_{m,H}(r,L)$ for a given K_n, i.e.,

$$\sup_{f \in \mathcal{S}_{m,H}(r,L)} \mathbb{E}\left(\|f - \widehat{f}_{P,T_\kappa}^B\|_\infty\right) \geq \frac{\widetilde{c}_m}{K_n^3}.$$

We will later see in Chapter V how this lower bound on the estimator performance prevents $\widehat{f}^{B}_{P,T_\kappa}$ from achieving the optimal convergence rate in the sup-norm uniformly over $\mathcal{S}_{m,H}(r, L)$ when $m > 3$ (c.f. Corollary 5.5.1, Remark 5.5.1, and the following discussion). In the next section, we demonstrate that although **(J)** fails for $m > 3$, a weaker version of this statement still holds for such m.

4.2.3 Spline Approximation of Functions with Derivatives Bounded Uniformly away from Zero

Choose constants L' and L, with $0 \le L' \le L$, and consider the class of functions

$$\mathcal{S}_{m,H}(r, L', L) := \left\{ f \in \mathcal{S}_m \,\middle|\, L'|x_1 - x_2|^\gamma \le |f^{(m-1)}(x_1) - f^{(m-1)}(x_2)| \le L|x_1 - x_2|^\gamma, \right.$$
$$\left. \forall x_1, x_2 \in [0,1] \right\} \subseteq \mathcal{S}_{m,H}(r, L). \tag{4.3}$$

The goal of this section is to prove the following result. Note that if $L' = 0$, this result does not hold for $m > 3$, by Proposition 4.2.2.

Proposition 4.2.3. *Suppose that $L' > 0$, and let $\gamma := r - (m-1)$. Then there exists*

$$c_B := \left(Lc_{\kappa,2}^{1+\gamma}\right)^{m-1} \left(\frac{m-2}{L'c_{\kappa,1}^{\gamma}}\right)^{m-2} \left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{(m-1)\log(m-1)} (m-1)^{(m-1)\log(m-1)} > 0,$$

such that for all $K_n \in \mathbb{N}$, $T_\kappa \in \mathcal{T}_{K_n}$, and $f \in \mathcal{S}_{m,H}(r, L', L)$, there exists $f_B \in \mathbb{S}^{T_\kappa}_{+,m}$ satisfying $\|f - f_B\|_\infty \le c_B K_n^{-r}$.

Given $p \in \mathbb{N}$, let $\{B^{T_\kappa}_{p,k}\}_{k=1}^{K+p-1}$ again denote the $(K + p - 1)$ B-splines of order p with knot sequence $T_\kappa := \{\kappa_0 < \kappa_1 < \cdots < \kappa_K\}$, and the usual extension. Fix $K_n \in \mathbb{N}$ and $T_\kappa \in \mathcal{T}_{K_n}$. Recall the matrices $D^{(k)} \in \mathbb{R}^{k\times(k+1)}$ (c.f. (3.4)) and $\Delta_{p,T_\kappa} \in \mathbb{R}^{(K_n+p-1)\times(K_n+p-1)}$ (c.f. (3.5)) from the previous chapter. Additionally, define the matrices $\widetilde{D}^{(m)}_{p,T_\kappa} \in \mathbb{R}^{(K_n+m-1-p)\times(K_n+m-1)}$ for each $m \in \mathbb{N}$ and $p = 0, 1, \ldots, m$ inductively:

$$\widetilde{D}^{(m)}_{0,T_\kappa} := I, \quad \text{and} \quad \widetilde{D}^{(m)}_{p,T_\kappa} := \Delta^{-1}_{m-p,T_\kappa} \cdot D^{(K_n+m-1-p)} \cdot \widetilde{D}^{(m)}_{p-1,T_\kappa}. \tag{4.4}$$

Note that $\widetilde{D}^{(m)}_{m,T_\kappa}$ is equal to $\widetilde{D}_{m,T_\kappa}$ (c.f. (3.6)) from Chapter III. In order to establish Proposition 4.2.3, we will need the following lemma.

Lemma 4.2.1. *Suppose that $m > 2$ and let $\gamma := r - (m-1)$. Then for each $j = 0, 1, 2, \ldots, m-2$, there exists*

$$c_b^{(j+2)} := \left(Lc_{\kappa,2}^{1+\gamma}\right)^{j+1} \left(\frac{m-2}{L'c^{\gamma}_{\kappa,1}}\right)^{j} \left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{\frac{j+1}{j+1}+\frac{j+1}{j}+\cdots+\frac{j+1}{2}} \prod_{\ell=1}^{j}(\ell+1)^{\frac{j+1}{\ell}} > 0, \tag{4.5}$$

such that for $g \in \mathcal{S}_{j+2,H}(j+1+\gamma, L', L)$, there exists $\widehat{g} = \sum_{k=1}^{K_n+j+1} \widehat{b}^{(j+2)}_k B^{T_\kappa}_{j+2,k}$ satisfying

(i) $\|g - \widehat{g}\|_\infty \le c_b^{(j+2)}/K_n^{j+1+\gamma}$, and

(ii) $\widetilde{D}^{(j+2)}_{j+2,T_\kappa}\widehat{b}^{(j+2)} \ge \frac{m-2-j}{m-2}L'c^{\gamma}_{\kappa,1}K_n^{-\gamma}$,

where we define $\prod_{\ell=1}^{j}(\ell+1)^{\frac{j+1}{\ell}}$ and $\left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{\frac{j+1}{j+1}+\frac{j+1}{j}+\cdots+\frac{j+1}{2}}$ to be 1 when $j = 0$.

Proof. We proceed by induction on j. Consider $j = 0$ first. For any $g \in \mathcal{S}_{2,H}(1+\gamma, L', L)$, let $\widehat{g} = \sum_{k=1}^{K_n+1} \widehat{b}^{(2)}_k B^{T_\kappa}_{2,k}$ be the piecewise linear interpolant of g, so that $\widehat{b}^{(2)}_k = g(\kappa_{k-1})$ for all $k = 1, \ldots, K_n+1$. By the discussion following statement **(J)**, $\|g - \widehat{g}\|_\infty \le \frac{Lc^{1+\gamma}_{\kappa,2}}{K_n^{1+\gamma}}$, so (i) holds for $j = 0$.

Next, we show that (ii) holds for $j = 0$. For all $i = 1, \ldots, K_n - 1$, we have that

$$\left(\widetilde{D}^{(2)}_{2,T_\kappa}\widehat{b}_2\right)_i = \left[\frac{g(\kappa_{i+1}) - g(\kappa_i)}{\kappa_{i+1} - \kappa_i} - \frac{g(\kappa_i) - g(\kappa_{i-1})}{\kappa_i - \kappa_{i-1}}\right] = \left[\frac{\int_{\kappa_i}^{\kappa_{i+1}} g'(x)dx}{\kappa_{i+1} - \kappa_i} - \frac{\int_{\kappa_{i-1}}^{\kappa_i} g'(x)dx}{\kappa_i - \kappa_{i-1}}\right]$$

$$= \frac{1}{\kappa_i - \kappa_{i-1}} \int_{\kappa_{i-1}}^{\kappa_i} \left[g'\left(\frac{\kappa_{i+1} - \kappa_i}{\kappa_i - \kappa_{i-1}} (x - \kappa_{i-1}) + \kappa_i \right) - g'(x) \right] dx$$

$$\geq \frac{L'}{\kappa_i - \kappa_{i-1}} \int_{\kappa_{i-1}}^{\kappa_i} \left[\left(\frac{\kappa_{i+1} - \kappa_i}{\kappa_i - \kappa_{i-1}} (x - \kappa_{i-1}) + \kappa_i \right) - x \right]^{\gamma} dx$$

$$\geq \frac{L'}{\kappa_i - \kappa_{i-1}} (\kappa_i - \kappa_{i-1}) \min\{(\kappa_i - \kappa_{i-1})^{\gamma}, (\kappa_{i+1} - \kappa_i)^{\gamma}\} \geq L' c_{\kappa,1}^{\gamma} K_n^{-\gamma}.$$

The second to last inequality follows from the fact that if we define

$$\ell_i(x) := \left(\frac{\kappa_{i+1} - \kappa_i}{\kappa_i - \kappa_{i-1}} (x - \kappa_{i-1}) + \kappa_i \right) - x,$$

then

$$\ell_i'(x) = \begin{cases} \frac{\kappa_{i+1} - \kappa_i}{\kappa_i - \kappa_{i-1}} - 1 & \text{if } \frac{\kappa_{i+1} - \kappa_i}{\kappa_i - \kappa_{i-1}} \neq 1 \\ 0 & \text{otherwise.} \end{cases}$$

Thus, $\ell_i(x)$ is either constant on $[\kappa_{i-1}, \kappa_i]$ or achieves its minimum when $x = \kappa_{i-1}$ or $x = \kappa_i$. Hence, the result holds for $j = 0$.

Fix $j \in \{1, 2, \ldots, m-2\}$, and assume that the result holds for $(j-1)$. Let $g \in \mathcal{S}_{j+2,H}(j+1+\gamma, L', L)$. Then by the induction hypothesis, there exists

$$c_b^{(j+1)} = \left(L c_{\kappa,2}^{1+\gamma} \right)^j \left(\frac{m-2}{L' c_{\kappa,1}^{\gamma}} \right)^{(j-1)} \left(\frac{6 c_{\kappa,2}}{c_{\kappa,1}} \right)^{\left(\frac{j}{j} + \frac{j}{j-1} + \cdots + \frac{j}{2} \right)} \prod_{\ell=1}^{j-1} (\ell+1)^{\frac{j}{\ell}} > 0 \tag{4.6}$$

such that for some $\phi := \sum_{j=1}^{K_n+j} \widehat{b}_k^{(j+1)} B_{j+1,k}^{T_\kappa}$, we have both

$$\|g' - \phi\|_\infty \leq c_b^{(j+1)} / K_n^{j+\gamma} \quad \text{and} \quad \widetilde{D}_{j+1,T_\kappa}^{(j+1)} \widehat{b}^{(j+1)} \geq \frac{m-1-j}{m-2} L' c_{\kappa,1}^{\gamma} K_n^{-\gamma}.$$

Define

$$q_j := \left\lceil \frac{2}{c_{\kappa,1}} \sqrt[j]{\frac{(m-2)\, c_b^{(j+1)} (j+1)}{L' c_{\kappa,1}^{\gamma}}} \right\rceil, \tag{4.7}$$

and note that since

$$c_b^{(j+1)} = \left(Lc_{\kappa,2}^{1+\gamma}\right)^j \left(\frac{m-2}{L'c_{\kappa,1}^{\gamma}}\right)^{j-1} \left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{(\frac{j}{j}+\frac{j}{j-1}+\cdots+\frac{j}{2})} \prod_{\ell=1}^{j-1}(\ell+1)^{\frac{j}{\ell}}$$
$$\geq Lc_{\kappa,2}^{1+\gamma}\left(\frac{Lc_{\kappa,2}^{1+\gamma}(m-2)}{L'c_{\kappa,1}^{\gamma}}\right)^{j-1} \geq Lc_{\kappa,2}^{1+\gamma}$$

for all $j = 1, \ldots, m-2$, we have

$$\frac{2}{c_{\kappa,1}}\sqrt[j]{\frac{(m-2)\, c_b^{(j+1)}(j+1)}{L'c_{\kappa,1}^{\gamma}}} \geq \frac{2}{c_{\kappa,1}}\sqrt[j]{\frac{(m-2)Lc_{\kappa,2}^{1+\gamma}(j+1)}{L'c_{\kappa,1}^{\gamma}}} \geq 2.$$

Hence,

$$q_j := \left\lceil \frac{2}{c_{\kappa,1}}\sqrt[j]{\frac{(m-2)\, c_b^{(j+1)}(j+1)}{L'c_{\kappa,1}^{\gamma}}} \right\rceil \leq \frac{3}{c_{\kappa,1}}\sqrt[j]{\frac{(m-2)\, c_b^{(j+1)}(j+1)}{L'c_{\kappa,1}^{\gamma}}}. \tag{4.8}$$

Let $r_j := \left\lfloor \frac{K_n}{q_j(j+1)} \right\rfloor$, and define the points $\tau_{\ell,p} := \kappa_{[(j+1)\ell+p]q_j}$ for all $\ell = 0, 1, \ldots, r_j$ and $p = 0, 1, \ldots, j$. (If $[(j+1)\ell+p]q_j > K_n$, define $\tau_{\ell,p} := \kappa_{[(j+1)\ell+p]q_j} := 1$.) Consider the knot sequence

$$T_\tau := \{0 := \tau_{0,0} < \tau_{0,1} < \cdots < \tau_{0,j} < \tau_{1,0} < \tau_{1,1} < \cdots < \tau_{1,j} < \cdots < \tau_{r_j,0}\}.$$

Associated with the knot sequence T_τ, is the set of order $(j+1)$ B-splines $\{B_{j+1,s}^{T_\tau}\}_{s=1}^{r_j(j+1)+j}$ with the usual left and right extension such that $\sum_{s=1}^{r_j(j+1)+j} B_{j+1,s}^{T_\tau}(x) = 1$ for all $x \in [0,1]$. Note that for each $s = \ell(j+1)$, the support of $B_{j+1,s}^{T_\tau}$ is $[\tau_{\ell-1,0}, \tau_{\ell,0}]$ for $\ell = 1, \ldots, r_j$.

Define the vector $d := (d_s) \in \mathbb{R}^{r_j(j+1)+j}$ such that

$$d_s := \begin{cases} (j+1)\nu_\ell & \text{when } s = \ell(j+1) \\ \\ 0 & \text{otherwise} \end{cases} \qquad \text{where} \qquad \nu_\ell := \frac{\int_{\tau_{\ell-1,0}}^{\tau_{\ell,0}} \left(g'(x) - \phi(x)\right)\, dx}{\tau_{\ell,0} - \tau_{\ell-1,0}}, \quad (4.9)$$

for $\ell = 1, 2, \ldots, r_j$. Moreover, ν_ℓ denotes the average value of $g' - \phi$ on $[\tau_{\ell-1,0}, \tau_{\ell,0}]$. Also, let

$$\widetilde{\phi} := \phi + \sum_{s=1}^{r_j(j+1)+j} d_s\, B_{j+1,s}^{T_\tau} = \phi + \sum_{k=1}^{K_n+j} a_k\, B_{j+1,k}^{T_\kappa} = \sum_{k=1}^{K_n+j} (\widehat{b}^{(j+1)} + a)_k\, B_{j+1,k}^{T_\kappa}, \qquad (4.10)$$

where $a := (a_k) \in \mathbb{R}^{K_n+j}$ is determined by d. Finally, define $\widehat{g}$ such that $\widehat{g}(x) := g(0) + \int_0^x \widetilde{\phi}(t)dt$ for all $x \in [0,1]$.

We will first show that $\|g - \widehat{g}\|_\infty \leq c_b^{(j+2)}/K_n^{j+1+\gamma}$, where $c_b^{(j+2)}$ is given by (4.5). Note that for any $\ell = 1, 2, \ldots, r_j$,

$$\int_{\tau_{\ell-1,0}}^{\tau_{\ell,0}} g'(t) - \widetilde{\phi}(t)\, dt = \int_{\tau_{\ell-1,0}}^{\tau_{\ell,0}} g'(t) - \phi(t)\, dt - (j+1)\nu_\ell \int_{\tau_{\ell-1,0}}^{\tau_{\ell,0}} B_{j+1,\ell(j+1)}^{T_\tau}(t)\, dt \qquad (4.11)$$

$$= \nu_\ell(\tau_{\ell,0} - \tau_{\ell-1,0}) - (j+1)\nu_\ell \frac{\tau_{\ell,0} - \tau_{\ell-1,0}}{j+1} = 0.$$

Also, for any $x \in [0,1]$, $x \in [\tau_{\ell-1,0}, \tau_{\ell,0}]$ for some $\ell = 1, 2, \ldots, r_j$, or $x \in [\tau_{r_j,0}, 1]$. Consider the following two cases:

Case 1: $x \in [\tau_{\ell-1,0}, \tau_{\ell,0}]$ for some $\ell = 1, 2, \ldots, r_j$. Then by (4.11) and the induction hypothesis,

$$|g(x) - \widehat{g}(x)| = \left| \int_0^x g'(t) - \widetilde{\phi}(t)\, dt \right| \leq \int_{\tau_{\ell-1,0}}^x |g'(t) - \widetilde{\phi}(t)|\, dt$$

$$\leq \int_{\tau_{\ell-1,0}}^x |g'(t) - \phi(t)|\, dt + (j+1)\, |\nu_\ell| \int_0^{\tau_{r_j,0}} \left| B_{j+1,\ell(j+1)}^{T_\tau}(x) \right| dx$$

$$\leq 2(\tau_{\ell,0} - \tau_{\ell-1,0}) c_b^{(j+1)} / K_n^{j+\gamma} \leq \frac{2 c_b^{(j+1)} c_{\kappa,2} q_j (j+1)}{K_n^{j+1+\gamma}}.$$

Case 2: $x \in [\tau_{r_j,0}, 1]$. Then

$$|g(x) - \widehat{g}(x)| = \left| \int_0^x g'(t) - \widetilde{\phi}(t)\, dt \right| = \left| \int_{\tau_{r_j,0}}^x g'(t) - \phi(t)\, dt \right| \leq \int_{\tau_{r_j,0}}^x |g'(t) - \phi(t)|\, dt$$
$$\leq (x - \tau_{\tau_{r_j,0}}) \frac{c_b^{(j+1)}}{K_n^{j+\gamma}} \leq \frac{2 c_b^{(j+1)} c_{\kappa,2} q_j (j+1)}{K_n^{j+1+\gamma}}.$$

Therefore, for all $x \in [0,1]$, by (4.6) and (4.8)

$$|g(x) - \widehat{g}(x)| \leq \frac{2 c_b^{(j+1)} c_{\kappa,2} q_j (j+1)}{K_n^{j+1+\gamma}} \leq \frac{2 c_b^{(j+1)} c_{\kappa,2} (j+1)}{K_n^{j+1+\gamma}} \frac{3}{c_{\kappa,1}} \sqrt[j]{\frac{(m-2)\, c_b^{(j+1)} (j+1)}{L' c_{\kappa,1}^{\gamma}}}$$
$$= \frac{6 c_{\kappa,2}}{c_{\kappa,1}} (j+1)^{\frac{j+1}{j}} \left(\frac{m-2}{L' c_{\kappa,1}^{\gamma}} \right)^{\frac{1}{j}} \left(c_b^{(j+1)} \right)^{\frac{j+1}{j}} \frac{1}{K_n^{j+1+\gamma}}$$
$$= \frac{6 c_{\kappa,2}}{c_{\kappa,1}} \left(\frac{6 c_{\kappa,2}}{c_{\kappa,1}} \right)^{\left(\frac{j+1}{j} + \frac{j+1}{j-1} + \cdots + \frac{j+1}{2} \right)} (j+1)^{\frac{j+1}{j}} \prod_{\ell=1}^{j-1} (\ell+1)^{\frac{j+1}{\ell}} \left(\frac{m-2}{L' c_{\kappa,1}^{\gamma}} \right)^{\frac{1}{j}} \left(\frac{m-2}{L' c_{\kappa,1}^{\gamma}} \right)^{(j-1)\frac{j+1}{j}}$$
$$\times \left(L c_{\kappa,2}^{1+\gamma} \right)^{j \frac{j+1}{j}} \frac{1}{K_n^{j+1+\gamma}} = c_b^{(j+2)} / K_n^{j+1+\gamma}$$

Hence, (i) holds by induction.

Next we will show that $\widetilde{D}_{j+2,T_\kappa}^{(j+2)} \widehat{b}^{(j+2)} \geq \frac{m-2-j}{m-2} L' c_{\kappa,1}^{\gamma} K_n^{-\gamma}$, where

$$\widehat{g} = \sum_{k=1}^{K_n+j+1} \widehat{b}_k^{(j+2)} B_{j+2,k}^{T_\kappa}.$$

Consider the jth derivative of $\widetilde{\phi} - \phi$,

$$(\widetilde{\phi} - \phi)^{(j)} = \left(\sum_{s=1}^{r_j(j+1)+j} d_s\, B_{j+1,s}^{T_\tau} \right)^{(j)} = \sum_{s=1}^{r_j(j+1)} \left(\widetilde{D}_{j,T_\tau}^{(j+1)} d \right)_s \mathbf{1}_{[\kappa_{s(q_j-1)}, \kappa_{s q_j})}$$

on $[0,\tau_{r_j,0}) = [0,\kappa_{r_j q_j(j+1)})$ via Lemma 3.2.1 of Chapter III. Note that by (4.9), only every $(j+1)$th entry of d is nonzero, and hence $\|\widetilde{D}^{(j+1)}_{1,T_\tau} d\|_\infty \le \frac{K_n}{q_j c_{\kappa,1}} \frac{(j+1)c_b^{(j+1)}}{K_n^{j+\gamma}}$. By induction, and using (3.5), and (3.6), for $p = 2,\dots,j$ we have

$$\|\widetilde{D}^{(j+1)}_{p,T_\tau} d\|_\infty = \|\Delta^{-1}_{j+1-p,T_\tau} D^{(r_j(j+1)+j-p)} \widetilde{D}^{(j+1)}_{p-1,T_\tau} d\|_\infty \le \frac{2K_n}{q_j c_{\kappa,1}} \|\widetilde{D}^{(j+1)}_{p-1,T_\tau} d\|_\infty$$
$$\le 2^{p-1} \left(\frac{K_n}{q_j c_{\kappa,1}}\right)^p \frac{(j+1)c_b^{(j+1)}}{K_n^{j+\gamma}}.$$

Taking $p = j$ gives us that the jth derivative of $\sum_{s=1}^{r_j(j+1)+j} d_s\, B^{T_\tau}_{j+1,s}$ is bounded in the supremum norm by $\frac{2^{j-1}\,(j+1)c_b^{(j+1)}}{q_j^j c_{\kappa,1}^j K_n^\gamma}$.

Now, recall from (4.10) that $\widetilde{\phi} - \phi = \sum_{s=1}^{r_j(j+1)+j} d_s\, B^{T_\tau}_{j+1,s} = \sum_{k=1}^{K_n+j} a_k\, B^{T_\kappa}_{j+1,k}$ for some $a \in \mathbb{R}^{K_n+j}$ determined by d. By Lemma 3.2.1, the jth derivative of $\widetilde{\phi} - \phi$ is given by $\sum_{k=1}^{K_n} \left(\widetilde{D}^{(j+1)}_{j,T_\kappa} a\right)_k \mathbf{1}_{[\kappa_{k-1},\kappa_k)}$ on $[0,1)$, which is bounded in the supremum norm by $\frac{2^{j-1}\,(j+1)c_b^{(j+1)}}{q_j^j c_{\kappa,1}^j K_n^\gamma}$, via the above discussion. By (4.7),

$$\|\widetilde{D}^{(j+1)}_{j+1,T_\kappa} a\|_\infty = \|D^{(K_n-1)} \widetilde{D}^{(j+1)}_{j,T_\kappa} a\|_\infty \le \|D^{(K_n-1)}\|_\infty \|\widetilde{D}^{(j+1)}_{j,T_\kappa} a\|_\infty$$
$$\le \frac{2^j\,(j+1)c_b^{(j+1)}}{q_j^j c_{\kappa,1}^j K_n^\gamma} \le \frac{L' c_{\kappa,1}^\gamma}{m-2} K_n^{-\gamma}. \tag{4.12}$$

Finally, on $[0,1)$, the $(j+1)$th derivative of $\widehat{g}$ is given by

$$(\widehat{g})^{(j+1)} = \left(\sum_{k=1}^{K_n+j+1} \widehat{b}_k^{(j+2)} B^{T_\kappa}_{j+2,k}\right)^{(j+1)} = \sum_{k=1}^{K_n} (\widetilde{D}^{(j+2)}_{j+1,T_\kappa} \widehat{b}^{(j+2)})_k \mathbf{1}_{[\kappa_{k-1},\kappa_k)},$$

which is equal to the jth derivative of $\widetilde{\phi}$, given by

$$(\widetilde{\phi})^{(j)} = \left(\sum_{k=1}^{K_n+j} (\widehat{b}^{(j+1)} + a)_k\, B^{T_\kappa}_{j+1,k}\right)^{(j)} = \sum_{k=1}^{K_n} (\widetilde{D}^{(j+1)}_{j,T_\kappa} (\widehat{b}^{(j+1)} + a))_k \mathbf{1}_{[\kappa_{k-1},\kappa_k)}.$$

Hence,

$$\begin{aligned}\widetilde{D}^{(j+2)}_{j+2,T_\kappa}\widehat{b}^{(j+2)} &= D_{K_n-1}\widetilde{D}^{(j+2)}_{j+1,T_\kappa}\widehat{b}^{(j+2)} = D^{(K_n-1)}\widetilde{D}^{(j+1)}_{j,T_\kappa}\left(\widehat{b}^{(j+1)}+a\right)\\ &= \widetilde{D}^{(j+1)}_{j+1,T_\kappa}\left(\widehat{b}^{(j+1)}+a\right) \geq \widetilde{D}^{(j+1)}_{j+1,T_\kappa}\widehat{b}^{(j+1)} - \mathbf{1}\|\widetilde{D}^{(j+1)}_{j+1,T_\kappa}a\|_\infty\\ &\geq \frac{m-1-j}{m-2}L'c_{\kappa,1}^{\gamma}K_n^{-\gamma} - \frac{L'c_{\kappa,1}^{\gamma}}{m-2}K_n^{-\gamma} = \frac{m-2-j}{m-2}L'c_{\kappa,1}^{\gamma}K_n^{-\gamma},\end{aligned}$$

via the induction hypothesis, and (4.12). Thus, (ii) holds completing the proof. □

The following argument demonstrates that Proposition 4.2.3 holds.

Proof of Proposition 4.2.3. Taking $j = m-2$ and applying Lemma 4.2.1, we have that there exists

$$c_b^{(m)} := \left(Lc_{\kappa,2}^{1+\gamma}\right)^{m-1}\left(\frac{m-2}{L'c_{\kappa,2}^{\gamma}}\right)^{m-2}\left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{\frac{m-1}{m-1}+\frac{m-1}{m-2}+\cdots+\frac{m-1}{2}}\prod_{\ell=1}^{m-2}(\ell+1)^{\frac{m-1}{\ell}} > 0$$

such that for all $K_n \in \mathbb{N}$, $T_\kappa \in \mathcal{T}_{K_n}$, and $g \in \mathcal{S}_{m,H}(m-1+\gamma, L', L)$ there exists $\widehat{g} := \sum_{k=1}^{K_n+m-1}\widehat{b}_k^{(m)}B_{m,k}^{T_\kappa}$ such that $\|g-\widehat{g}\|_\infty \leq \frac{c_b^{(m)}}{K_n^{m-1+\gamma}}$ and $\widetilde{D}^{(m)}_{m,T_\kappa}\widehat{b}^{(m)} \geq 0$ implying that $\widehat{g} \in \mathbb{S}_{+,m}^{T_\kappa}$. Additionally, we have that

$$\sum_{\ell=2}^{m-1}\frac{m-1}{\ell} \leq (m-1)\int_1^{m-1}\frac{dx}{x} \leq (m-1)\log(m-1),$$

so, $\left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{\frac{m-1}{m-1}+\frac{m-1}{m-2}+\cdots+\frac{m-1}{2}} \leq \left(\frac{6c_{\kappa,2}}{c_{\kappa,1}}\right)^{(m-1)\log(m-1)}$. Also,

$$\begin{aligned}\log\left(\prod_{\ell=1}^{m-2}(\ell+1)^{\frac{m-1}{\ell}}\right) &= (m-1)\sum_{\ell=1}^{m-2}\frac{\log(\ell+1)}{\ell} \leq 2(m-1)\sum_{\ell=1}^{m-2}\frac{\log(\ell+1)}{\ell+1}\\ &\leq 2(m-1)\int_1^{m-1}\frac{\log x}{x}\,dx = (m-1)(\log(m-1))^2,\end{aligned}$$

and thus $\prod_{\ell=1}^{m-2}(\ell+1)^{\frac{m-1}{\ell}} \leq (m-1)^{(m-1)(\log(m-1))}$. Combining these results, we have that $c_b^{(m)} \leq c_B$. Taking $f_B := \widehat{g}$ completes the proof of Proposition 4.2.3. $\square$

We have presented several different results on the accuracy and limitations of approximating functions $f \in \mathcal{S}_{m,H}(r,L)$ with splines $f_B \in \mathbb{S}_{+,m}^{T_\kappa}$. We will utilize these results, along with the uniform Lipschitz property, to measure the performance of the nonnegative derivative constrained B-spline estimator from Chapter III in the next section.

4.3 Bias and Stochastic Error

In this section we apply the uniform Lipschitz property of the constrained B-spline estimator established in Theorem 3.2.1, along with the spline approximation results from Section 4.2, to the nonparametric estimation of smooth nonnegative derivative constrained functions in a Hölder class. Let L and r be positive constants and $m := \lceil r \rceil \in \mathbb{N}$ so that $r \in (m-1, m]$. Given a sequence of design points $(x_i)_{i=0}^n$ on $[0,1]$, consider the following regression problem:

$$y_i = f(x_i) + \sigma\varepsilon_i, \quad i = 0, 1, \ldots, n, \tag{4.13}$$

where f is an unknown true function in $\mathcal{S}_{m,H}(r,L)$, the ε_i's are independent standard normal errors, σ is a positive constant, and the y_i's are samples. The goal of shape constrained estimation is to construct an estimator $\widehat{f}$ that preserves the specified shape of the true function characterized by $\mathcal{S}_m$. In the asymptotic analysis of such an estimator, we are particularly interested in its uniform convergence on the entire interval $[0,1]$, as well as the convergence rate of $\sup_{f\in\mathcal{S}_{m,H}(r,L)} \mathbb{E}(\|\widehat{f}-f\|_\infty)$, when the sample size n is sufficiently large. With the help of the uniform Lipschitz property and the results from Section 4.2, we show that for general nonnegative derivative constraints (i.e., $m \in \mathbb{N}$ is arbitrary), the constrained B-spline estimator (3.7) achieves uniform convergence on $[0,1]$ for possibly unevenly spaced design points and knots. We also provide a convergence rate. In Chapter V, we will see that this convergence rate is optimal in certain instances (c.f. Corollary 5.5.1 and Remark 5.5.1). These results pave the way for further study of the convergence rate of estimators subject to general nonnegative derivative constraints.

We discuss the asymptotic performance of the constrained B-spline estimator (3.7) as follows. Consider the set $\mathcal{P}_n$ in (3.13) for a given $c_\omega \geq 1$ and the collection of knot sequences $\mathcal{T}_{K_n}$ in (3.14) for fixed $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$. For each $n \in \mathbb{N}$, let $P := (x_i)_{i=1}^n \in \mathcal{P}_n$ be a sequence of design points on $[0,1]$ and let $T_\kappa \in \mathcal{T}_{K_n}$ be a given sequence of knots, where (K_n) is an increasing sequence of natural numbers. Let $y = (y_i)_{i=0}^n \in \mathbb{R}^{n+1}$ be the sample data vector given in (4.13). For a given m and a true function $f \in \mathcal{S}_{m,H}(r,L)$, consider the constrained B-spline estimator, denoted by $\widehat{f}^B_{P,T_\kappa}$ in (3.7), and its B-spline coefficient vector $\widehat{b}_{P,T_\kappa}$ defined in (3.9). Moreover, we introduce the vector of noise-free data $\vec{f} := (f(x_0), f(x_1), \ldots, f(x_n))^T \in \mathbb{R}^{n+1}$ and define $\overline{f}_{P,T_\kappa} := \sum_{k=1}^N \bar{b}_k B^{T_\kappa}_{m,k}$, where $N := K_n + m - 1$, $\{B^{T_\kappa}_{m,k}\}_{k=1}^N$ denotes the set of N order m B-splines with knot sequence T_κ and the usual extension, and $\bar{b}_{P,T_\kappa} = (\bar{b}_k) \in \mathbb{R}^N$ is the B-spline coefficient vector characterized by the optimization problem in (3.9) when $\bar{y}$ is replaced by $K_n \widehat{X}^T \Theta_n \vec{f}$:

$$\bar{b}_{P,T_\kappa} := \underset{\widetilde{D}_{m,T_\kappa} b \geq 0}{\arg\min} \ \frac{1}{2} b^T \Lambda_{K_n,P,T_\kappa} b - b^T \big(K_n \widehat{X}^T \Theta_n \vec{f} \,\big). \tag{4.14}$$

Note that for each true f, $\mathbb{E}(\|\widehat{f}^B_{P,T_\kappa} - f\|_\infty) \leq \|f - \overline{f}_{P,T_\kappa}\|_\infty + \mathbb{E}(\|\overline{f}_{P,T_\kappa} - \widehat{f}^B_{P,T_\kappa}\|_\infty)$, where $\|f - \overline{f}_{P,T_\kappa}\|_\infty$ pertains to the estimator bias and $\mathbb{E}(\|\overline{f}_{P,T_\kappa} - \widehat{f}^B_{P,T_\kappa}\|_\infty)$ corresponds to the stochastic error. We develop uniform bounds for these two terms in the succeeding propositions via the uniform Lipschitz property and the results from Section 4.2. For notational simplicity, define $\gamma := r - (m-1)$ for $\mathcal{S}_{m,H}(r, L)$.

Proposition 4.3.1. *Let $q := \min\{2+\gamma, r\}$. Fix $m \in \mathbb{N}$, and constants $c_\omega \geq 1$ (c.f. (3.13)), $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$ (c.f. (3.14)), $L > 0$, and $r \in (m-1, m]$ (c.f. (4.1)). Let (K_n) be an increasing sequence of natural numbers with $K_n \to \infty$ and $K_n/n \to 0$ as $n \to \infty$. Then there exists $C_b > 0$ depending only on $m, L, c_{\kappa,1}$, and $c_{\kappa,2}$, as well as $\widehat{n}_1 \in \mathbb{N}$ depending only on (K_n) (and the fixed constants $m, c_\omega, c_{\kappa,1}, c_{\kappa,2}$) such that*

$$\sup_{f \in \mathcal{S}_{m,H}(r,L),\, P \in \mathcal{P}_n,\, T_\kappa \in \mathcal{T}_{K_n}} \left\| f - \overline{f}_{P,T_\kappa} \right\|_\infty \leq C_b \cdot \big(K_n\big)^{-q}, \qquad \forall\, n \geq \widehat{n}_1.$$

Proof. Fix an arbitrary true function $f \in \mathcal{S}_{m,H}(r, L)$. For any given $P \in \mathcal{P}_n$ and $T_\kappa \in \mathcal{T}_{K_n}$, we write $\overline{f}_{P,T_\kappa}$ as $\overline{f}$ to simplify notation.

By Proposition 4.2.1 and the discussion following statement **(J)**, if $m = 1, 2$, or 3, then there exists a spline $f_B \in \mathbb{S}^{T_\kappa}_{+,m}$ and a constant $c_{\infty,m}$ such that $\|f - f_B\|_\infty \leq c_{\infty,m} K_n^{-r} \leq \frac{3Lc^3_{\kappa,2}}{2} K_n^{-q}$. Alternatively, if $m > 3$, then define $g := f^{(m-3)} \in \mathcal{S}_{3,H}(r + 3 - m, L)$. By Proposition 4.2.1, there exists a constant $c_{\infty,3}$, as well as a spline $g_B \in \mathbb{S}^{T_\kappa}_{+,m}$ such that $\|g - g_B\|_\infty \leq c_{\infty,3} K_n^{m-r-3} \leq \frac{3Lc^3_{\kappa,2}}{2} K_n^{-(2+\gamma)}$. If we define $f_B : [0, 1] \to \mathbb{R}$ such that

$$f_B(x) := \sum_{k=0}^{m-4} \frac{f^{(k)}(0)}{k!} x^k + \int_0^x \int_0^{t_1} \cdots \int_0^{t_{m-4}} g_B(t_{m-3})\, dt_{m-3} \cdots dt_2\, dt_1,$$

then $f_B \in \mathcal{S}_{m,H}(r, L)$ and

$$\begin{aligned} \big|f(x) - f_B(x)\big| &\leq \int_0^x \int_0^{t_1} \cdots \int_0^{t_{m-4}} |g(t_{m-3}) - g_B(t_{m-3})|\, dt_{m-3} \cdots dt_2\, dt_1 \\ &\leq \int_0^x \int_0^{t_1} \cdots \int_0^{t_{m-4}} \frac{3Lc^3_{\kappa,2}}{2} K_n^{-(2+\gamma)}\, dt_{m-3} \cdots dt_2\, dt_1 \end{aligned}$$

$$\leq \frac{3Lc_{\kappa,2}^3}{2(m-3)!} K_n^{-(2+\gamma)} \leq \frac{3Lc_{\kappa,2}^3}{2} K_n^{-q},$$

for all $x \in [0,1]$, where we define $\int_0^x \int_0^{t_1} \cdots \int_0^{t_{m-4}} h(t_{m-3})\, dt_{m-3} \cdots dt_2\, dt_1 := \int_0^x h(t_1)\, dt_1$ for any integrable function h if $m = 4$. In either case, we have $\|f - f_B\|_\infty \leq \frac{3Lc_{\kappa,2}^3}{2} K_n^{-q}$.

In view of $\|f - \overline{f}\|_\infty \leq \|f - f_B\|_\infty + \|f_B - \overline{f}\|_\infty$, it remains to establish a uniform bound on $\|f_B - \overline{f}\|_\infty$. We introduce the vector $\vec{f_B} := (f_B(x_0), f_B(x_1), \ldots, f_B(x_n))^T \in \mathbb{R}^{n+1}$. Since $f_B \in \mathbb{S}_{+,m}^{T_\kappa}$ is an order m spline with knot sequence T_κ, there exists $\widetilde{b} \in \mathbb{R}^N$ such that $f_B = \sum_{k=1}^N \widetilde{b}_k B_{m,k}^{T_\kappa}$. Thus, we have $\widehat{X}\widetilde{b} = \vec{f_B}$, where $\widehat{X}$ is the design matrix corresponding to the design point sequence P and the B-splines $\{B_{m,k}^{T_\kappa}\}_{k=1}^N$ (cf. Section 3.2.1). This shows that $\frac{1}{2}\|K_n^{1/2}\Theta_n^{1/2}(\widehat{X}\widetilde{b} - \vec{f_B})\|_2^2 = 0$. Moreover, since $\widetilde{D}_{m,T_\kappa}\widetilde{b} \geq 0$ (c.f. (3.5)) via Lemma 3.2.1, we deduce that

$$\widetilde{b} = \underset{\widetilde{D}_{m,T_\kappa} b \geq 0}{\arg\min} \frac{1}{2} b^T \Lambda_{K_n,P,T_\kappa} b - b^T \Big(K_n \widehat{X}^T \Theta_n \vec{f_B} \Big).$$

(See Section 3.2.1 for the definitions of Θ_n and Λ_{K_n,P,T_κ}.) By using the definition of $\overline{f}$ before (4.14) and the uniform Lipschitz property of Theorem 3.2.1, we obtain a positive constant c_∞, depending only on m and $c_{\kappa,1}$, and a natural number n_*, depending only on $(K_n), m, c_\omega, c_{\kappa,1}$, and $c_{\kappa,2}$, such that for any $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \geq n_*$,

$$\begin{aligned}
\big\|\overline{f} - f_B\big\|_\infty \leq \big\|\overline{b}_{P,T_\kappa} - \widetilde{b}\big\|_\infty &\leq c_\infty \cdot \Big\| K_n \widehat{X}^T \Theta_n \vec{f} - K_n \widehat{X}^T \Theta_n \vec{f_B} \Big\|_\infty \\
&\leq c_\infty \cdot \big\| K_n \widehat{X}^T \Theta_n \big\|_\infty \cdot \Big\| \vec{f} - \vec{f_B} \Big\|_\infty \\
&\leq c_\infty \cdot \big\| K_n \widehat{X}^T \Theta_n \big\|_\infty \cdot \frac{3Lc_{\kappa,2}^3}{2} K_n^{-q}, \qquad (4.15)
\end{aligned}$$

where we use $\left\|\vec{f}-\vec{f_B}\right\|_\infty \le \|f-f_B\|_\infty$ and the uniform bound for $\|f-f_B\|_\infty$ established above. We further show that $\left\|K_n\widehat{X}^T\Theta_n\right\|_\infty$ attains a uniform bound independent of $P\in\mathcal{P}_n$, K_n, and $T_\kappa\in\mathcal{T}_{K_n}$ as long as n is large enough. It follows from the definition of $\widehat{X}$ and the non-negativity, upper bound, and support of the $B^{T_\kappa}_{m,k}$'s (given at the beginning of Section 3.2) that for each $k=1,\ldots,N$,

$$\begin{aligned}\left\|(K_n\widehat{X}^T\Theta_n)_{k\bullet}\right\|_\infty &= K_n\sum_{i=0}^n B^{T_\kappa}_{m,k}(x_i)\cdot(x_{i+1}-x_i) \;\le\; K_n\sum_{i=0}^n \mathbf{I}_{[\kappa_{k-m},\,\kappa_k]}(x_i)\cdot(x_{i+1}-x_i)\\ &\le K_n\left(\kappa_k-\kappa_{k-m}+\frac{c_\omega}{n}\right) \;\le\; c_{\kappa,2}\,m+\frac{c_\omega K_n}{n},\end{aligned}$$

where the term c_ω/n comes from the fact that κ_k is in the interval $[x_r, x_{r+1})$ for some design points x_r, x_{r+1}. Since $K_n/n\to 0$ as $n\to\infty$, we obtain $\bar{n}_1\in\mathbb{N}$ (depending only on (K_n) and c_ω) such that for any $n\ge\bar{n}_1$, $\left\|(K_n\widehat{X}^T\Theta_n)_{k\bullet}\right\|_\infty\le c_{\kappa,2}(m+1)$ for each $k=1,\ldots,N$ so that $\left\|K_n\widehat{X}^T\Theta_n\right\|_\infty\le c_{\kappa,2}(m+1)$ for any $P\in\mathcal{P}_n$, K_n, and $T_\kappa\in\mathcal{T}_{K_n}$. Combining this with (4.15) yields that for any $n\ge\max(n_*,\bar{n}_1)$, $\|\overline{f}-f_B\|_\infty\le\frac{c_\infty 3L(m+1)\,c^4_{\kappa,2}}{2}K_n^{-q}$ for any $f\in\mathcal{S}_{m,H}(r,L)$, $P\in\mathcal{P}_n$, K_n, and $T_\kappa\in\mathcal{T}_{K_n}$.

Setting $\widehat{n}_1:=\max(n_*,\bar{n}_1)$ (depending only on (K_n) and the fixed constants m, c_ω, $c_{\kappa,1}$, $c_{\kappa,2}$), we conclude that

$$\sup_{f\in\mathcal{S}_{m,H}(r,L),\,P\in\mathcal{P}_n,\,T_\kappa\in\mathcal{T}_{K_n}}\|\,f-\overline{f}\,\|_\infty\;\le\;C_b\cdot K_n^{-q},\quad\forall\,n\ge\widehat{n}_1,$$

where $C_b:=\frac{[c_\infty(m+1)c_{\kappa,2}+1]3Lc^3_{\kappa,2}}{2}$. □

The next result provides a uniform bound on the bias of $\widehat{f}^B_{P,T_\kappa}$ over the function class $\mathcal{S}_{m,H}(r,L',L)\subseteq\mathcal{S}_{m,H}(r,L)$ (defined in (4.3)), when $L'>0$. This bound is asymptotically better than the bound in Proposition 4.3.1. However, a uniform bound with this asymptotic rate cannot be extended to all of $\mathcal{S}_{m,H}(r, L)$ when $m > 3$ (c.f. Remark 4.2.1). The proof of this result is similar to that of Proposition 4.3.1 and is therefore omitted; the argument relies on Proposition 4.2.3 and the uniform Lipschitz property.

Proposition 4.3.2. *Fix $m \in \mathbb{N}$, and constants $c_\omega \geq 1$, $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$, $L \geq L' > 0$, and $r \in (m-1, m]$. Let (K_n) be an increasing sequence of natural numbers with $K_n \to \infty$ and $K_n/n \to 0$ as $n \to \infty$. Then there exists $C_b' > 0$ depending only on $m, r, L, L', c_{\kappa,1}$, and $c_{\kappa,2}$, as well as $\widehat{n}_1 \in \mathbb{N}$ depending only on (K_n) (and the fixed constants $m, c_\omega, c_{\kappa,1}, c_{\kappa,2}$) such that*

$$\sup_{f \in \mathcal{S}_{m,H}(r,L',L),\, P \in \mathcal{P}_n,\, T_\kappa \in \mathcal{T}_{K_n}} \left\| f - \overline{f}_{P,T_\kappa} \right\|_\infty \leq C_b' \cdot \left(K_n\right)^{-r}, \qquad \forall\, n \geq \widehat{n}_1.$$

In the following proposition, we derive a uniform bound on the stochastic error of the estimator $\widehat{f}^B_{P,T_\kappa}$ over all of $\mathcal{S}_{m,H}(r, L)$.

Proposition 4.3.3. *Fix $m \in \mathbb{N}$, and constants $c_\omega \geq 1$, $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$, $L > 0$, $r \in (m-1, m]$, and define $q := \min\{2+\gamma, r\}$. Let (K_n) be an increasing sequence of natural numbers with $K_n \to \infty$, $K_n/n \to 0$, $K_n/(n^{1/q} \cdot \sqrt{\log n}) \to 0$ as $n \to \infty$. Then there exist a positive constant C_s and $\widehat{n}_2 \in \mathbb{N}$, both depending only on (K_n) (and the fixed constants $m, c_\omega, c_{\kappa,1}, c_{\kappa,2}, \sigma$), such that*

$$\sup_{f \in \mathcal{S}_{m,H}(r,L),\, P \in \mathcal{P}_n,\, T_\kappa \in \mathcal{T}_{K_n}} \mathbb{E}\left(\left\| \widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa} \right\|_\infty \right) \leq C_s \cdot \sqrt{\frac{K_n \log n}{n}}, \qquad \forall\, n \geq \widehat{n}_2.$$

Proof. Fix a true function $f \in \mathcal{S}_{m,H}(r, L)$. Given arbitrary $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$, let $\vec{\varepsilon} := (\varepsilon_i) \in \mathbb{R}^{n+1}$, $\omega_i := x_{i+1} - x_i$ for $i = 0, 1, \ldots, n$, and define $\xi_k := \left(\sqrt{nK_n}\, \widehat{X}^T \Theta_n\right)_{k\bullet} \vec{\varepsilon} = \sqrt{nK_n} \sum_{i=0}^n \omega_i B^{T_\kappa}_{m,k}(x_i) \varepsilon_i$ for each $k = 1, \ldots, N$. (See Section 3.2.1 for the definitions of

$\widehat{X}$ and Θ_n.) Since each $\varepsilon_i \sim \mathcal{N}(0,1)$ and the ε_i's are independent, we have $\xi_k \sim \mathcal{N}(0, \bar\sigma_k^2)$, where $\bar\sigma_k^2 = \|(\sqrt{nK_n}\,\widehat{X}^T\Theta_n)_{k\bullet}\|_2^2 \ge 0$. By the proof of Proposition 4.3.1, there exists $\bar n_1 \in \mathbb{N}$ (depending only on (K_n) and c_ω) such that if $n \ge \bar n_1$, then for any $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$, $\|(K_n \widehat{X}^T\Theta_n)_{k\bullet}\|_\infty \le c_{\kappa,2}(m+1)$ for each $k = 1, \ldots, N$. Therefore, by using $n \cdot \big(B^{T_\kappa}_{m,k}(x_i)\,\omega_i\big)^2 \le n\omega_i \cdot \big(B^{T_\kappa}_{m,k}(x_i)\,\omega_i\big) \le c_\omega \cdot \big(B^{T_\kappa}_{m,k}(x_i)\,\omega_i\big)$ for each i, we have, for any $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \ge \bar n_1$,

$$\Big\|\big(\sqrt{nK_n}\,\widehat{X}^T\Theta_n\big)_{k\bullet}\Big\|_2^2 = \sum_{i=0}^n K_n \cdot n\left(B^{T_\kappa}_{m,k}(x_i)\,\omega_i\right)^2 \le c_\omega \sum_{i=0}^n K_n B^{T_\kappa}_{m,k}(x_i)\,\omega_i$$
$$= c_\omega \Big\|(K_n\widehat{X}^T\Theta_n)_{k\bullet}\Big\|_\infty \le c_\omega c_{\kappa,2}(m+1), \qquad \forall\, k = 1, \ldots, N.$$

This shows that $\bar\sigma_k^2 \le c_\omega c_{\kappa,2}(m+1)$ for each $k = 1, \ldots, N$. Letting $\xi := (\xi_1, \ldots, \xi_N)^T \in \mathbb{R}^N$, we see that $\sigma\xi = \sqrt{nK_n}\widehat{X}^T\Theta_n\sigma\vec\varepsilon = \sqrt{nK_n}\widehat{X}^T\Theta_n(y - \vec f)$. Hence, we deduce, via the uniform Lipschitz property of Theorem 3.2.1, that there exist a positive constant c_∞ and $n_* \in \mathbb{N}$ (depending on $(K_n), m, c_\omega, c_{\kappa,1}, c_{\kappa,2}$ only) such that for any $f \in \mathcal{S}_{m,H}(r, L)$, $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \ge n_*$,

$$\Big\|\widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa}\Big\|_\infty \le \big\|\widehat{b}_{P,T_\kappa} - \bar b_{P,T_\kappa}\big\|_\infty \le c_\infty \cdot \sqrt{K_n/n} \cdot \Big\|\sqrt{nK_n}\widehat{X}^T\Theta_n\big(y - \vec f\big)\Big\|_\infty$$
$$= c_\infty \cdot \sqrt{K_n/n} \cdot \sigma \cdot \|\xi\|_\infty = \widetilde{c} \cdot \sqrt{K_n/n} \cdot \bar\xi, \tag{4.16}$$

where $\bar\xi := \|\xi\|_\infty = \max_{k=1,\ldots,N} |\xi_k|$ and $\widetilde{c} := c_\infty\sigma > 0$.

Define $\grave\sigma := \sqrt{c_\omega c_{\kappa,2}(m+1)}$, and consider the random variable $Z_\xi \sim \mathcal{N}(0, \grave\sigma^2)$. Since the variance of ξ_k satisfies $\bar\sigma_k^2 \le c_\omega c_{\kappa,2}(m+1) = \grave\sigma^2$ for each k, we have, for any $u \ge 0$,

$$\mathbb{P}\left(|Z_\xi| \ge \frac{u}{\widetilde{c}}\sqrt{\frac{n}{K_n}}\right) \ge \mathbb{P}\left(|\xi_k| \ge \frac{u}{\widetilde{c}}\sqrt{\frac{n}{K_n}}\right), \qquad \forall\, k = 1, \ldots, N.$$

Recall $\widehat{n}_1 := \max(\bar{n}_1, n_*)$ from the proof of Proposition 4.3.1. By (4.16), the above inequality, and the implication: $Y \sim \mathcal{N}(0, \sigma^2) \implies \mathbb{P}(|Y| \geq v) \leq \exp\left(-\frac{v^2}{2\sigma^2}\right)$ for any $v \geq 0$, we have that for any $u \geq 0$, $f \in \mathcal{S}_{m,H}(r, L)$, $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \geq \widehat{n}_1$,

$$\mathbb{P}\left(\|\widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa}\|_\infty \geq u\right) \leq \mathbb{P}\left(\bar{\xi} \geq \frac{u}{\widetilde{c}}\sqrt{\frac{n}{K_n}}\right) \leq N \cdot \mathbb{P}\left(|Z_\xi| \geq \frac{u}{\widetilde{c}}\sqrt{\frac{n}{K_n}}\right)$$
$$\leq N \cdot \exp\left(-\frac{u^2 n}{2\,\grave{\sigma}^2\,\widetilde{c}^2\,K_n}\right).$$

Let $W_n := \widetilde{c}\,\grave{\sigma}\sqrt{\frac{2K_n \log n}{q \cdot n}}$. It follows from the above result and

$$\int_v^\infty e^{-t^2/(2\sigma^2)} dt \leq e^{-v^2/(2\sigma^2)} \sigma\sqrt{\pi/2}$$

for any $v \geq 0$ that for any $f \in \mathcal{S}_{m,H}(r, L)$, $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \geq \widehat{n}_1$,

$$\mathbb{E}\left(\left\|\widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa}\right\|_\infty\right) = \int_0^\infty \mathbb{P}\left(\left\|\widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa}\right\|_\infty \geq t\right) dt$$
$$\leq W_n + \int_{W_n}^\infty \mathbb{P}\left(\left\|\widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa}\right\|_\infty \geq t\right) dt \leq W_n + N \cdot \int_{W_n}^\infty \exp\left(-\frac{n\,t^2}{2\,\widetilde{c}^2\,\grave{\sigma}^2 K_n}\right) dt$$
$$\leq W_n + N\widetilde{c}\,\grave{\sigma}\sqrt{\frac{\pi K_n}{2n}} \exp\left(-\frac{W_n^2 n}{2\widetilde{c}^2\grave{\sigma}^2 K_n}\right) = W_n + \widetilde{c}\,\grave{\sigma} \cdot \sqrt{\frac{\pi K_n}{2n}} \cdot (K_n + m - 1) \cdot n^{-\frac{1}{q}}.$$

Since $K_n/(n^{1/q} \cdot \sqrt{\log n}) \to 0$ as $n \to \infty$, there exist a constant $C_s > 0$ and $\widehat{n}_2 \in \mathbb{N}$ with $\widehat{n}_2 \geq \widehat{n}_1$ (depending on $(K_n), m, c_\omega, c_{\kappa,1}, c_{\kappa,2}$, and σ only) such that for any $f \in \mathcal{S}_{m,H}(r, L)$, $P \in \mathcal{P}_n$, K_n, and $T_\kappa \in \mathcal{T}_{K_n}$ with $n \geq \widehat{n}_2$,

$$\mathbb{E}\left(\left\|\widehat{f}^B_{P,T_\kappa} - \overline{f}_{P,T_\kappa}\right\|_\infty\right) \leq C_s \cdot \sqrt{\frac{K_n \log n}{n}}.$$

This leads to the desired uniform bound for the stochastic error. □

Combining Propositions 4.3.1 and 4.3.3, we obtain the following theorem.

Theorem 4.3.1. *Fix $m \in \mathbb{N}$, and constants $c_\omega \geq 1$, $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$, $L > 0$, $r \in (m-1, m]$, and let $q := \min\{2+\gamma, r\}$. Let (K_n) be a sequence of natural numbers with $K_n \to \infty$, $K_n/n \to 0$, $K_n/(n^{1/q} \cdot \sqrt{\log n}) \to 0$ as $n \to \infty$. Then there exist two positive constants C_b, C_s and $\widehat{n}_\star \in \mathbb{N}$ depending on $(K_n), m, r, L, c_\omega, c_{\kappa,1}, c_{\kappa,2}$, and σ only such that*

$$\sup_{f \in \mathcal{S}_{m,H}(r,L),\, P \in \mathcal{P}_n\, T_\kappa \in \mathcal{T}_{K_n}} \mathbb{E}\left(\left\| f - \widehat{f}^B_{P,T_\kappa} \right\|_\infty \right) \leq C_b \cdot (K_n)^{-q} + C_s \cdot \sqrt{\frac{K_n \log n}{n}}, \qquad \forall\, n \geq \widehat{n}_\star.$$

A specific choice of (K_n) that satisfies the conditions in Theorem 4.3.1 is $K_n = \left\lceil \left(\frac{n}{\log n}\right)^{1/(2q+1)} \right\rceil$. This result demonstrates the uniform convergence of the constrained B-spline estimator $\widehat{f}^B_{P,K_n}$ to the true function f on the entire interval $[0,1]$, and the consistency of this B-spline estimator, including the consistency at the two boundary points, even if design points are not equally spaced. Note that the monotone and convex least-squares estimators are inconsistent at the boundary points due to non-negligible asymptotic bias [27, 51, 81], which is known as the spiking problem.

Remark 4.3.1. In addition to the uniform convergence, Theorem 4.3.1 also gives an asymptotic convergence rate of the constrained B-spline estimator in the sup-norm, subject to general nonnegative derivative constraints. Moreover, the convergence rate is on the order of $\left(\frac{\log n}{n}\right)^{\frac{q}{2q+1}}$, where $q := \min\{2+\gamma, r\}$. We will see in Chapter V that this rate is optimal when $m = 1, 2$, or 3 (c.f. Corollary 5.5.1 and Remark 5.5.1).

We conclude this section with the following theorem, which follows from Propositions 4.3.2 and 4.3.3. Suppose we restrict the true function f to $\mathcal{S}_{m,H}(r, L', L) \subseteq \mathcal{S}_{m,H}(r, L)$ (c.f. (4.3)), for a fixed $L' > 0$. This last result gives us a faster rate of convergence over the subclass $\mathcal{S}_{m,H}(r, L', L)$ when $m > 3$. To this end, we take $K_n = \left\lceil \left(\frac{n}{\log n}\right)^{1/(2r+1)} \right\rceil$ to obtain a convergence rate on the order of $\left(\frac{\log n}{n}\right)^{r/(2r+1)}$.

Theorem 4.3.2. *Fix $m \in \mathbb{N}$, and constants $c_\omega \geq 1$, $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$, $L \geq L' > 0$, and $r \in (m-1, m]$. Let (K_n) be a sequence of natural numbers with $K_n \to \infty$, $K_n/n \to 0$, $K_n/(n^{1/q} \cdot \sqrt{\log n}) \to 0$ as $n \to \infty$. Then there exist two positive constants C_b', C_s and $\widehat{n}_\star \in \mathbb{N}$ depending on $(K_n), m, r, L, L', c_\omega, c_{\kappa,1}, c_{\kappa,2}$, and σ only such that*

$$\sup_{f \in \mathcal{S}_{m,H}(r,L',L),\, P \in \mathcal{P}_n\, T_\kappa \in \mathcal{T}_{K_n}} \mathbb{E}\left(\left\| f - \widehat{f}^B_{P,T_\kappa} \right\|_\infty \right) \leq C_b \cdot \big(K_n\big)^{-r} + C_s \cdot \sqrt{\frac{K_n \log n}{n}}, \qquad \forall\, n \geq \widehat{n}_\star.$$

4.4 Summary

In this chapter, we obtained several results on the accuracy and limitations of approximating smooth nonnegative derivative constrained functions by splines with the same nonnegative derivative constraint. These results were then used in conjunction with the uniform Lipschitz property of Chapter III to provide asymptotic upper bounds on the bias and stochastic error of the nonnegative derivative constrained B-spline estimator.

CHAPTER V

Nonnegative Derivative Constrained Estimation: Minimax Lower Bound in the Supremum Norm

In the previous chapter, we applied the uniform Lipschitz property of Chapter III to establish asymptotic upper bounds on the bias and stochastic error of a constrained B-spline estimator with respect to the supremum-norm. In this chapter, we will develop minimax asymptotic lower bounds on certain nonparametric estimation problems with nonnegative derivative constraints. It follows from results in Chapters III-V that under suitable conditions on either the order of the derivative constraint or the function class under consideration, the constrained B-spline estimator proposed in Chapter III achieves the optimal asymptotic performance under the supremum-norm.

5.1 Introduction

With various applications in science and engineering, there has been a substantial interest in the nonparametric estimation of functions subject to nonnegative derivative constraints such as monotonicity or convexity [22, 52, 73, 70, 79]. However, the nonsmooth inequality constraints of such problems complicate the asymptotic performance analysis of constraint preserving estimators. In particular, the minimax performance analysis of constrained estimators becomes even more difficult when the supremum-norm is used as the performance metric. In this chapter, we establish minimax lower bounds for a large variety of nonparametric estimation problems over suitable Hölder or Sobolev function classes subject to nonnegative derivative constraints, with respect to the supremum-norm. This is done by constructing an appropriate collection of functions (called hypotheses [77, Section 2]) that satisfy the pre-specified nonnegative derivative constraint. We then combine these results with those from Chapters III-IV to demonstrate, in certain cases, the optimal performance of the previously introduced constrained B-spline estimator.

This chapter is organized as follows. In Section 5.2, descriptions of the minimax lower bounds for general constrained nonparametric estimation problems are given; the main result of this chapter, Theorem 5.2.1, is stated, and the required conditions on the hypothesis functions are presented. The hypothesis functions are then constructed in Section 5.3. In Section 5.4 it is demonstrated that these hypotheses meet the required conditions of Section 5.2, thus proving Theorem 5.2.1. Several important corollaries to this theorem that tie in results from earlier chapters are presented in Section 5.5. Finally, a summary is given in Section 5.6.

Notation: Given a function $g : [a, b] \to \mathbb{R}$, denote its supremum-norm (or simply sup-norm) by $\|g\|_\infty := \sup_{x\in[a,b]} |g(x)|$, and its L_2-norm by $\|g\|_{L_2} := \left(\int_a^b (g(x))^2 \, dx\right)^{1/2}$. Let $\mathbb{E}$ denote the expectation operator and let $f^{(\ell)}$ denote the ℓth derivative of the function

f. Additionally, denote the pth integral of g from a to b by

$$\mathcal{I}_{[a,b]}^{(p)}(g) := \begin{cases} \int_a^b g(t_1)\ dt_1 & \text{if } p = 1 \\ \int_a^b \int_a^{t_p} \dots \int_a^{t_2} g(t_1)\ dt_1 \dots\ dt_{p-1}\ dt_p & \text{otherwise.} \end{cases}$$

Finally, for two sequences of positive numbers (a_n) and (b_n), we write that $a_n \asymp b_n$ if there exist positive constants c_1, c_2, such that $c_1 \leq \liminf_{n\to\infty} a_n/b_n \leq \limsup_{n\to\infty} a_n/b_n \leq c_2$.

5.2 Problem Formulation

Fix $m \in \mathbb{N}$, $r \in (m-1, m]$ and $L > 0$. Let $\gamma := r - m + 1$. Recall the family $\mathcal{S}_m$ of univariate functions on $[0,1]$ subject to a general nonnegative derivative constraint, from (3.1) in Chapter III, the Hölder class of functions H_L^r defined in (4.1) in Chapter IV, and $\mathcal{S}_{m,H}(r, L) := \mathcal{S}_m \cap H_L^r$.

Consider the regression problem

$$y_i = f(x_i) + \sigma\epsilon_i, \tag{5.1}$$

where the x_i's are evenly spaced design points on the unit interval, i.e., $x_i = i/n$ for all $i = 0, 1, \dots, n$, n denotes the sample size, $f : [0,1] \to \mathbb{R}$ is an unknown function in $\mathcal{S}_{m,H}(r, L)$, and the ϵ_i's are iid standard normal errors. Our goal is to establish a lower bound under the sup-norm on the minimax risk associated with the collection of estimators that preserve the nonnegative derivative constraint of $f \in \mathcal{S}_{m,H}(r, L)$, for this nonparametric model. Specifically, the main result of this chapter is presented in the following theorem.

Theorem 5.2.1. *Fix $m \in \mathbb{N}$, and $r \in (m-1, m]$ and consider the regression problem given by (5.1). There exists a positive constant c such that*

$$\liminf_{n\to\infty} \inf_{\widehat{f}_n} \sup_{f\in\mathcal{S}_{m,H}(r,L)} \left(\frac{n}{\log n}\right)^{\frac{r}{2r+1}} \mathbb{E}\big(\|\widehat{f}_n - f\|_\infty\big) \ \geq\ c, \tag{5.2}$$

where $\inf_{\widehat{f}_n}$ *denotes the infimum over all constrained estimators* $\widehat{f}_n \in \mathcal{S}_m$ *on* $[0,1]$.

It follows from Theorem 5.2.1 that for $m = 1, 2$, or 3 the constrained B-spline estimator $\widehat{f}^B_{P,T_\kappa}$ proposed in Chapter III (c.f. (3.7)-(3.8)) satisfies

$$\begin{aligned} c\left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}} &\leq \inf_{\widehat{f}_n} \sup_{f\in\mathcal{S}_{m,H}(r,L)} \mathbb{E}\big(\|\widehat{f}_n - f\|_\infty\big) \\ &\leq \sup_{f\in\mathcal{S}_{m,H}(r,L)} \mathbb{E}\big(\|\widehat{f}^B_{P,T_\kappa} - f\|_\infty\big) \leq C\Big(\frac{\log n}{n}\Big)^{\frac{r}{2r+1}}, \end{aligned} \tag{5.3}$$

for all n sufficiently large, via Theorem 4.3.1 and Remark 4.3.1 of Chapter IV. Consequently,

$$\inf_{\widehat{f}_n} \sup_{f\in\mathcal{S}_{m,H}(r,L)} \mathbb{E}\big(\|\widehat{f}_n - f\|_\infty\big) \asymp \left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}} \asymp \sup_{f\in\mathcal{S}_{m,H}(r,L)} \mathbb{E}\big(\|\widehat{f}^B_{P,T_\kappa} - f\|_\infty\big), \tag{5.4}$$

proving that $\widehat{f}^B_{P,T_\kappa}$ is an (asymptotically) optimally performing estimator over the constrained function class $\mathcal{S}_{m,H}(r,L)$, for such m.

Our strategy to substantiate Theorem 5.2.1, motivated by [77, Theorem 2.10], amounts to constructing a class of hypothesis functions that lie in the function class $\mathcal{S}_{m,H}(r,L)$. These functions will maintain a suitable distance from each other in the sup-norm, while staying sufficiently close to each other under the L_2-norm. Moreover, this family of M_n hypotheses $f_{j,n}, j = 0, 1, \ldots, M_n$ must satisfy the following three conditions:

(C1) each $f_{j,n} \in \mathcal{S}_{m,H}(r,L)$, $j = 0, 1, \ldots, M_n$;

(C2) whenever $j \neq k$, $\|f_{j,n} - f_{k,n}\|_\infty \geq 2s_n > 0$, where $s_n \asymp (\log n/n)^{r/(2r+1)}$;

(C3) there must exist a fixed constant $c_0 \in (0, 1/8)$ such that for all n sufficiently large,

$$\frac{1}{M_n}\sum_{j=1}^{M_n} K(P_j, P_0) \;\leq\; c_0 \log(M_n),$$

where P_j denotes the distribution of $(Y_{j,1}, \ldots, Y_{j,n})$, $Y_{j,i} = f_{j,n}(X_i) + \xi_i$, $i = 1, \ldots, n$, $X_i = i/n$, the ξ_i's are iid random variables, and $K(P, Q)$ denotes the Kullback divergence between the two probability measures P and Q [41], i.e.,

$$K(P, Q) := \begin{cases} \displaystyle\int \log \frac{dP}{dQ}\, dP, & \text{if } P \ll Q \\ +\infty, & \text{otherwise.} \end{cases}$$

We will specify M_n in the later development. In addition, we assume that there exists a constant $p_* > 0$ (independent of n and $f_{j,n}$) such that $K(P_j, P_0) \leq p_* \sum_{i=1}^n \big(f_{j,n}(X_i) - f_{0,n}(X_i)\big)^2$. This assumption holds true if the iid random variables $\xi_i \sim N(0, \sigma^2)$ (cf. [77, (2.36)] or [77, Section 2.5, Assumption B]). Hence, the constrained regression problem defined in (5.1) satisfies this assumption.

In other words, once a family of functions $\{f_{j,n}\}$ satisfying the above three conditions is constructed, then the minimax lower bound over $\mathcal{S}_{m,H}(r, L)$ given by Theorem 5.2.1 will hold, for some constant $c > 0$ depending on m, r, L, and p_* only. In view of this, the goal of this chapter is to construct a family of suitable functions $f_{j,n}$ satisfying (C1)-(C3).

5.3 Construction of Hypothesis Functions

Let (K_n) be the increasing sequence of positive integers given by

$$K_n := \left\lceil \left(\frac{n}{\log n} \right)^{\frac{1}{2r+1}} \right\rceil, \tag{5.5}$$

and fix n large. For that fixed n, define $\kappa_i := \frac{i}{K_n}$ for each $i = 0, 1, \ldots, K_n$. In this section, we construct the functions $f_{j,n}, j = 0, 1, \ldots, M_n$ that satisfy conditions (C1)-(C3) of the previous section. To this end, we begin by constructing increasing functions $h^{[1]}_{p,n}$, $h^{[2]}_{p,n}$: $[0, \kappa_{2^p}] \to \mathbb{R}$ inductively for $p = 1, 2, \ldots, m$. Our procedure for constructing the $f_{j,n}$'s involves (i) using $h^{[1]}_{m,n}$ and $h^{[2]}_{m,n}$ to construct the $g_{j,n}$'s (cf. (5.14)-(5.15) and (5.16)-(5.17)) and (ii) integrating the $g_{j,n}$'s a total of $(m-1)$ times to produce the $f_{j,n}$'s (c.f. (5.18)). We choose $h^{[1]}_{m,n}$ and $h^{[2]}_{m,n}$ for this procedure for the following reasons.

(i) In order to meet (C1), each $g_{j,n} = f^{(m-1)}_{j,n}$ must be increasing. Both $h^{[1]}_{m,n}$ and $h^{[2]}_{m,n}$ (used in the construction of each $g_{j,n}$) meet this requirement.

(ii) In view of (C2), the distance (measured with respect to the sup-norm) between $f_{j,n}$ and $f_{k,n}$ for $j \neq k$ must be non-small. The $f_{j,n}$'s are constructed such that $f_{j,n}(x) = f_{k,n}(x)$ when $j \neq k$ for all x outside of two small subintervals of $[0, 1]$. On these subintervals, $f_{j,n} - f_{k,n}$ will be equal to the $(m-1)$th integral of either $h^{[2]}_{m,n} - h^{[1]}_{m,n}$ or $h^{[1]}_{m,n} - h^{[2]}_{m,n}$ (c.f. Lemma 5.3.3). This integral is on the order of K_n^{m-1} times smaller than $h^{[2]}_{m,n} - h^{[1]}_{m,n}$ in the sup-norm. Although this integral is relatively small, it will still be large enough for the $f_{j,n}$'s to meet (C2).

(iii) The $(m-1)$th integral of $h^{[2]}_{m,n} - h^{[1]}_{m,n}$, is on the order of K_n^{m-1} times smaller than $h^{[2]}_{m,n} - h^{[1]}_{m,n}$ in the sup-norm, and even smaller in the L_2-norm. Since the $f_{j,n}$'s are constructed such that $|f_{j,n} - f_{k,n}|$ is equal to $|\mathcal{I}^{(m-1)}_{[0,\cdot]}(h^{[2]}_{m,n} - h^{[1]}_{m,n})|$ (where $\mathcal{I}^{(m-1)}$ is defined in Section 5.1) on two small subintervals of $[0,1]$ and zero elsewhere for $j \neq k$ (c.f. Lemma 5.3.3), the L_2-norm of $f_{j,n} - f_{k,n}$ will be sufficiently small and allow the $f_{j,n}$'s to meet (C3).

With these ideas in mind, we proceed to construct the auxiliary functions $h^{[1]}_{p,n}$ and $h^{[2]}_{p,n}$, for $p = 1, \ldots, m$ and establish two technical lemmas in Section 5.3.1. In Section 5.3.2, we use the constructions and results from Section 5.3.1 to (i) construct the $g_{j,n}$'s, (ii) construct the hypotheses $f_{j,n},\ j = 0, 1, \ldots, M_n$ by integrating each $g_{j,n}$ a total of $(m-1)$ times, and (iii) establish Lemma 5.3.3, which will pave the way for the proof of Theorem 5.2.1.

5.3.1 Construction of Auxiliary Functions

We will now construct the auxiliary functions $h^{[1]}_{p,n}$ and $h^{[2]}_{p,n}$ to be used in the subsequent constructions. Let $c_0 \in (0, \frac{1}{8})$, and p_* be the positive constant indicated at the end of condition (C3) in the previous section. Choose

$$\overline{L} = \min\left\{ \frac{L}{2^{\,m}}, \frac{m!}{2^{m^m}} \sqrt{\frac{\gamma\ c_0}{2^{m+3} p_* (2r+1)}} \right\}. \tag{5.6}$$

Define the following functions $h^{[1]}_{p,n}, h^{[2]}_{p,n} : [0, \kappa_{2^p}] \to \mathbb{R}$ recursively for $p = 1, 2, \ldots, m$ as follows. First let

$$h^{[1]}_{1,n}(x) = \begin{cases} 0 & \text{if } x \in [0, \kappa_1] \\ \overline{L} K_n^{1-\gamma} (x - \kappa_1) & \text{if } x \in (\kappa_1, \kappa_2] \end{cases} \tag{5.7}$$

and

$$h^{[2]}_{1,n}(x) = \begin{cases} \overline{L} K_n^{1-\gamma} x & \text{if } x \in [0, \kappa_1] \\ \overline{L} K_n^{-\gamma} & \text{if } x \in (\kappa_1, \kappa_2]. \end{cases} \tag{5.8}$$

Then for $p = 2, \dots, m$, define

$$h_{p,n}^{[1]}(x) = \begin{cases} h_{p-1,n}^{[1]}(x) & \text{if } x \in [0, \kappa_{2^{p-1}}] \\ h_{p-1,n}^{[2]}(x - \kappa_{2^{p-1}}) + h_{p-1,n}^{[1]}(\kappa_{2^{p-1}}) & \text{if } x \in (\kappa_{2^{p-1}}, \kappa_{2^p}] \end{cases} \tag{5.9}$$

and

$$h_{p,n}^{[2]}(x) = \begin{cases} h_{p-1,n}^{[2]}(x) & \text{if } x \in [0, \kappa_{2^{p-1}}] \\ h_{p-1,n}^{[1]}(x - \kappa_{2^{p-1}}) + h_{p-1,n}^{[2]}(\kappa_{2^{p-1}}) & \text{if } x \in (\kappa_{2^{p-1}}, \kappa_{2^p}] \end{cases} . \tag{5.10}$$

Figure 5.1 contains plots of these functions for $p = 1, 2, 3, 4$. Note that both $h_{1,n}^{[1]}$ and $h_{1,n}^{[2]}$ are continuous. By induction, so are $h_{p,n}^{[1]}$ and $h_{p,n}^{[2]}$ for $p = 2, \dots, m$. Additionally, for $1 < p \leq m$, the first "half" of $h_{p,n}^{[1]}$ (i.e., the part defined on $[0, \kappa_{2^{p-1}}]$) is identical to $h_{p-1,n}^{[1]}$, and the second "half" of $h_{p,n}^{[1]}$ (i.e., the part defined on $(\kappa_{2^{p-1}}, \kappa_{2^p}]$), when shifted appropriately, is identical to $h_{p-1,n}^{[2]}$. An analogous relationship holds for $h_{p,n}^{[2]}$, $h_{p-1,n}^{[2]}$ on $[0, \kappa_{2^{p-1}}]$, and $h_{p-1,n}^{[1]}$ on $(\kappa_{2^{p-1}}, \kappa_{2^p}]$.

For each $p = 1, \dots, m$, define $\varphi_p : [0, \kappa_{2^m}] \to \mathbb{R}$ such that for all $x \in [0, \kappa_{2^m}]$,

$$\varphi_1(x) := (h_{m,n}^{[2]} - h_{m,n}^{[1]})(x) \text{ and } \varphi_p(x) := \mathcal{I}_{[0,x]}^{(p-1)}(\varphi_1),\ p = 2, \dots, m. \tag{5.11}$$

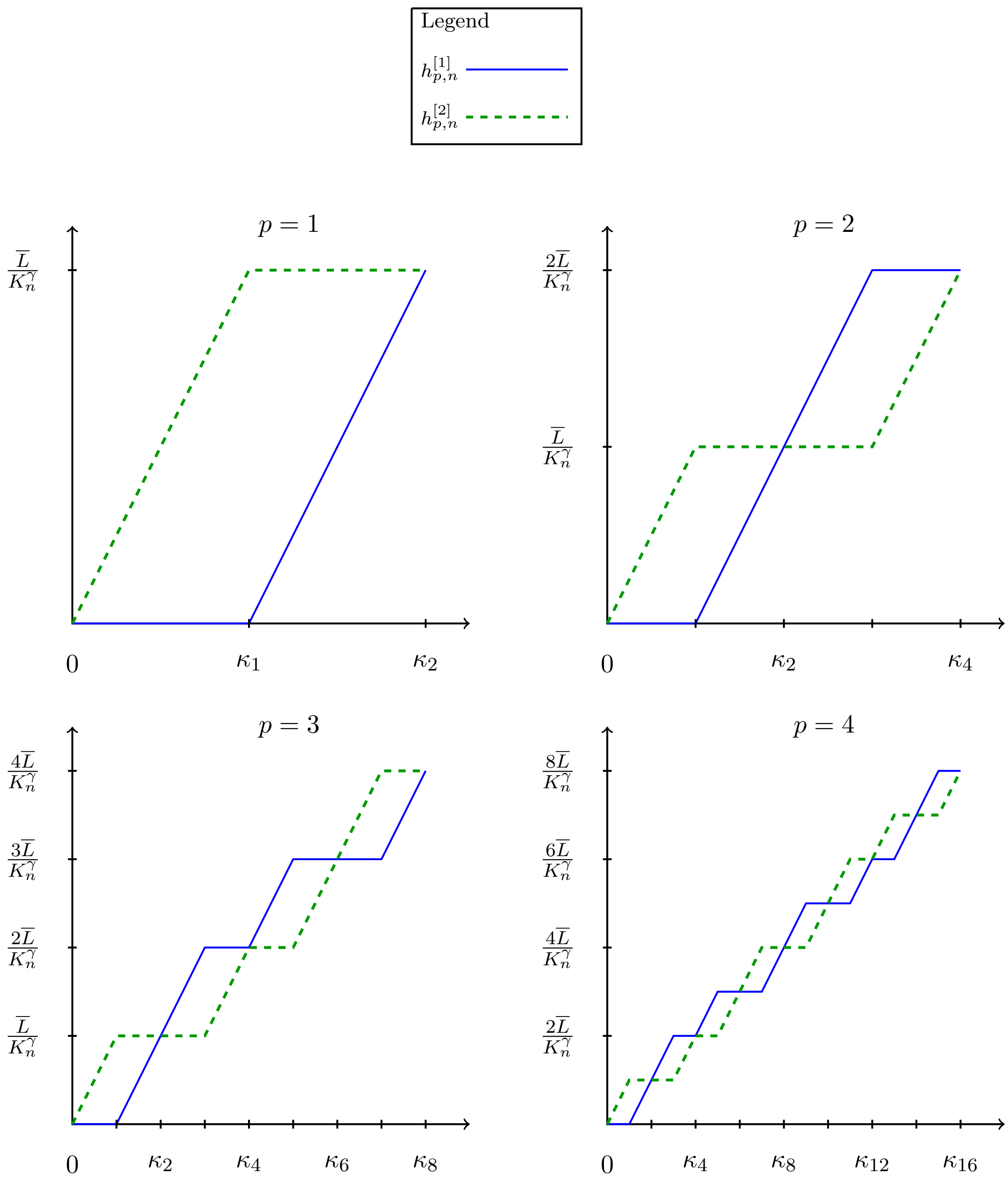
Note that on $[0, \kappa_{2^p}]$,

$$\varphi_1(x) = (h_{m,n}^{[2]} - h_{m,n}^{[1]})(x) = (h_{m-1,n}^{[2]} - h_{m-1,n}^{[1]})(x) = \cdots = (h_{p,n}^{[2]} - h_{p,n}^{[1]})(x). \tag{5.12}$$

Also, on $[0, \kappa_{2^m}]$, the ℓth derivative

$$\varphi_p^{(\ell)}(x) = \varphi_{p-\ell}(x), \text{ for all } \ell = 1, \dots, p-1. \tag{5.13}$$

Figure 5.1: Plot of $h_{p,n}^{[1]}$ and $h_{p,n}^{[2]}$ for $p = 1, 2, 3, 4$.



The following two lemmas will be useful in Section 5.3.2.

Lemma 5.3.1. *For each $p = 1, \ldots, m$, $\varphi_p^{(\ell)}(\kappa_{2^p}) = 0$ for $\ell = 0, 1, \ldots, p-1$. Note that for $p = m$, we define $\varphi_m^{(\ell)}(\kappa_{2^m})$ as the ℓth right derivative of φ_m at κ_{2^m}.*

Proof. We prove this result by induction on p. For $p = 1$, by virtue of (5.12),

$$\varphi_1(\kappa_2) = (h_{1,n}^{[2]} - h_{1,n}^{[1]})(\kappa_2) = \overline{L}K_n^{-\gamma} - \overline{L}K_n^{-\gamma} = 0.$$

Hence, the result holds for $p = 1$. Fix $p \in \mathbb{N}$ with $1 < p \leq m$ and assume that the result holds for $(p-1)$. In what follows, we show that the result then holds for p.

Consider $\ell = 0$ first. Since φ_p is $(p-1)$ times differentiable, by Taylor expansion

$$\varphi_p(\kappa_{2^p}) = \sum_{q=0}^{p-2} \frac{\varphi_p^{(q)}(\kappa_{2^{p-1}}) \left(\frac{2^{p-1}}{K_n}\right)^q}{q!} + \mathcal{I}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}^{(p-1)}(\varphi_p^{(p-1)}).$$

By (5.13) and the induction hypothesis, we have $\varphi_p^{(q)}(\kappa_{2^{p-1}}) = \varphi_{p-q}(\kappa_{2^{p-1}}) = \varphi_{p-1}^{(q-1)}(\kappa_{2^{p-1}})$ $= 0$ for $q = 1, \ldots, p-2$. Hence, by the above display,

$$\begin{aligned}
\varphi_p(\kappa_{2^p}) &= \varphi_p(\kappa_{2^{p-1}}) + \mathcal{I}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}^{(p-1)}(\varphi_p^{(p-1)}) = \varphi_p(\kappa_{2^{p-1}}) + \mathcal{I}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}^{(p-1)}(h_{m,n}^{[2]} - h_{m,n}^{[1]}) \\
&= \varphi_p(\kappa_{2^{p-1}}) + \mathcal{I}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}^{(p-1)}\Big((h_{p-1,n}^{[1]} - h_{p-1,n}^{[2]})(\,\cdot\, - \kappa_{2^{p-1}}) + \varphi_1(\kappa_{2^{p-1}})\Big) \\
&= \varphi_p(\kappa_{2^{p-1}}) + \mathcal{I}_{[0, \kappa_{2^{p-1}}]}^{(p-1)}(h_{p-1,n}^{[1]} - h_{p-1,n}^{[2]}) = \varphi_p(\kappa_{2^{p-1}}) - \varphi_p(\kappa_{2^{p-1}}) = 0,
\end{aligned}$$

where we use (5.7)-(5.13), and $\varphi_1(\kappa_{2^{p-1}}) = \varphi_{p-1}^{(p-2)}(\kappa_{2^{p-1}}) = 0$ via (5.13) and the induction hypothesis.

Next consider $\ell = 1, \dots, p-2$. We have that

$$\varphi_p^{(\ell)}(\kappa_{2^p}) = \sum_{q=0}^{p-\ell-2} \frac{\varphi_p^{(\ell+q)}(\kappa_{2^{p-1}}) \left(\frac{2^{p-1}}{K_n}\right)^q}{q!} + \mathcal{I}^{(p-\ell-1)}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}(\varphi_p^{(p-1)}).$$

In view of $\varphi_p^{(\ell+q)}(\kappa_{2^{p-1}}) = \varphi_{p-\ell-q}(\kappa_{2^{p-1}}) = 0$ for all $q = 0, 1, \dots, p-\ell-2$ via (5.13) and the induction hypothesis, we have by the above display, and (5.7)-(5.13),

$$\begin{aligned}
\varphi_p^{(\ell)}(\kappa_{2^p}) &= \mathcal{I}^{(p-\ell-1)}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}(\varphi_1) = \mathcal{I}^{(p-\ell-1)}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}(h^{[2]}_{p,n} - h^{[1]}_{p,n}) \\
&= \mathcal{I}^{(p-\ell-1)}_{[\kappa_{2^{p-1}}, \kappa_{2^p}]}\left[(h^{[1]}_{p-1,n} - h^{[2]}_{p-1,n})(\,\cdot\, - \kappa_{2^{p-1}}) + \varphi_1(\kappa_{2^{p-1}})\right] \\
&= -\mathcal{I}^{(p-\ell-1)}_{[0, \kappa_{2^{p-1}}]}(\varphi_1) = -\varphi_{p-\ell}(\kappa_{2^{p-1}}) = 0.
\end{aligned}$$

Finally, if $\ell = p-1$, then by (5.7)-(5.13),

$$\begin{aligned}
&\varphi_p^{(p-1)}(\kappa_{2^p}) = \varphi_1(\kappa_{2^p}) = h^{[2]}_{p,n}(\kappa_{2^p}) - h^{[1]}_{p,n}(\kappa_{2^p}) \\
&= \left(h^{[1]}_{p-1,n}(\kappa_{2^{p-1}}) + h^{[2]}_{p-1,n}(\kappa_{2^{p-1}})\right) - \left(h^{[2]}_{p-1,n}(\kappa_{2^{p-1}}) + h^{[1]}_{p-1,n}(\kappa_{2^{p-1}})\right) = 0.
\end{aligned}$$

Hence the result holds by induction. □

Lemma 5.3.2. *Let* $r \in (m-1, m]$ *and* $\gamma = r - (m-1)$*. For* $\varphi_m : [0, \kappa_{2^m}] \to \mathbb{R}$,

$$\frac{\overline{L}}{m!} K_n^{-r} \le \|\varphi_m\|_\infty \le \frac{\overline{L}\ 2^{m^m}}{m!} K_n^{-r}.$$

Proof. Suppose that $m = 1$. Then it is easy to see via Figure 5.1 that

$$\|\varphi_1\|_\infty = \|h^{[2]}_{1,n} - h^{[1]}_{1,n}\|_\infty = \overline{L} K_n^{-\gamma},$$

so the result holds for $m = 1$.

Therefore, consider $m > 1$. Let dT_{m-1} denote $dt_1 \dots dt_{m-2}\, dt_{m-1}$. On $[0, \kappa_1]$, we have that $\varphi_1(x) = h^{[2]}_{1,n}(x) - h^{[1]}_{1,n}(x) = \overline{L} K_n^{1-\gamma} x$. Hence, if $m = 2$,

$$\|\varphi_2\|_\infty \geq \varphi_2\left(\kappa_1\right) = \mathcal{I}^{(1)}_{[0,\kappa_1]}(\varphi_1) = \int_0^{\kappa_1} \overline{L} K_n^{1-\gamma} t_1\, dt_1 = \frac{\overline{L}}{2!} K_n^{-r},$$

and if $m > 2$,

$$\|\varphi_m\|_\infty \geq \varphi_m\left(\kappa_1\right) = \mathcal{I}^{(m-1)}_{[0,\kappa_1]}(\varphi_1) = \int_0^{\kappa_1} \int_0^{t_{m-1}} \dots \int_0^{t_2} \overline{L} K_n^{1-\gamma} t_1\, dT_{m-1} = \frac{\overline{L}}{m!} K_n^{-r}.$$

We claim that $|\varphi_1(x)| \leq \overline{L} K_n^{-\gamma}$ for all $x \in [0, \kappa_{2^p}]$ for $p = 1, \dots, m$, and prove this claim by induction on p. Certainly this claim holds for $p = 1$, via (5.7)-(5.8) and (5.11). If $1 < p \leq m$, and the result holds for $(p-1)$, we need only show that $|\varphi_1(x)| \leq \overline{L} K_n^{-\gamma}$ on $(\kappa_{2^{p-1}}, \kappa_{2^p}]$. If $x \in (\kappa_{2^{p-1}}, \kappa_{2^p}]$, then by (5.9)-(5.12) and Lemma 5.3.1,

$$\begin{aligned} |\varphi_1(x)| &= |(h^{[2]}_{p,n} - h^{[1]}_{p,n})(x)| = |(h^{[1]}_{p-1,n} - h^{[2]}_{p-1,n})(x - \kappa_{2^{p-1}}) + \varphi_1(\kappa_{2^{p-1}})| \\ &= |(h^{[1]}_{p-1,n} - h^{[2]}_{p-1,n})(x - \kappa_{2^{p-1}})| \leq \overline{L} K_n^{-\gamma}, \end{aligned}$$

since $(x - \kappa_{2^{p-1}}) \in [0, \kappa_{2^{p-1}}]$.

Now by the established claim, we complete the proof by observing that

$$\|\varphi_m\|_\infty \leq \mathcal{I}^{(m-1)}_{[0,\kappa_{2^m}]}(\|\varphi_1\|_\infty) \leq \mathcal{I}^{(m-1)}_{[0,\kappa_{2^m}]}(\overline{L} K_n^{-\gamma}) = \frac{\overline{L}\; 2^{m^{m-1}}}{(m-1)!} K_n^{-r} \leq \frac{\overline{L}\; 2^{m^m}}{m!} K_n^{-r}.$$

□

Now that we have established the previous two preliminary results, we are ready to construct the hypothesis functions using $h^{[1]}_{m,n}$ and $h^{[2]}_{m,n}$ in the next section.

5.3.2 Construction of the Hypotheses

In what follows, we construct the $(m-1)$th derivatives of the $f_{j,n}$'s, namely the $g_{j,n}$'s, $j = 0, 1, \ldots, M_n$. We then integrate the $g_{j,n}$'s to create the $f_{j,n}$'s. Later in Section 5.4, we will demonstrate that the $f_{j,n}$'s meet conditions (C1)-(C3) of Section 5.2.

To this end, we consider two different cases in constructing the $g_{j,n}$'s.

Case 1: $r \in (m-1, m)$, so that $\gamma = r - m + 1 \in (0, 1)$. In this case, let $M_n := \lfloor K_n^{\gamma} \rfloor - 1 \in \mathbb{N}$ and define $g_{0,n} : [0,1] \to \mathbb{R}$ such that

$$g_{0,n}(x) := \begin{cases} i\ 2^{m-1}\overline{L}K_n^{-\gamma} + h^{[\mathbf{1}]}_{m,n}(x - iK_n^{-\gamma}) & \text{if } x \in [iK_n^{-\gamma}, iK_n^{-\gamma} + \kappa_{2^m}) \\ (i+1)2^{m-1}\overline{L}K_n^{-\gamma} & \text{if } x \in [iK_n^{-\gamma} + \kappa_{2^m}, (i+1)K_n^{-\gamma}) \end{cases} \tag{5.14}$$

for all appropriate $i \in \mathbb{Z}_+$, where $h^{[1]}_{m,n}$ is defined in (5.9). Note that we assume that n is large enough so that $\kappa_{2^m} < K_n^{-\gamma}$, and hence, $g_{0,n}$ is well defined. Define the intervals

$$I_j := [(j-1)K_n^{-\gamma}, (j-1)K_n^{-\gamma} + \kappa_{2^m}) \subseteq [0,1]$$

for each $j = 1, \ldots, M_n$. For each such j, we define $g_{j,n} : [0,1] \to \mathbb{R}$ such that

$$g_{j,n}(x) := \begin{cases} (j-1)2^{m-1}\overline{L}K_n^{-\gamma} + h^{[\mathbf{2}]}_{m,n}(x - (j-1)K_n^{-\gamma}) & \text{if } x \in I_j \\ g_{0,n}(x) & \text{otherwise,} \end{cases} \tag{5.15}$$

where $h^{[2]}_{m,n}$ is defined in (5.10). Hence, $g_{j,n}(x) = g_{0,n}(x)$ for all $x \in [0,1] \setminus I_j$. For $x \in I_j$,

$$g_{j,n}(x) - g_{0,n}(x) = h^{[2]}_{m,n}(x - (j-1)K_n^{-\gamma}) - h^{[1]}_{m,n}(x - (j-1)K_n^{-\gamma}) = \varphi_1(x - (j-1)K_n^{-\gamma}).$$

Furthermore, $g_{0,n}$ is continuous, since (i) $h^{[1]}_{m,n}$ is continuous on $[0, \kappa_{2^m}]$, and (ii) it can be shown by induction that $h^{[1]}_{m,n}(\kappa_{2^m}) = 2^{m-1}\overline{L}K_n^{-\gamma}$; thus for each i,

$$i\ 2^{m-1}\overline{L}K_n^{-\gamma} + h^{[1]}_{m,n}(iK_n^{-\gamma} + \kappa_{2^m} - iK_n^{-\gamma}) = (i+1)2^{m-1}\overline{L}K_n^{-\gamma}.$$

A similar argument shows that $g_{j,n}$ is continuous, for $j = 1, \ldots, M_n$.

In Figure 5.2 a plot of several of the $g_{j,n}$'s near the origin is given for $m = 1, 2, 3$.

Case 2: $r = m$, so that $\gamma = 1$. In this case, let $M_n := \lfloor \frac{K_n}{2^m} \rfloor - 1 \in \mathbb{N}$ and define $g_{0,n} : [0,1] \to \mathbb{R}$ such that

$$g_{0,n}(x) := i\ 2^{m-1}\overline{L}K_n^{-1} + h^{[\mathbf{1}]}_{j,n}(x - i\ 2^m K_n^{-1}) \text{ if } x \in [i\ 2^m K_n^{-1}, (i+1)2^m K_n^{-1}) \tag{5.16}$$

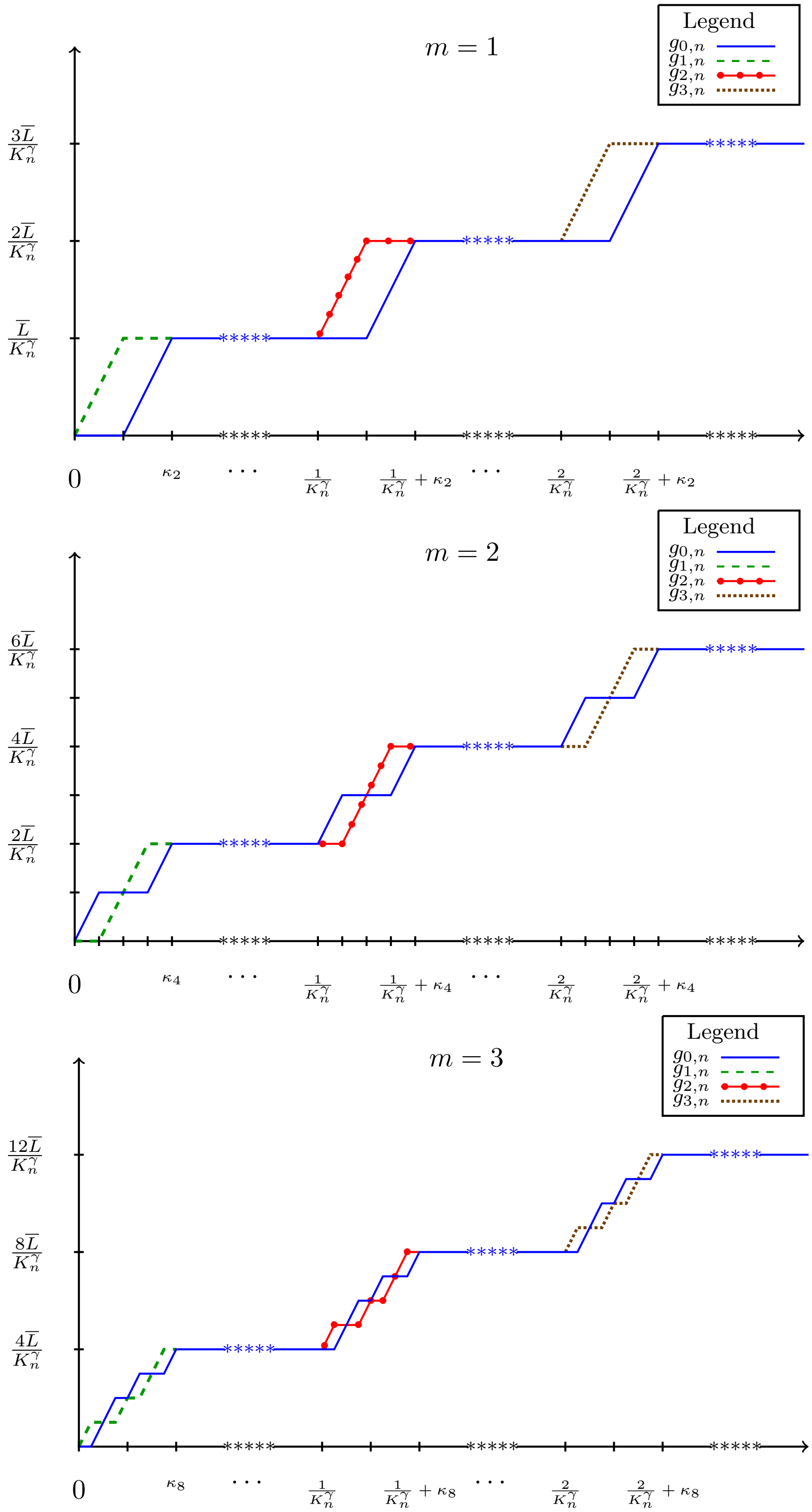
for all appropriate $i \in \mathbb{Z}_+$, where $h^{[1]}_{m,n}$ is defined in (5.9). Also, define the intervals

$$I_j := [(j-1)2^m K_n^{-1}, j\ 2^m K_n^{-1}) \subseteq [0,1]$$

for each $j = 1, \ldots, M_n$ and let $g_{j,n} : [0,1] \to \mathbb{R}$ be such that

$$g_{j,n}(x) := \begin{cases} (j-1)2^{m-1}\overline{L}K_n^{-1} + h^{[\mathbf{2}]}_{m,n}(x - (j-1)2^m K_n^{-1}) & \text{if } x \in I_j \\ g_{0,n}(x) & \text{otherwise,} \end{cases} \tag{5.17}$$

Figure 5.2: Plot of the $g_{j,n}$'s near the origin, $\gamma \in (0, 1)$



where $h^{[2]}_{m,n}$ is defined in (5.10). In this case, we again have that, $g_{j,n}(x) = g_{0,n}(x)$ for all $x \in [0,1] \setminus I_j$ and for all $x \in I_j$,

$$g_{j,n}(x) - g_{0,n}(x) = (h^{[2]}_{m,n} - h^{[1]}_{m,n})(x - (j-1)2^m K_n^{-1}) = \varphi_1(x - (j-1)2^m K_n^{-1}).$$

In Figure 5.3 a plot of several of the $g_{j,n}$'s near the origin is given for $m = 1, 2, 3$. By an argument similar to Case 1, each $g_{j,n}$, $j = 0, 1, \ldots, M_n$, is continuous on $[0,1]$.

Finally, in either case, define the jth hypothesis function $f_{j,n} : [0,1] \to \mathbb{R}$ such that

$$f_{j,n}(x) := \mathcal{I}^{(m-1)}_{[0,x]}(g_{j,n}), \ \forall\, x \in [0,1]. \tag{5.18}$$

Now that we have constructed the hypothesis functions, we will establish one more lemma, before demonstrating that the hypotheses satisfy conditions (C1)-(C3) in Section 5.4.

Lemma 5.3.3. *If $\gamma \in (0,1)$, then for each $j = 1, \ldots, M_n$, we have that*

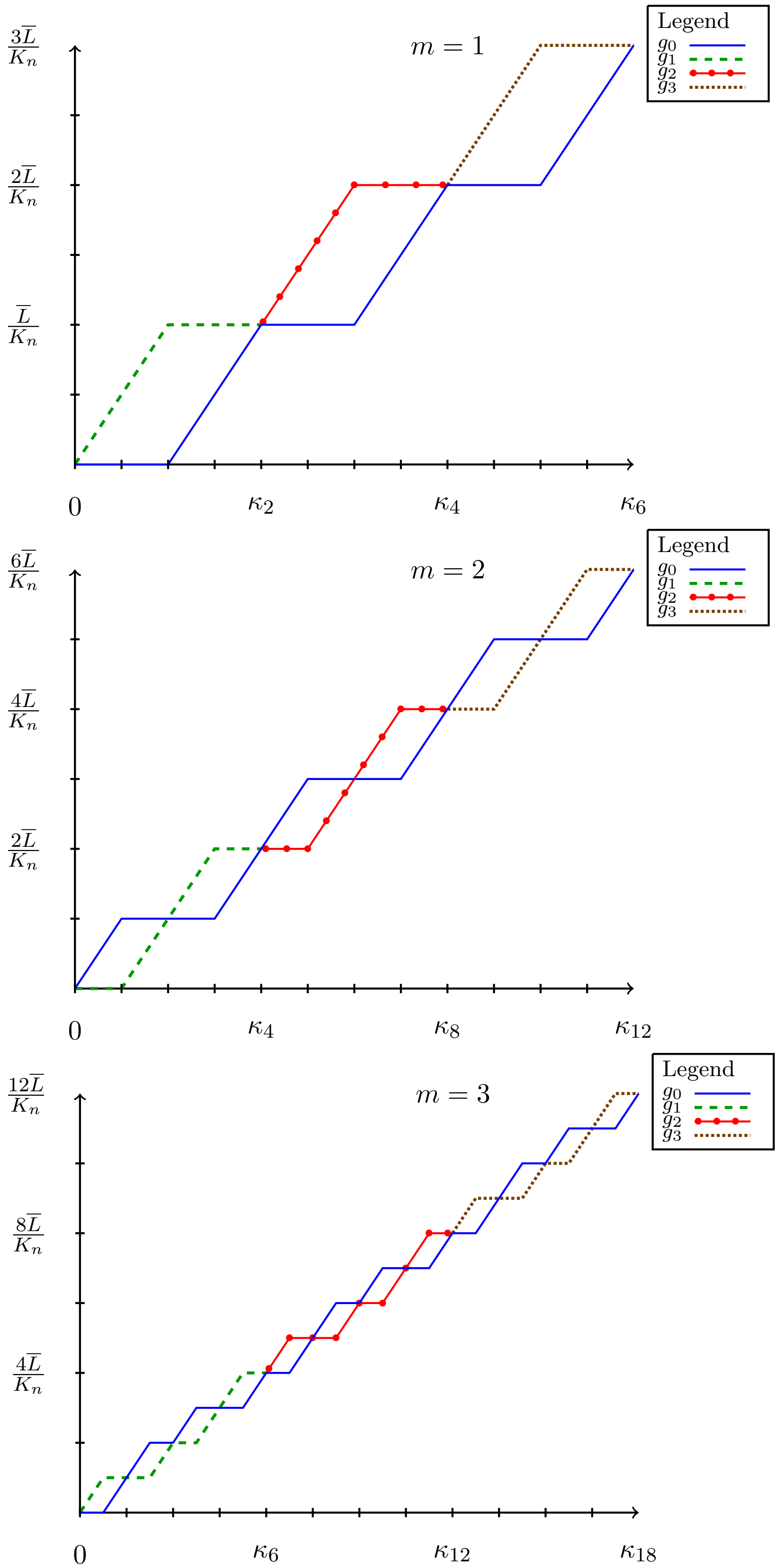
$$f_{j,n}(x) - f_{0,n}(x) = \begin{cases} \varphi_m(x - (j-1)K_n^{-\gamma}) & \text{if } x \in I_j \\ 0 & \text{otherwise,} \end{cases}$$

and alternatively, if $\gamma = 1$, then for each $j = 1, \ldots, M_n$, we have that

$$f_{j,n}(x) - f_{0,n}(x) = \begin{cases} \varphi_m(x - (j-1)2^m K_n^{-1}) & \text{if } x \in I_j \\ 0 & \text{otherwise,} \end{cases}$$

where φ_m is defined in (5.11).

Figure 5.3: Plot of the $g_{j,n}$'s near the origin, $\gamma = 1$



Proof. Certainly, the result holds for $m = 1$ by (5.11) and (5.14)-(5.18). In what follows, consider $m > 1$. We have the following two cases.

Case 1: $\gamma \in (0, 1)$, so each $f_{j,n}$ is given by (5.14)-(5.15), and (5.18). Fix $j = 1, \ldots, M_n$.

If $x \in [0, (j-1)K_n^{-\gamma})$, then via (5.15), and (5.18),

$$(f_{j,n} - f_{0,n})(x) = \mathcal{I}^{(m-1)}_{[0,x]}(g_{j,n} - g_{j,0}) = 0. \tag{5.19}$$

Suppose that $x \in I_j := [(j-1)K_n^{-\gamma}, (j-1)K_n^{-\gamma} + \kappa_{2^m})$. Then by (5.11), (5.14)-(5.15), and (5.18),

$$\begin{aligned}(f_{j,n} - f_{0,n})(x) &= \mathcal{I}^{(m-1)}_{[0,x]}(g_{j,n} - g_{j,0}) = \mathcal{I}^{(m-1)}_{[(j-1)K_n^{-\gamma},x]}\Big((h^{[2]}_{m,n} - h^{[1]}_{m,n})(\,\cdot\, - (j-1)K_n^{-\gamma})\Big) \\ &= \mathcal{I}^{(m-1)}_{[0,\ x-(j-1)K_n^{-\gamma}]}(\varphi_1) = \varphi_m(x - (j-1)K_n^{-\gamma}). \end{aligned} \tag{5.20}$$

Finally, consider $x \in [(j-1)K_n^{-\gamma} + \kappa_{2^m}, 1]$. By Lemma 5.3.1, (5.11)-(5.15), and (5.18),

$$\begin{aligned} 0 = \varphi^{(p)}_m(\kappa_{2^m}) &= \varphi_{m-p}(\kappa_{2^m}) = \mathcal{I}^{(m-p-1)}_{[0,\kappa_{2^m}]}(h^{[2]}_{m,n} - h^{[1]}_{m,n}) \\ &= \mathcal{I}^{(m-p-1)}_{[(j-1)K_n^{-\gamma},\ (j-1)K_n^{-\gamma}+\kappa_{2^m}]}\Big((h^{[2]}_{m,n} - h^{[1]}_{m,n})(\,\cdot\, - (j-1)K_n^{-\gamma})\Big) \\ &= \mathcal{I}^{(m-p-1)}_{[(j-1)K_n^{-\gamma},\ (j-1)K_n^{-\gamma}+\kappa_{2^m}]}\Big(g_{j,n} - g_{0,n}\Big) = \mathcal{I}^{(m-p-1)}_{[0,\ (j-1)K_n^{-\gamma}+\kappa_{2^m}]}\Big(g_{j,n} - g_{0,n}\Big) \\ &= (f_{j,n} - f_{0,n})^{(p)}((j-1)K_n^{-\gamma} + \kappa_{2^m}), \end{aligned} \tag{5.21}$$

for $p = 0, 1, \ldots, m-1$. Since $g_{j,n} - g_{0,n}$ is continuous by the discussion below (5.14)-(5.15), $f_{j,n} - f_{0,n}$ is $(m-1)$ times continuously differentiable. Hence, via Taylor expansion and (5.21),

$$(f_{j,n} - f_{0,n})(x) = (f_{j,n} - f_{0,n})(x)$$

$$- \sum_{p=0}^{m-2} \frac{(f_{j,n} - f_{0,n})^{(p)} \left((j-1)K_n^{-\gamma} + \kappa_{2^m}\right) \left(x - [(j-1)K_n^{-\gamma} + \kappa_{2^m}]\right)^p}{p!}$$

$$= \mathcal{I}^{(m-1)}_{\left[(j-1)K_n^{-\gamma} + \kappa_{2^m},\ x\right]} \left((f_{j,n} - f_{0,n})^{(m-1)}\right) = \mathcal{I}^{(m-1)}_{\left[(j-1)K_n^{-\gamma} + \kappa_{2^m},\ x\right]} (g_{j,n} - g_{0,n})$$

$$= 0, \tag{5.22}$$

and the result holds for Case 1.

Case 2: $\gamma = 1$ so each $f_{j,n}$ is given by (5.16)-(5.17), and (5.18). Again, fix $j = 1, \ldots, M_n$. Using arguments similar to those in (5.19), (5.20), and (5.21)-(5.22), demonstrates that Case 2 holds for all $x \in [0, (j-1)2^m K_n^{-1})$, $[(j-1)2^m K_n^{-1}, j\ 2^m K_n^{-1})$, and $[j\ 2^m K_n^{-1}, 1]$, respectively. □

Now that we have constructed the hypotheses and established the previous result, we are ready to show that these functions meet conditions (C1)-(C3) from Section 5.2.

5.4 Proof of the Main Result

We use the previous constructions and results to establish Theorem 5.2.1 in the following proof.

Proof. In each of the following two cases, we demonstrate that the $f_{j,n}$'s of (5.18) meet conditions (C1)-(C3).

Case 1: $\gamma \in (0, 1)$, so that $M_n = \lfloor K_n^\gamma \rfloor - 1$, and the $g_{j,n}$'s are given by (5.14)-(5.15). We show that the $f_{j,n}$'s meet conditions (C1), (C2), and (C3), in (1), (2), and (3) respectively.

(1) For all n (and K_n) sufficiently large, the following properties of each $g_{j,n}$ can be easily verified via Figure 5.2: for $x, y \in [0, 1]$, suppose that

(i) $0 < |x-y| \le \kappa_{2^m}$. Then

$$\max_j \frac{|g_{j,n}(x) - g_{j,n}(y)|}{|x-y|} \le \frac{|g_{1,n}(x) - g_{1,n}(y)|}{|x-y|}\Big|_{x=\kappa_1,\, y=\kappa_{2^m-1}} \le \overline{L}K_n^{1-\gamma}.$$

(ii) $\kappa_{2^m} < |x-y| \le K_n^{-\gamma}$. Then

$$\max_j |g_{j,n}(x) - g_{j,n}(y)| \le |g_{0,n}(x) - g_{0,n}(y)|\big|_{x=0,\, y=\kappa_{2^m}} \le 2^{m-1}\overline{L}K_n^{-\gamma}.$$

(iii) $K_n^{-\gamma} < |x-y| \le 1$. Without loss of generality, let $x < y$ with $y = qK_n^{-\gamma} + s(x,y)$ for some $q \in \mathbb{N}$ and $0 \le s(x,y) < K_n^{-\gamma}$. It follows from (5.6) that

$$\max_j \frac{|g_{j,n}(x) - g_{j,n}(y)|}{|x-y|} \le \frac{|g_{1,n}(x) - g_{1,n}(y)|}{|x-y|}\Big|_{x=\kappa_1,\ y=qK_n^{-\gamma}+\kappa_{2^m-1}}$$
$$\le \frac{2^{m-1}(q+1)\overline{L}K_n^{-\gamma}}{qK_n^{-\gamma} + (2^m-2)K_n^{-1}} \le \frac{2^{m-1}(q+1)\overline{L}K_n^{-\gamma}}{qK_n^{-\gamma}} \le 2^m\overline{L} \le L.$$

Since each $g_{j,n}$ is nondecreasing, each $f_{j,n}$ given by (5.18) belongs to $\mathcal{S}_m$ (c.f. (3.1)). To see that each $f_{j,n}$ is in the Hölder class H_L^r, we consider the following three scenerios:

(1.1) $0 < |x-y| \le \kappa_{2^m}$. Then, by (i) and (5.6), we have that

$$\frac{|f_{j,n}^{(m-1)}(x) - f_{j,n}^{(m-1)}(y)|}{|x-y|^\gamma} = \frac{|f_{j,n}^{(m-1)}(x) - f_{j,n}^{(m-1)}(y)|}{|x-y|}|x-y|^{1-\gamma}$$
$$\le \bar{L}K_n^{1-\gamma}\kappa_{2^m}^{1-\gamma} \le 2^m\overline{L} \le L.$$

(1.2) $\kappa_{2^m} < |x-y| \le K_n^{-\gamma}$. Then, by (ii) and (5.6), we have that

$$\frac{|f_{j,n}^{(m-1)}(x) - f_{j,n}^{(m-1)}(y)|}{|x-y|^\gamma} \le \frac{2^{m-1}\overline{L}K_n^{-\gamma}}{|x-y|^\gamma} \le 2^{m-1}\bar{L}K_n^{-\gamma}\kappa_{2^m}^{-\gamma} \le 2^m\overline{L} \le L.$$

(1.3) $\frac{1}{K_n^\gamma} < |x-y| \leq 1$. By (iii), we obtain

$$\frac{|f_{j,n}^{(m-1)}(x) - f_{j,n}^{(m-1)}(y)|}{|x-y|^\gamma} \leq \frac{|f_{j,n}^{(m-1)}(x) - f_{j,n}^{(m-1)}(y)|}{|x-y|} \leq L.$$

Thus, each $f_{j,n} \in \mathcal{S}_{m,H}(r, L)$, so the $f_{j,n}$'s satisfy (C1).

(2) Suppose that $j \neq k$. By Lemma 5.3.3, we have that $f_{j,n}(x) = f_{0,n}(x) = f_{k,n}(x)$ for all $x \in [0,1] \setminus (I_j \cup I_k)$. Hence, $|f_{j,n}(x) - f_{k,n}(x)| = 0$ on $[0,1] \setminus (I_j \cup I_k)$. Also,

$$|f_{j,n}(x) - f_{k,n}(x)| = |f_{j,n}(x) - f_{0,n}(x)| = |\varphi_m(x - (j-1)K_n^{-\gamma})| \ \forall \ x \in I_j,$$

and similarly, $|f_{j,n}(x) - f_{k,n}(x)| = |\varphi_m(x - (k-1)K_n^{-\gamma})| \ \forall \ x \in I_k$. Therefore, in view of Lemma 5.3.2, we see that the $f_{j,n}$'s meet condition (C2) with $s_n := \frac{\overline{L}}{2m!}\left\lceil \left(\frac{n}{\log n}\right)^{\frac{1}{2r+1}} \right\rceil^{-r} \asymp \left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}}$, as

$$\|f_{j,n} - f_{k,n}\|_\infty = \|\varphi_m\|_\infty \geq \frac{\overline{L}}{m!} K_n^{-r} = 2s_n.$$

(3) By the discussion following the statement of (C3) in Section 5.2, there exists $p_* > 0$, independent of n and $f_{j,n}$, such that $K(P_j, P_0) \leq p_* \sum_{i=1}^n (f_{j,n}(X_i) - f_{0,n}(X_i))^2$ where $X_i = \frac{i}{n}$, for all $j = 1, \ldots, M_n$. Also,

$$\frac{i}{n} \in \left[(j-1)K_n^{-\gamma}, (j-1)K_n^{-\gamma} + \kappa_{2^m}\right) \implies \lceil n(j-1)K_n^{-\gamma} \rceil \leq i \leq \left\lfloor n\left((j-1)K_n^{-\gamma} + \kappa_{2^m}\right)\right\rfloor.$$

Let $a_j := \left\lceil n(j-1)K_n^{-\gamma} \right\rceil$ and $b_j := \left\lfloor n\left((j-1)K_n^{-\gamma} + \kappa_{2^m}\right)\right\rfloor$. Then by Lemma 5.3.2, Lemma 5.3.3, (5.5), and (5.6), for n sufficiently large,

$$K(P_j, P_0) \leq p_* \sum_{i=1}^n \left(f_{j,n}\left(\frac{i}{n}\right) - f_{0,n}\left(\frac{i}{n}\right)\right)^2 = p_* \sum_{i=a_j}^{b_j} \left(f_{j,n}\left(\frac{i}{n}\right) - f_{0,n}\left(\frac{i}{n}\right)\right)^2$$

$$
\begin{aligned}
&= p_* \sum_{i=a_j}^{b_j} \left(\varphi_m\left(\frac{i}{n} - (j-1)K_n^{-\gamma}\right) \right)^2 \leq p_* \sum_{i=a_j}^{b_j} \left(\frac{\overline{L}2^{m^m}}{m!}K_n^{-r}\right)^2 \\
&\leq p_* 2n \ \kappa_{2^m} \left(\frac{\overline{L}2^{m^m}}{m!}K_n^{-r}\right)^2 = p_* 2^{m+1} \left(\frac{\overline{L}2^{m^m}}{m!}\right)^2 n K_n^{-(2r+1)} \\
&\leq \frac{\gamma c_0}{4(2r+1)} n \ K_n^{-(2r+1)} \leq \frac{\gamma c_0}{4(2r+1)} \log n \leq \frac{\gamma c_0}{2(2r+1)} \log\left(\frac{n}{\log n}\right) \\
&\leq \frac{\gamma c_0}{2} \log(K_n) \leq c_0 \log(\lfloor K_n^{\gamma} \rfloor - 1) = c_0 \log M_n
\end{aligned}
$$

for all $j = 1, \ldots, M_n$. Thus, $\frac{1}{M_n}\sum_{j=1}^{M_n} K(P_j, P_0) \leq c_0 \log M_n$, and (C3) holds in Case 1.

Case 2: $\gamma = 1$, so that $M_n = \lfloor \frac{K_n}{2^m} \rfloor - 1$, and the $g_{j,n}$'s are now given by (5.16)-(5.17). We now demonstrate that conditions (C1)-(C3) hold for Case 2 in (1)-(3).

(1) It is easy to see that each $g_{j,n}$ is increasing via Figure 5.3. Hence, each $f_{j,n}$ given by (5.18) belongs to $\mathcal{S}_m$. Also, it is easy to verify that for any $0 \leq x < y \leq 1$, $\frac{|g_{j,n}(x) - g_{j,n}(y)|}{|x-y|} \leq \overline{L} \leq L$ for each $j = 0, 1, \ldots, M_n$. This thus implies that each $f_{j,n} \in \mathcal{S}_{m,H}(r, L)$. Hence, the $f_{j,n}$'s meet condition (C1).

(2) Suppose that $j \neq k$. By the same argument as in Case 1,

$$
|f_{j,n}(x) - f_{k,n}(x)| = \begin{cases} |\varphi_m(x - (j-1)\kappa_{2^m})| & \text{if } x \in I_j \\ |\varphi_m(x - (k-1)\kappa_{2^m})| & \text{if } x \in I_k \\ 0 & \text{otherwise.} \end{cases}
$$

Hence the $f_{j,n}$'s meet condition (C2) with $s_n := \frac{\overline{L}}{2m!}\left\lceil \left(\frac{n}{\log n}\right)^{\frac{1}{2r+1}} \right\rceil^{-r} \asymp \left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}}$, as

$$
\|f_{j,n} - f_{k,n}\|_\infty = \|\varphi_m\|_\infty \geq \frac{\overline{L}}{m!}K_n^{-r} = 2s_n.
$$

(3) Let $a_j := \lceil n(j-1)\kappa_{2^m} \rceil$ and $b_j := \lfloor n\ j\ \kappa_{2^m} \rfloor$. By an argument similar to that in Case 1, for n sufficiently large, we have that for all $j = 1, \ldots, M_n$,

$$K(P_j, P_0) \le p_* \sum_{i=a_j}^{b_j} \left(\varphi_m \left(\frac{i}{n} - (j-1)\kappa_{2^m} \right) \right)^2 \le p_* \sum_{i=a_j}^{b_j} \left(\frac{\overline{L} 2^{m^m}}{m!} K_n^{-r} \right)^2$$
$$\le p_* 2n\ \kappa_{2^m} \left(\frac{\overline{L} 2^{m^m}}{m!} K_n^{-r} \right)^2 \le \frac{c_0}{2} \log(K_n) \le c_0 \log \left(\left\lfloor \frac{K_n}{2^m} \right\rfloor \right) = c_0 \log(M_n)$$

Hence $\frac{1}{M_n} \sum_{j=1}^{M_n} K(P_j, P_0) \le c_0 \log M_n$ and condition (C3) holds for Case 2 as well.

We have demonstrated that conditions (C1)-(C3) are satisfied by $f_{j,n}$, $j = 0, 1 \ldots, M_n$. By virtue of the discussion following the statement of Theorem 5.2.1 in Section 5.2, Theorem 5.2.1 holds. □

5.5 Implications and Extensions

In this section, we state and establish several corollaries to Theorem 5.2.1. The first two corollaries combine Theorem 5.2.1 with the results from Chapter IV to demonstrate that, in certain instances, the constrained B-spline estimator proposed in Chapter III achieves the optimal performance under the sup-norm. The second two corollaries establish a minimax lower bound in the sup-nom for nonnegative derivative constrained Sobolev function classes.

Combining the results from Chapters III-V, we have the following results on the constrained nonparametric estimation problem given by (5.1).

Corollary 5.5.1. *Fix $m \in \mathbb{N}$, $r \in (m-1, m]$, and $L > 0$. Consider the regression problem given by (5.1). If $m = 1, 2,$ or 3, then*

$$\inf_{\widehat{f}} \sup_{f \in \mathcal{S}_{m,H}(r,L)} \mathbb{E}\big(\|\widehat{f} - f\|_\infty\big) \asymp \Big(\frac{\log n}{n}\Big)^{\frac{r}{2r+1}}, \tag{5.23}$$

where $\inf_{\widehat{f}}$ *denotes the infimum over all estimators in* $\mathcal{S}_m$ *on* $[0, 1]$.

Proof. For fixed n (and K_n), let the set of design points $P = (x_i)_{i=0}^n$ be given by $x_i = \frac{i}{n}$ (c.f. (3.13)). Fix positive constants $c_{\kappa,1}, c_{\kappa,2}$ such that $0 < c_{\kappa,1} \leq 1 \leq c_{\kappa,2}$. Then for any $T_\kappa \in \mathcal{T}_{K_n}$, let $\widehat{f}^B_{P,T_\kappa}$ denote the nonnegative derivative constrained B-spline from Chapter III given by (3.7)-(3.8). The result follows from (5.3). □

Remark 5.5.1. By (5.4), $\widehat{f}^B_{P,T_\kappa}$ is an (asymptotically) optimally performing estimator over $\mathcal{S}_{m,H}(r, L)$, for $m = 1, 2, 3$.

Recall from Chapter IV that by Proposition 4.2.2 and Remark 4.2.1, the maximum risk associated with the nonnegative constrained B-spline $\widehat{f}^B_{P,T_\kappa}$ estimator

$$\sup_{f \in \mathcal{S}_{m,H}(r,L)} \mathbb{E}\big(\|\widehat{f}^B_{P,T_\kappa} - f\|_\infty\big) \geq \frac{\widetilde{c}_m}{K_n^3} \asymp \left(\frac{\log n}{n}\right)^{\frac{3}{2r+1}}$$

when $m > 3$ and $K_n \asymp \left(\frac{n}{\log n}\right)^{\frac{1}{2r+1}}$, which is much larger than the minimax lower bound given in Theorem 5.2.1. Therefore, we believe that $\widehat{f}^B_{P,T_\kappa}$ does not perform optimally over $\mathcal{S}_{m,H}(r, L)$ for such m. However, the next result demonstrates that this estimator still performs optimally over the restricted Hölder class of strictly positive derivative constrained functions $\mathcal{S}_{m,H}(r, L', L)$ (c.f (4.3)) for any fixed m, r, L', and L. The proof the next corollary follows immediately from Theorems 4.3.2 and 5.2.1.

Corollary 5.5.2. *Fix* $m \in \mathbb{N}$, $r \in (m-1, m]$, *and* $L \geq L' > 0$. *Let* $\mathcal{S}_{m,H}(r, L', L)$ *denote the previously defined restricted Hölder class of strictly positive derivative constrained functions given by (4.3). Then for the regression problem given by (5.1),*

$$\inf_{\widehat{f}} \sup_{f \in \mathcal{S}_{m,H}(r,L',L)} \mathbb{E}\big(\|\widehat{f} - f\|_\infty\big) \asymp \left(\frac{\log n}{n}\right)^{\frac{r}{2r+1}},$$

where $\inf_{\widehat{f}}$ *denotes the infimum over all estimators in* $\mathcal{S}_m$ *on* $[0,1]$.

In this chapter, we have studied minimax lower bounds for constrained Hölder clasees, where the ceiling of the Hölder exponent, $\lceil r \rceil$, is equal to m, the order of the nonnegative derivative constraint. In the next corollary, we establish the same minimax lower bounds when $\lceil r \rceil$ is greater than the order of the derivative constraint. Let $\mathcal{S}_{p,H}(r,L) := \mathcal{S}_p \cap H_L^r$ for any $p \in \mathbb{N}$, with $1 \le p < m$. Consider the regression problem given by (5.1) with $\mathcal{S}_{m,H}(r,L)$ replaced by $\mathcal{S}_{p,H}(r,L)$. We have the following corollary.

Corollary 5.5.3. *Fix* $m \in \mathbb{N}$, $r \in (m-1, m]$, $L > 0$, *and* $p \in \mathbb{N}$, *with* $1 \le p < m$. *Then there exists a positive constant* c *such that*

$$\liminf_{n\to\infty} \inf_{\widehat{f}} \sup_{f \in \mathcal{S}_{p,H}(r,L)} \mathbb{E}\big(\|\widehat{f} - f\|_\infty\big) \ \ge\ c\Big(\frac{\log n}{n}\Big)^{\frac{r}{2r+1}},$$

where $\inf_{\widehat{f}}$ *denotes the infimum over all estimators in* $\mathcal{S}_p$ *on* $[0,1]$.

Proof. In view of the proof of Theorem 5.2.1, it is sufficient to show that there exists a family hypothesis functions $f_{j,n}$, $j = 0, 1, \ldots, M_n$ satisfying (i) $f_{j,n} \in \mathcal{S}_{p,H}(r,L)$ for all j, (ii) (C2) of Section 5.2, and (iii) (C3) of Section 5.2. Because the $g_{j,n}$'s constructed in (5.14)-(5.17) satisfy $g_{j,n} \ge 0$,

$$f_{j,n}^{(p)}(x) = \mathcal{I}_{[0,x]}^{(m-p-1)}(g_{j,n}) \ge 0,$$

so each of the $f_{j,n}$'s given by (5.18) belong to $\mathcal{S}_p$. Moreover, by the proof of Theorem 5.2.1, each $f_{j,n} \in H_L^r$ (and thus is also in $\mathcal{S}_{p,H}(r,L)$) and satisfies (C2) and (C3). □

We have studied the nonparametric estimation of nonnegative derivative constrained functions in the sup-norm, over suitable Hölder classes. In this final corollary, we consider the same problem over a Sobolev class. Fix $m \in \mathbb{N}$ and $L > 0$. We define the Sobolev class of functions

$$\mathcal{W}(m,L) := \Big\{ f : [0,1] \to \mathbb{R} \;\Big|\; f \text{ is } (m-1) \text{ times differentiable,} \\ \text{with } f^{(m-1)} \text{ absolutely continuous, and } \|f^{(m)}\|_{L_2} \le L \Big\}.$$

Let $\mathcal{S}_{p,\mathcal{W}}(m,L) := \mathcal{S}_p \cap \mathcal{W}(m,L)$. Consider the regression problem given by (5.1) with $\mathcal{S}_{m,H}(r,L)$ replaced by $\mathcal{S}_{p,\mathcal{W}}(m,L)$. We have the following last corollary.

Corollary 5.5.4. *Fix $m \in \mathbb{N}$, $L > 0$, and $p \in \mathbb{N}$, with $1 \le p \le m$. Then there exists a positive constant c such that*

$$\liminf_{n\to\infty} \inf_{\widehat{f}} \sup_{f \in \mathcal{S}_{p,\mathcal{W}}(m,L)} \mathbb{E}\big(\|\widehat{f} - f\|_\infty\big) \;\ge\; c\Big(\frac{\log n}{n}\Big)^{\frac{r}{2r+1}},$$

where $\inf_{\widehat{f}}$ denotes the infimum over all estimators in $\mathcal{S}_p$ on $[0,1]$.

Proof. In view of the proof of the previous corollary, it is sufficient show that the $f_{j,n}$'s given by (5.18) belong to the function class $\mathcal{S}_{p,\mathcal{W}}(m,L)$. Note that each $g_{j,n}$ is Lipschitz continuous, with Lipschitz constant L. Hence, each $f_{j,n}^{(m-1)} = g_{j,n}$ is absolutely continuous. In addition, by the Lipschitz continuity of $g_{j,n}$,

$$\int_0^1 \Big(f_{j,n}^{(m)}(x)\Big)^2 \, dx = \int_0^1 \big(g_{j,n}'(x)\big)^2 \, dx \le \int_0^1 L^2 \, dx = L^2.$$

Thus, $\|f_{j,n}^{(m)}\|_{L_2} \le L$, and each $f_{j,n} \in \mathcal{S}_{m,\mathcal{W}}(m,L)$, completing the proof. ∎

5.6 Summary

In this chapter, we constructed a family of hypothesis functions in order to establish a minimax lower bound for a family of nonnegative derivative constrained nonparametric estimation problems under the supremum norm. Combining this result with those from the previous chapters demonstrated that in certain cases, the nonnegative derivative constrained B-spline estimator from Chapter III achieves the optimal performance when the supremum norm is used as the performance metric.

CHAPTER VI

Conclusions

We have studied a number of problems in shape constrained estimation, concerning (i) the analysis and computation of constrained smoothing splines, and (ii) the asymptotic analysis of general nonnegative derivative constrained nonparametric estimation. In this chapter, we summarize the results that we have established in these areas, and discuss several future research directions.

6.1 Analysis and Computation of Constrained Smoothing Splines

In Chapter II, we formulated smoothing splines subject to general linear dynamics and control constraints in terms of optimal control problems. We then used Hilbert space methods and variational techniques to derive optimality conditions for the solutions of these problems. In order to compute the constrained smoothing splines, a modified nonsmooth Newton's algorithm with line search was employed. A detailed argument for the convergence analysis of this algorithm was given; several nontrivial constrained smoothing spline numerical examples were considered.

6.1.1 Future Work

A variety of extensions will be considered in the future. For instance, we aspire to reduce the size requirement on the smoothing parameter needed to guarantee the convergence of the nonsmooth Newton's algorithm (c.f. Theorems 2.5.1-2.5.2). Such a size reduction would ensure the algorithm's convergence for smoothing parameters similar to those used in the numerical examples in Section 2.6. Another interesting research extension would involve studying the effect of the smoothing parameter on the constrained smoothing spline performance. A third direction would include examining a constrained spline model for nonlinear dynamical systems. Other possibilities include the study of smoothing splines subject to both control and state constraints. Finally, we hope to address the statistical performance analysis of constrained smoothing splines in the future.

6.2 Asymptotic Analysis of General Nonnegative Derivative Constrained Nonparametric Estimation

In Chapter III, we introduced a general nonnegative derivative constrained B-spline estimator, for which we developed a critical uniform Lipschitz property. This uniform Lipschitz property was then invoked in Chapter IV to provided asymptotic upper bounds on the bias and stochastic error of the constrained B-spline estimator, with respect to the supremum norm. These upper bounds allowed us to establish the B-spline estimator consistency, and provided us with an estimator convergence rate. After establishing a variety of minimax asymptotic lower bounds over suitable Hölder and Sobolev classes under the supremum norm in Chapter V, it was observed that such minimax asymptotic lower bounds corresponded to the asymptotic upper bounds developed for the nonnegative derivative constrained B-spline estimator risk for the first, second, and third order derivative constraints. This demonstrates that the proposed constrained B-spline estimator performs optimally over certain constrained Hölder classes for such nonnegative derivative constraints with respect to the supremum norm.

6.2.1 Future Work

Although the proposed B-spline estimator achieves the optimal performance rate under the supremum norm uniformly over many constrained Hölder classes for the first, second, and third order derivative constraints, this optimal performance is not achieved for fourth and higher order derivative constraints due to an undesirably large estimator bias. Consequently, in order to meet the minimax asymptotic lower bounds from Chapter V, other constrained estimators must be considered. One possible candidate is a nonnegative derivative constrained B-spline estimator with variable knots. Moreover, the large bias of the constrained B-spline estimator with fixed knots, introduced in Chapter III, stems from the inability of certain smooth higher order nonnegative derivative constrained functions to achieve Jackson type approximations with the same constraint for a fixed knot sequence, as illustrated in Proposition 4.2.2. However, it is demonstrated in [32] that such Jackson type approximations are attainable when the spline knot sequence is not fixed. Therefore, one possible extension of the work presented in Chapters III-V would be to consider the performance of a nonnegative derivative constrained B-spline estimator, whose variable knots are somehow influenced by the data.

Other possible extensions to this second topic include the asymptotic analysis of nonparametric estimation for (i) problems with more general shape constraints, or (ii) problems with more than one shape constraint such as the k-monotone constraints given in [2]. Finally, we may wish to examine other implications of the uniform Lipschitz property for the general nonnegative derivative constrained B-spline estimator such as the pointwise L_2-risk and the pointwise mean squared error; these matters are addressed in [80, Theroem 4.1, Statement 2], for a convex B-spline estimator.

APPENDIX A

An Alternative Proof of Proposition 4.2.1

In this appendix, we give an independent proof of Proposition 4.2.1. We continue to use the notation from Chapter IV. In what follows, we will show that there exists a constant $c_{\infty,3} := \frac{3}{2} L\, c_{\kappa,2}^{2+\gamma}$ such that for all $f \in \mathcal{S}_{3,H}(r, L)$, with $2 < r \leq 3$, $T_\kappa \in \mathcal{T}_{K_n}$, and $K_n \in \mathbb{N}$, there exists $f_B \in \mathbb{S}_{+,3}^{T_\kappa}$ satisfying $\|f - f_B\|_\infty \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$. In order to do this, first fix $K_n \in \mathbb{N}$ and $T_\kappa \in \mathcal{T}_{K_n}$. Consider $g := f' \in \mathcal{S}_{2,H}(r-1, L)$ for any $f \in \mathcal{S}_{3,H}(r, L)$, $r \in (2, 3]$. Our goal is to construct a piecewise linear function $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$ such that

$$\left| \int_0^x (g(t) - \widetilde{g}(t))\, dt \right| \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}} \text{ for all } x \in [0, 1]. \tag{A.1}$$

We will then define f_B such that $f_B(x) = f(0) + \int_0^x \widetilde{g}(t)\, dt$ for all $x \in [0, 1]$. The function f_B must lie in $\mathbb{S}_{+,3}^{T_\kappa}$ since its derivative $\widetilde{g}$ lies in the family $\mathbb{S}_{+,2}^{T_\kappa}$ of convex piecewise linear functions with knot sequence T_κ. Furthermore, by (A.1), we will have $\|f - f_B\|_\infty \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$. This purpose of this appendix is to construct such $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$ and $f_B \in \mathbb{S}_{+,3}^{T_\kappa}$.

A.1 Overview of Construction

The construction of $\widetilde{g}$ is somewhat technical. Therefore, we will first give a brief overview of the construction of this function.

To construct $\widetilde{g}$, we will first subdivide $[0,1]$ into either N or $(N+1)$ smaller intervals: $[\tau_{j-1},\tau_j]$, for $j=1,\ldots,N$ with $\tau_0=0$, and $[\tau_N,1]$, if $\tau_N<1$. Moreover, each τ_j will be a point in the knot sequence T_κ. Furthermore, in selecting the τ_j's via Algorithm 2, we will ensure that $\int_{\tau_{j-1}}^{\tau_j}(\widehat{g}-g)(t)\,dt \le \frac{c_{\infty,3}}{K_n^{2+\gamma}}$ (shown in Lemma A.2.1), for all $j=1,\ldots,N$, where $\widehat{g}\ge g$ is the linear interpolant of the convex function g at the knots in T_κ. (The importance of bounding $\int_{\tau_{j-1}}^{\tau_j}(\widehat{g}-g)(t)\,dt$ in this way will become apparent later.) The goal is to construct a function $\widetilde{g}_j$ on each $[\tau_{j-1},\tau_j]$ such that $\int_{\tau_{j-1}}^{\tau_j}(g-\widetilde{g}_j)(t)\,dt=0$ for all j, and setting

$$\widetilde{g}(t)=\begin{cases}\widetilde{g}_j(t) & \text{if } t\in[\tau_{j-1},\tau_j]\\[2ex] \widehat{g}(t) & \text{if } t\in[\tau_N,1]\end{cases}$$

will produce a well-defined convex continuous piecewise linear $\widetilde{g}\in\mathbb{S}_{+,2}^{T_\kappa}$ satisfying (A.1).

On $[\tau_{j-1},\tau_j]$, each $\widetilde{g}_j$ will be a weighted average of $\widehat{g}$ and another piecewise linear convex function $\grave{g}_j$ (see (A.14)) with knots in $[\tau_{j-1},\tau_j]\cap T_\kappa$. Since $g\le\widehat{g}$, we have $\int_{\tau_{j-1}}^{\tau_j}g(t)\,dt \le \int_{\tau_{j-1}}^{\tau_j}\widehat{g}(t)\,dt$ for all $j=1,\ldots,N$. Alternatively, each $\grave{g}_j$ will be constructed such that $\int_{\tau_{j-1}}^{\tau_j}g(t)\,dt \ge \int_{\tau_{j-1}}^{\tau_j}\grave{g}_j(t)\,dt$ (see Lemma A.3.2) and $\int_{\tau_{j-1}}^{\tau_j}(\grave{g}_j-g)(t)\mathbf{1}_{[\grave{g}_j-g\ge 0]}(t)\,dt \le \frac{c_{\infty,3}}{K_n^{2+\gamma}}$ (see the proof of Lemma A.4.1) for all $j=1,\ldots,N$. By choosing an appropriate weight $r_j\in[0,1]$, and setting $\widetilde{g}_j:=r_j\widehat{g}+(1-r_j)\grave{g}_j$ on $[\tau_{j-1},\tau_j]$, we will have that $\int_{\tau_{j-1}}^{\tau_j}(g-\widetilde{g}_j)(t)\,dt=0$ for all j. Combining this with the fact that

$$0\le\int_{\tau_{j-1}}^{\tau_j}(\widehat{g}-g)(t)\,dt,\ \int_{\tau_{j-1}}^{\tau_j}(\grave{g}_j-g)(t)\mathbf{1}_{[\grave{g}_j-g\ge 0]}(t)\,dt \ \le\ \frac{c_{\infty,3}}{K_n^{2+\gamma}},$$

will allow us to establish that $\left|\int_{\tau_{j-1}}^{x}(g-\widetilde{g}_j)(t)\,dt\right| \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$ for all $x \in [\tau_{j-1},\tau_j]$. The construction of the $\grave{g}_j$'s and $\widetilde{g}_j$'s will also take into account the continuity and convexity of $\widetilde{g}$ (see Lemmas A.3.1 and A.4.1).

Putting all of this together gives us that $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$ satisfies (A.1) as

$$\left|\int_0^x (g-\widetilde{g})(t)\,dt\right| = \sum_{i=1}^{j-1}\left|\int_{\tau_{i-1}}^{\tau_i}(g-\widetilde{g}_i)(t)\,dt\right| + \left|\int_{\tau_{j-1}}^{x}(g-\widetilde{g}_j)(t)\,dt\right| \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}},$$

for all $x \in [\tau_{j-1},\tau_j]$, and $j = 1,\ldots,N$. (If $x \in [\tau_N, 1]$, a similar argument can be made.)

The rest of this appendix is concerned with the construction of $\widetilde{g}$ and f_B. In Section A.2, we choose the τ_j's via Algorithm 2 in order to form the intervals $[\tau_{j-1},\tau_j]$, $j = 1,\ldots,N$, on which we may define the $\grave{g}_j$'s and the $\widetilde{g}_j$'s. In Section A.3 we construct the piecewise linear convex $\grave{g}_j$'s so that $\int_{\tau_{j-1}}^{\tau_j} g(t)\,dt \geq \int_{\tau_{j-1}}^{\tau_j}\grave{g}_j(t)\,dt$ and $\int_{\tau_{j-1}}^{\tau_j}(\grave{g}_j - g)(t)\mathbf{1}_{[\grave{g}_j-g\geq 0]}(t)\,dt \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$. Finally, in Section A.4, we use the $\grave{g}_j$'s to construct the $\widetilde{g}_j$'s, the function $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$, and finally $f_B \in \mathbb{S}_{+,3}^{T_\kappa}$ satisfying (A.1).

A.2 Construction of $\widetilde{g}$: Choosing the τ_j's

In this section we choose points $\tau_j \in T_\kappa$ via Algorithm 2. The choice of these points is of crucial importance in the construction of the $\grave{g}_j$'s, the $\widetilde{g}_j$'s, as well as $\widetilde{g}$ in subsequent sections.

Define $c_2^* := \frac{1}{2}Lc_{\kappa,2}^{1+\gamma}$, and recall that $c_{\infty,3} := \frac{3}{2}Lc_{\kappa,2}^{2+\gamma}$. These quantities will be frequently used throughout this and subsequent sections. Note that $g = f' \in \mathcal{S}_{2,H}(r-1,L)$ is differentiable. Define the function $h : [0,1]\times[0,1] \to \mathbb{R}$ so that

$$h(x,y) = g(y) + g'(y)(x-y) \tag{A.2}$$

for all $(x, y) \in [0,1] \times [0,1]$. Moreover, for each pair of $x, y \in [0,1]$, the quantity $h(x, y)$ is the value of the tangent line to g at y evaluated at x. The following properties hold for all $(x, y) \in [0,1] \times [0,1]$ and are illustrated in Figure A.1.

(P1) Since g is a convex function, the value of any tangent line to g will always be less than or equal to the value of g at any point $x \in [0,1]$. Moreover,

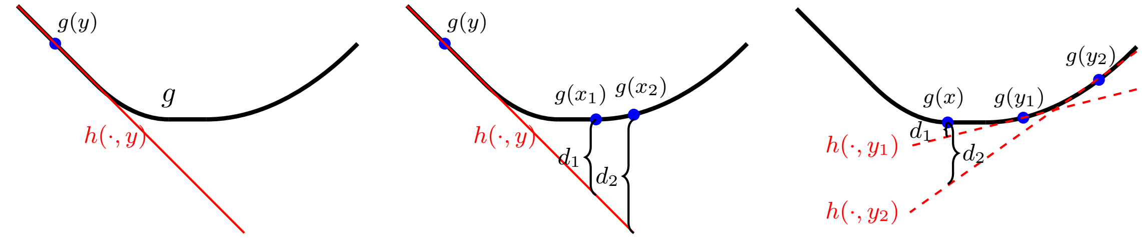
$$h(x, y) \leq g(x) \text{ for all } x, y \in [0,1]. \tag{A.3}$$

(P2) Consider $h(\cdot, y)$, the tangent line to the function g at the point y. Since g is a convex function, the difference between g and its tangent line $h(\cdot, y)$ evaluated at the point x increases as the distance between x and y increases. Moreover, combining this idea with (A.3), we have that

$$0 \leq g(x) - h(x, y) \text{ increases as } |x - y| \text{ increases with } y \text{ fixed.} \tag{A.4}$$

(P3) For fixed $x \in [0,1]$, we may also consider the function $g(x) - h(x, \cdot) : [0,1] \to \mathbb{R}$, i.e., we consider $g(x) - h(x, y)$ as a function of y since $x \in [0,1]$ is fixed. This function gives us the difference between the function g and its tangent line h evaluated at the point x, as we vary the point y at which h is tangent to g. Since g is convex, increasing the distance between the fixed point x and the point y, where h is tangent to g, will increase the difference between g and $h(\cdot, y)$ evaluated at the point x. Hence, (A.3) gives us that

$$0 \leq g(x) - h(x, y) \text{ increases as } |x - y| \text{ increases with } x \text{ fixed.} \tag{A.5}$$



(a) P1: Observe that $g(x) \geq h(x, y)$ for all x.

(b) P2: As x moves farther away from y, the difference between $g(x)$ and $h(x, y)$ increases.

(c) P3: As y moves farther away from x, the difference between $g(x)$ and $h(x, y)$ increases.

Figure A.1: An illustration of properties P1, P2, and P3.

With these properties in mind, we use Algorithm 2 to choose the points $\tau_0, \tau_1, \ldots, \tau_N$.

An illustration of Algorithm 2 is given in Figure A.2.

Algorithm 2 Choose $\tau_0, \tau_1, \ldots, \tau_N$.

Step 1: Let $\tau_0 = 0$, and $j = 0$.

Step 2: Let $\widetilde{\tau}_j$ be the first $\kappa_i > \tau_j$ such that $g(\kappa_i) - h(\kappa_i, \tau_j) \geq \frac{c_2^*}{K_n^{1+\gamma}}$, if such a $\kappa_i \in [0, 1]$ exists. (If no such $\kappa_i \in [0, 1]$ exists, set $N = j$, and terminate the algorithm.)

Step 3: Let τ_{j+1} be the first $\kappa_i > \widetilde{\tau}_j$ such that $g(\widetilde{\tau}_j) - h(\widetilde{\tau}_j, \kappa_i) \geq \frac{c_2^*}{K_n^{1+\gamma}}$ if such a κ_i exists. (If no such $\kappa_i \in [0, 1]$ exists, set $N = j$, and terminate the algorithm.)

Step 4: If $\tau_{j+1} = 1$, set $N = j + 1$, and terminate the algorithm. Otherwise, replace j with $j + 1$, and return to Step 2.

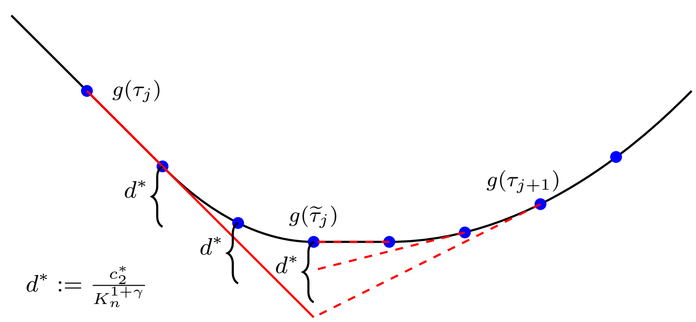


Figure A.2: In Algorithm 2, $\widetilde{\tau}_j$ is the first knot $\kappa_i \in T_\kappa$ to the right of τ_j such that $g(\kappa_i) - h(\kappa_i, \tau_j) \geq d^* := \frac{c_2^*}{K_n^{1+\gamma}}$; τ_{j+1} is the first $\kappa_i \in T_\kappa$ to the right of $\widetilde{\tau}_j$ such that $g(\kappa_i) - h(\kappa_i, \tau_{j+1}) \geq d^*$.

Recall that $\widehat{g}$ is the linear interpolant of the convex function g at the knots in the sequence T_κ. Later on, we will use $\widehat{g}$ to construct $\widetilde{g}$ as described in Section A.1, and will need the following lemma concerning the area between $\widehat{g}$ and g on each $[\tau_{j-1}, \tau_j]$.

Lemma A.2.1. *Suppose that $N \in \mathbb{N}$. Then for each $j \in \{1, \ldots, N\}$, we have that*

$$0 \leq \int_{\tau_{j-1}}^{\tau_j} \widehat{g}(x) - g(x)\, dx \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}. \tag{A.6}$$

Additionally, we have

$$\int_{\tau_N}^{1} \widehat{g}(x) - g(x)\, dx \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}, \tag{A.7}$$

even if $N = 0$.

Proof. First note that $g(\kappa_i) = \widehat{g}(\kappa_i)$ for all $\kappa_i \in T_\kappa$, as $\widehat{g}$ is the linear interpolant of g at the knots in T_κ. Therefore, for all $\kappa_i > \kappa_\ell$, we have that

$$\int_{\kappa_\ell}^{\kappa_i} (\widehat{g}(x) - g(x))\, dx = \sum_{r=\ell+1}^{i} \int_{\kappa_{r-1}}^{\kappa_r} (\widehat{g}(x) - g(x))\, dx = \sum_{r=\ell+1}^{i} \int_{\kappa_{r-1}}^{\kappa_r} \int_{\kappa_{r-1}}^{x} (\widehat{g}'(t) - g'(t))\, dt\, dx.$$

Now, since $\widehat{g}$ is the linear interpolant of g at the knots in T_κ, we have that

$$\widehat{g}'(t) = \frac{1}{\kappa_r - \kappa_{r-1}} \int_{\kappa_{r-1}}^{\kappa_r} g'(s)\, ds \text{ for all } t \in (\kappa_{r-1}, \kappa_r), \tag{A.8}$$

i.e., $\widehat{g}'$ is constant on each (κ_{r-1}, κ_r) and equal to the average value of g' on that same interval. Therefore, since g' is an increasing function, $\widehat{g}'(t) - g'(t) \leq (g'(\kappa_r) - g'(\kappa_{r-1}))$ for all $t \in (\kappa_{r-1}, \kappa_r)$. Hence, since $\kappa_r - \kappa_{r-1} \leq \frac{c_{\kappa,2}}{K_n}$ for all r, we also have

$$\sum_{r=\ell+1}^{i} \int_{\kappa_{r-1}}^{\kappa_r} \int_{\kappa_{r-1}}^{x} (\widehat{g}'(t) - g'(t))\, dt\, dx \leq \sum_{r=\ell+1}^{i} \int_{\kappa_{r-1}}^{\kappa_r} \int_{\kappa_{r-1}}^{x} (g'(\kappa_r) - g'(\kappa_{r-1}))\, dt\, dx$$

$$\leq \sum_{r=\ell+1}^{i} \frac{c_{\kappa,2}^2}{2K_n^2}(g'(\kappa_r) - g'(\kappa_{r-1})) = \frac{c_{\kappa,2}^2}{2K_n^2}(g'(\kappa_i) - g'(\kappa_\ell)).$$

Combining the above information, we see that for all $\kappa_i > \kappa_\ell$,

$$\int_{\kappa_\ell}^{\kappa_i} (\widehat{g}(x) - g(x))\, dx \leq \frac{c_{\kappa,2}^2}{2K_n^2}(g'(\kappa_i) - g'(\kappa_\ell)). \tag{A.9}$$

Define

$$a_{\ell,i} := \kappa_i - \left(\frac{g'(\kappa_i) - g'(\kappa_\ell)}{L}\right)^{\frac{1}{\gamma}} \in [\kappa_\ell, \kappa_i],$$

since $g \in H_L^{1+\gamma}$. Note that by the properties of $g \in \mathcal{S}_{2,H}(1+\gamma, L)$,

$$\begin{aligned} g(\kappa_i) - h(\kappa_i, \kappa_\ell) &= \int_{\kappa_\ell}^{\kappa_i} g'(x) - g'(\kappa_\ell)\, dx \geq \int_{a_{\ell,i}}^{\kappa_i} g'(x) - g'(\kappa_\ell)\, dx \\ &\geq \int_{a_{\ell,i}}^{\kappa_i} (g'(\kappa_i) - g'(\kappa_\ell)) - (g'(\kappa_i) - g'(x))\, dx \\ &\geq \int_{a_{\ell,i}}^{\kappa_i} (g'(\kappa_i) - g'(\kappa_\ell)) - L(\kappa_i - x)^\gamma\, dx = \frac{\gamma}{1+\gamma} \frac{(g'(\kappa_i) - g'(\kappa_\ell))^{1+\frac{1}{\gamma}}}{L^{\frac{1}{\gamma}}}. \end{aligned}$$

Hence,

$$g'(\kappa_i) - g'(\kappa_\ell) \leq \left(L^{\frac{1}{\gamma}}\left(\frac{1+\gamma}{\gamma}\right)(g(\kappa_i) - h(\kappa_i, \kappa_\ell))\right)^{\frac{\gamma}{1+\gamma}} \leq L^{\frac{1}{1+\gamma}}(g(\kappa_i) - h(\kappa_i, \kappa_\ell))^{\frac{\gamma}{1+\gamma}}. \tag{A.10}$$

Combining (A.9) and (A.10), we have that

$$\int_{\kappa_\ell}^{\kappa_i} (\widehat{g}(x) - g(x))\, dx \leq \frac{L^{\frac{1}{1+\gamma}} c_{\kappa,2}^2}{2K_n^2}(g(\kappa_i) - h(\kappa_i, \kappa_\ell))^{\frac{\gamma}{1+\gamma}}, \tag{A.11}$$

for all κ_ℓ and κ_i with $\kappa_\ell < \kappa_i$. By a similar argument, (A.11) holds when $\kappa_\ell > \kappa_i$.

In what follows, we will show that (A.6) holds for all $j = 1, \dots, N$, when $N \geq 1$. Fix $j \in \{1, \dots, N\}$, and note $\widetilde{\tau}_{j-1} = \kappa_{i_1^*}$ and $\tau_j = \kappa_{i_2^*}$ for some $i_1^*, i_2^* \in \mathbb{N}$. We have that

$$\int_{\tau_{j-1}}^{\tau_j} (\widehat{g} - g)(x)\, dx = \int_{\tau_{j-1}}^{\kappa_{i_1^*-1}} (\widehat{g} - g)(x)\, dx + \int_{\kappa_{i_1^*-1}}^{\kappa_{i_1^*}} (\widehat{g} - g)(x)\, dx + \int_{\kappa_{i_1^*}}^{\kappa_{i_2^*-1}} (\widehat{g} - g)(x)\, dx + \int_{\kappa_{i_2^*-1}}^{\tau_j} (\widehat{g} - g)(x)\, dx.$$

and will now bound each of the four quantities on the right hand side of this equation.

(i) We have that $\tau_{j-1} \leq \kappa_{i_1^*-1}$, since $\tau_{j-1} < \kappa_{i_1^*} = \widetilde{\tau}_{j-1}$. Hence,

$$\int_{\tau_{j-1}}^{\kappa_{i_1^*-1}} (\widehat{g} - g)(x)\, dx \leq \frac{L^{\frac{1}{1+\gamma}} c_{\kappa,2}^2}{2K_n^2} (g(\kappa_i) - h(\kappa_i, \kappa_\ell))^{\frac{\gamma}{1+\gamma}} \leq \frac{L c_{\kappa,2}^{2+\gamma}}{2K_n^{2+\gamma}} = \frac{1}{3} \frac{c_{\infty,3}}{K_n^{2+\gamma}}, \quad \text{(A.12)}$$

via the choice of $\widetilde{\tau}_{j-1}$ in Step 2 of Algorithm 2 and (A.11).

(ii) For any $i = 1, \dots, K_n$, let $\kappa_{i-1/2} := \frac{\kappa_{i-1}+\kappa_i}{2}$. Then, for any such i, we have $g(\kappa_{i-1}) = \widehat{g}(\kappa_{i-1})$, $g(\kappa_i) = \widehat{g}(\kappa_i)$, and $\widehat{g}'(x) \in [g'(\kappa_{i-1}), g'(\kappa_i)]$ on (κ_{i-1}, κ_i), since $\widehat{g}$ is the linear interpolant of g at the knots in T_κ, and g' is increasing. Therefore,

$$\begin{aligned}
\int_{\kappa_{i-1}}^{\kappa_i} (\widehat{g} - g)(x)\, dx &= \int_{\kappa_{i-1}}^{\kappa_{i-\frac{1}{2}}} (\widehat{g} - g)(x)\, dx + \int_{\kappa_{i-\frac{1}{2}}}^{\kappa_i} (\widehat{g} - g)(x)\, dx \\
&= \int_{\kappa_{i-1}}^{\kappa_{i-\frac{1}{2}}} \int_{\kappa_{i-1}}^{t} (\widehat{g} - g)'(t)\, dt\, dx + \int_{\kappa_{i-\frac{1}{2}}}^{\kappa_i} \int_{t}^{\kappa_i} (\widehat{g} - g)'(t)\, dt\, dx \\
&\leq \int_{\kappa_{i-1}}^{\kappa_{i-\frac{1}{2}}} \int_{\kappa_{i-1}}^{t} (g(\kappa_i) - g(\kappa_{i-1}))\, dt\, dx + \int_{\kappa_{i-\frac{1}{2}}}^{\kappa_i} \int_{t}^{\kappa_i} (g(\kappa_i) - g(\kappa_{i-1}))\, dt\, dx \\
&\leq \int_{\kappa_{i-1}}^{\kappa_{i-\frac{1}{2}}} \int_{\kappa_{i-1}}^{t} L \left(\frac{c_{\kappa,2}}{K_n} \right)^{\gamma} dt\, dx + \int_{\kappa_{i-\frac{1}{2}}}^{\kappa_i} \int_{t}^{\kappa_i} L \left(\frac{c_{\kappa,2}}{K_n} \right)^{\gamma} dt\, dx \\
&\leq 2L \left(\frac{c_{\kappa,2}}{K_n} \right)^{\gamma} \frac{c_{\kappa,2}^2}{8K_n^2} = \frac{L}{4} \left(\frac{c_{\kappa,2}}{K_n} \right)^{2+\gamma} = \frac{1}{6} \frac{c_{\infty,3}}{K_n^{2+\gamma}}.
\end{aligned} \quad \text{(A.13)}$$

Setting $i = i_1^*$ gives us that $\int_{\kappa_{i_1^*-1}}^{\kappa_{i_1^*}} \widehat{g}(x) - g(x)\, dx \leq \frac{1}{6} \frac{c_{\infty,3}}{K_n^{2+\gamma}}$.

(iii) Similar to (i), we have $\kappa_{i_1^*} = \widetilde{\tau}_{j-1} < \tau_j = \kappa_{i_2^*}$, so $\kappa_{i_1^*} \leq \kappa_{i_2^*-1}$, and

$$\int_{\kappa_{i_1^*}}^{\kappa_{i_2^*-1}} \widehat{g}(x) - g(x)\,dx \leq \frac{L^{\frac{1}{1+\gamma}} c_{\kappa,2}^2}{2K_n^2} (g(\kappa_{i_1^*}) - h(\kappa_{i_1^*}, \kappa_{i_2^*-1}))^{\frac{\gamma}{1+\gamma}} \leq \frac{1}{3}\frac{c_{\infty,3}}{K_n^{2+\gamma}}.$$

(iv) Setting $i = i_2^*$ in (A.13) gives us that $\int_{\kappa_{i_2^*-1}}^{\tau_j} \widehat{g}(x) - g(x)\,dx \leq \frac{1}{6}\frac{c_{\infty,3}}{K_n^{2+\gamma}}$, since $\tau_j = \kappa_{i_2^*}$.

Combining (i)-(iv), and the fact that $\widehat{g} \geq g$, we have that (A.6) holds.

Next, we will show that (A.7) holds, by considering the following three different cases.

Case 1: Algorithm 2 is terminated at Step 2. In this case, we have $g(\kappa_i) - h(\kappa_i, \tau_N) < \frac{c_2^*}{K_n^{1+\gamma}}$ for all $\kappa_i \geq \tau_N$ including $\kappa_{K_n} = 1$, so

$$\int_{\tau_N}^{1} (\widehat{g} - g)(x)\,dx \leq \frac{L^{\frac{1}{1+\gamma}} c_{\kappa,2}^2}{2K_n^2} (g(1) - h(1, \tau_N))^{\frac{\gamma}{1+\gamma}} \leq \frac{L c_{\kappa,2}^{2+\gamma}}{2K_n^{2+\gamma}} < \frac{c_{\infty,3}}{K_n^{2+\gamma}}.$$

Case 2: Algorithm 2 is terminated at Step 3. In this case, $\widetilde{\tau}_N = \kappa_{i_1^*}$ for some $i_1^* \in \mathbb{N}$ and $g(\widetilde{\tau}_N) - h(\widetilde{\tau}_N, \kappa_i) \leq \frac{c_2^*}{K_n^{1+\gamma}}$ for all $\kappa_i \geq \widetilde{\tau}_N$, including $\kappa_{K_n} = 1$. Note that

$$\begin{aligned}\int_{\tau_N}^{1} \widehat{g}(x) - g(x)\,dx = \int_{\tau_N}^{\kappa_{i_1^*-1}} \widehat{g}(x) - g(x)\,dx + \int_{\kappa_{i_1^*-1}}^{\kappa_{i_1^*}} \widehat{g}(x) - g(x)\,dx \\ + \int_{\kappa_{i_1^*}}^{\kappa_{K_n}} \widehat{g}(x) - g(x)\,dx.\end{aligned}$$

Using an argument similar to that in (A.12), we have that $\int_{\tau_N}^{\kappa_{i_1^*-1}} (\widehat{g} - g)(x)\,dx \leq \frac{1}{3}\frac{c_{\infty,3}}{K_n^{2+\gamma}}$, and by (A.13), we have that $\int_{\kappa_{i_1^*-1}}^{\kappa_{i_1^*}} (\widehat{g} - g)(x)\,dx \leq \frac{1}{6}\frac{c_{\infty,3}}{K_n^{2+\gamma}}$. Finally, since $g(\kappa_{i_1^*}) - h(\kappa_{i_1^*}, 1) < \frac{c_2^*}{K_n^{1+\gamma}}$, we have that

$$\int_{\kappa_{i_1^*}}^{1} \widehat{g}(x) - g(x)\,dx \leq \frac{L^{\frac{1}{1+\gamma}} c_{\kappa,2}^2}{2K_n^2} \left(g(\kappa_{i_1^*}) - h(\kappa_{i_1^*}, 1)\right)^{\frac{\gamma}{1+\gamma}} \leq \frac{L c_{\kappa,2}^{2+\gamma}}{2K_n^{2+\gamma}} = \frac{1}{3}\frac{c_{\infty,3}}{K_n^{2+\gamma}}.$$

From all of this, we can conclude that $\int_{\tau_N}^{1} \widehat{g}(x) - g(x)\, dx \leq \frac{5}{6}\frac{c_{\infty,3}}{K_n^{2+\gamma}} < \frac{c_{\infty,3}}{K_n^{2+\gamma}}$.

Case 3: Algorithm 2 is terminated at Step 4. We have that $\tau_N = 1$, so $\int_{\tau_N}^{1} \widehat{g}(x) - g(x)\, dx = 0 \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$.

This completes the proof of (A.7). □

Now that we have chosen the intervals $[\tau_{j-1}, \tau_j]$, $j = 1, \dots, N$ and proven Lemma A.2.1, we will construct piecewise linear continuous convex functions $\grave{g}_j$, on each $[\tau_{j-1}, \tau_j]$, which will be later used in the construction of $\widetilde{g}$.

A.3 Construction of $\widetilde{g}$: the $\grave{g}_j$'s

In the previous section, we chose points $\tau_0, \tau_1, \dots, \tau_N \in T_\kappa$. In this section, we will define continuous piecewise linear convex functions $\grave{g}_j : [\tau_{j-1}, \tau_j] \to \mathbb{R}$ for each $j = 1, \dots, N$. In order to do this, we must first identify certain knots in $[\tau_{j-1}, \tau_j] \cap T_\kappa$ that are needed to construct $\grave{g}_j$:

(i) Let $\tau_{j-1}^{(1)} \in T_\kappa$ be the knot immediately to the left of $\widetilde{\tau}_{j-1}$, i.e., if $\widetilde{\tau}_{j-1} = \kappa_i$, then $\tau_{j-1}^{(1)} = \kappa_{i-1}$.

(ii) Observe that $g(x) - h(x, \tau_j)$ increases as $x \leq \tau_j$ decreases by (A.4). Let $\tau_{j-1}^{(2)}$ be the largest $\kappa_i \in T_\kappa$ with $\kappa_i < \tau_j$, such that $g(\kappa_i) - h(\kappa_i, \tau_j) \geq \frac{c_2^*}{K_n^{1+\gamma}}$.

(iii) Finally, let $\tau_{j-1}^{(3)}$ be the knot in T_κ immediately to the right of $\tau_{j-1}^{(2)}$.

Note that for each j, we have $\tau_{j-1} \leq \tau_{j-1}^{(1)} < \widetilde{\tau}_{j-1} \leq \tau_{j-1}^{(2)} < \tau_{j-1}^{(3)} \leq \tau_j$. We define each $\grave{g}_j$ such that

$$\grave{g}_j(x) := \begin{cases} h(x, \tau_{j-1}) & \text{if } x \in [\tau_{j-1}, \tau_{j-1}^{(1)}) \\ h(\tau_{j-1}^{(1)}, \tau_{j-1}) + \left(g(\widetilde{\tau}_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}} - h(\tau_{j-1}^{(1)}, \tau_{j-1}) \right) \frac{x - \tau_{j-1}^{(1)}}{\widetilde{\tau}_{j-1} - \tau_{j-1}^{(1)}} & \text{if } x \in [\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}) \\ \widehat{g}(x) - \frac{c_2^*}{K_n^{1+\gamma}} & \text{if } x \in [\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}] \\ h(\tau_{j-1}^{(3)}, \tau_j) + \left(g(\tau_{j-1}^{(2)}) - \frac{c_2^*}{K_n^{1+\gamma}} - h(\tau_{j-1}^{(3)}, \tau_j) \right) \frac{\tau_{j-1}^{(3)} - x}{\tau_{j-1}^{(3)} - \tau_{j-1}^{(2)}} & \text{if } x \in (\tau_{j-1}^{(2)}, \tau_{j-1}^{(3)}] \\ h(x, \tau_j) & \text{if } x \in (\tau_{j-1}^{(3)}, \tau_j], \end{cases} \tag{A.14}$$

where we note that $[\tau_{j-1}, \tau_{j-1}^{(1)})$, $(\tau_{j-1}^{(3)}, \tau_j]$ may be empty, and $[\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}]$ may contain only a single point. An illustration of constructing $\grave{g}_j$ is given in Figure A.3.

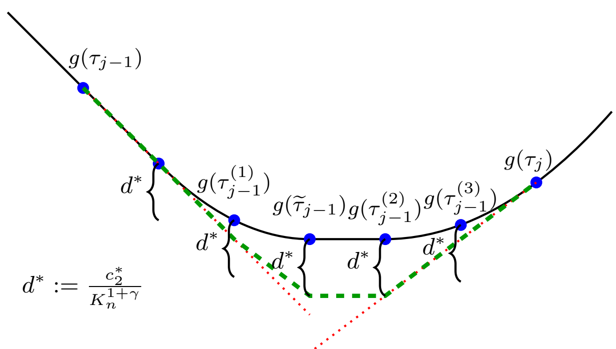


Figure A.3: Construction of $\grave{g}_j$ (dashed line).

As discussed in Section A.1, the goal in constructing each of the $\grave{g}_j$'s is that each $\grave{g}_j$ is a continuous, convex, piecewise linear function with knots in $[\tau_{j-1}, \tau_j] \cap T_\kappa$, such that $\int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(x)\, dx \leq 0$, and $\int_{\tau_{j-1}}^{x} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \geq 0]}(t)\, dt \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$ for all $x \in [\tau_{j-1}, \tau_j]$. Heuristically, $\grave{g}_j$ should be on average below g more than it is above g; it is possible that $\grave{g}_j$ may be below g on all of (τ_{j-1}, τ_j). We choose $\grave{g}_j$ in this way, so that later on, we may construct $\widetilde{g}_j$ as a weighted average of $\grave{g}_j$ and $\widehat{g}$ on $[\tau_{j-1}, \tau_j]$; since $\widehat{g}$ satisfies

$\int_{\tau_{j-1}}^{\tau_j} (\widehat{g} - g)(x)\, dx \geq 0$, we may choose a suitable weight so that $\int_{\tau_{j-1}}^{\tau_j} (\widetilde{g}_j - g)(t)\, dt = 0$. The next two Lemmas establish the desired properties of the $\grave{g}_j$'s.

Lemma A.3.1. *For each $j \in \{1, \ldots, N\}$, the function $\grave{g}_j$ is piecewise linear with knots in $T_\kappa \cap [\tau_{j-1}, \tau_j]$, continuous, and convex on $[\tau_{j-1}, \tau_j]$.*

Proof. Certainly $\grave{g}_j$ is a piecewise linear function with knots in $T_\kappa \cap [\tau_{j-1}, \tau_j]$, as $h(\cdot, \tau_{j-1})$ and $h(\cdot, \tau_j)$ are both linear, and $\widehat{g}$ is the linear interpolant of g with knots in T_κ.

To see that $\grave{g}_j$ is continuous, first observe that $\grave{g}_j$ is continuous on each of $[\tau_{j-1}, \tau_{j-1}^{(1)})$, $(\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1})$, $(\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)})$, $(\tau_{j-1}^{(2)}, \tau_{j-1}^{(3)})$, and $(\tau_{j-1}^{(3)}, \tau_j]$, some of which may have empty interior. By noting that $\widehat{g}(\widetilde{\tau}_{j-1}) = g(\widetilde{\tau}_{j-1})$, $\widehat{g}(\tau_{j-1}^{(2)}) = g(\tau_{j-1}^{(2)})$, and substituting in the endpoints of these subintervals of $[\tau_{j-1}, \tau_j]$, we can see that $\grave{g}_j$ is continuous on all of $[\tau_{j-1}, \tau_j]$ as well.

Finally, we must show that $\grave{g}_j$ is convex on $[\tau_{j-1}, \tau_j]$. This is equivalent to showing that the slopes of the line segments forming $\grave{g}_j$ increase when going from left to right on $[\tau_{j-1}, \tau_j]$. Since $\grave{g}_j$ is linear (and thus convex) on each of $[\tau_{j-1}, \tau_{j-1}^{(1)}]$, $[\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}]$, $[\tau_{j-1}^{(2)}, \tau_{j-1}^{(3)}]$, and $[\tau_{j-1}^{(3)}, \tau_j]$, as well as convex on $[\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}]$, the slopes of the line segments forming $\grave{g}_j$ increase when going from left to right on each of these subintervals of $[\tau_{j-1}, \tau_j]$. Therefore, it is sufficient to show that the slope of the line segment immediately to the left of each $\kappa_i = \tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}, \tau_{j-1}^{(3)}$ is less than or equal to the slope of the corresponding line segment immediately to the right of each of these points, i.e., that $(\grave{g}_j)'_-(\kappa_i) \leq (\grave{g}_j)'_+(\kappa_i)$ for each $\kappa_i = \tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}, \tau_{j-1}^{(3)}$. We establish this inequality for each of these points. (Note that we assume that $[\tau_{j-1}, \tau_{j-1}^{(1)}]$, $[\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}]$, and $[\tau_{j-1}^{(3)}, \tau_j]$ all have nonempty interior. If this is not the case, similar arguments can be made.)

(i) By (A.14), $(\grave{g}_j)'_-(\tau^{(1)}_{j-1}) = \frac{d}{dx}\left[h(x,\tau_{j-1})\right]\big|_{\tau^{(1)}_{j-1}} = g'(\tau_{j-1})$. Likewise by (A.14) and the choice of $\widetilde{\tau}_{j-1}$ via Algorithm 2,

$$\begin{aligned}
(\grave{g}_j)'_+(\tau^{(1)}_{j-1}) &= \frac{g(\widetilde{\tau}_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}} - h(\tau^{(1)}_{j-1},\tau_{j-1})}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} \\
&= \frac{g(\widetilde{\tau}_{j-1}) - g(\tau_{j-1}) - g'(\tau_{j-1})(\tau^{(1)}_{j-1} - \tau_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}}}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} \\
&= \frac{g(\widetilde{\tau}_{j-1}) - g(\tau_{j-1}) - g'(\tau_{j-1})(\widetilde{\tau}_{j-1} - \tau_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}}}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} + g'(\tau_{j-1}) \\
&= \frac{g(\widetilde{\tau}_{j-1}) - h(\widetilde{\tau}_{j-1},\tau_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}}}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} + g'(\tau_{j-1}) \\
&\geq g'(\tau_{j-1}) = (\grave{g}_j)'_-(\tau^{(1)}_{j-1}).
\end{aligned}$$

(ii) Let κ_p be the knot immediately to the right of $\widetilde{\tau}_{j-1}$, so that $\widetilde{\tau}_{j-1} = \kappa_{p-1}$. Then by (A.8) and the fact that g' is an increasing function,

$$\begin{aligned}
(\grave{g}_j)'_+(\widetilde{\tau}_{j-1}) &= \widehat{g}'_+(\widetilde{\tau}_{j-1}) = \frac{1}{\kappa_p - \widetilde{\tau}_{j-1}} \int_{\widetilde{\tau}_{j-1}}^{\kappa_p} g'(x)\,dx \geq g'(\widetilde{\tau}_{j-1}) \geq \frac{g(\widetilde{\tau}_{j-1}) - g(\tau^{(1)}_{j-1})}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} \\
&\geq \frac{g(\widetilde{\tau}_{j-1}) - g(\tau^{(1)}_{j-1}) + g(\tau^{(1)}_{j-1}) - h(\tau^{(1)}_{j-1},\tau_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}}}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} \\
&= \frac{g(\widetilde{\tau}_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}} - h(\tau^{(1)}_{j-1},\tau_{j-1})}{\widetilde{\tau}_{j-1} - \tau^{(1)}_{j-1}} = (\grave{g}_j)'_-(\widetilde{\tau}_{j-1}).
\end{aligned}$$

(iii) Let $\kappa_p \in T_\kappa$ be the knot immediately to the left of $\tau^{(2)}_{j-1}$, so that $\tau^{(2)}_{j-1} = \kappa_{p+1}$. Then, by an argument similar to (ii),

$$\begin{aligned}
(\grave{g}_j)'_-(\tau^{(2)}_{j-1}) &= \widehat{g}'_-(\tau^{(2)}_{j-1}) = \frac{1}{\tau^{(2)}_{j-1} - \kappa_p} \int_{\kappa_p}^{\tau^{(2)}_{j-1}} g'(x)\,dx \leq g'(\tau^{(2)}_{j-1}) \\
&\leq \frac{g(\tau^{(3)}_{j-1}) - g(\tau^{(2)}_{j-1})}{\tau^{(3)}_{j-1} - \tau^{(2)}_{j-1}} \leq \frac{g(\tau^{(3)}_{j-1}) - g(\tau^{(2)}_{j-1}) - g(\tau^{(3)}_{j-1}) + h(\tau^{(3)}_{j-1},\tau_j) + \frac{c_2^*}{K_n^{1+\gamma}}}{\tau^{(3)}_{j-1} - \tau^{(2)}_{j-1}}
\end{aligned}$$

$$= -\frac{g(\tau_{j-1}^{(2)}) - \frac{c_2^*}{K_n^{1+\gamma}} - h(\tau_{j-1}^{(3)}, \tau_j)}{\tau_{j-1}^{(3)} - \tau_{j-1}^{(2)}} = (\grave{g}_j)'_+(\tau_{j-1}^{(2)}).$$

(iv) Finally, we have that

$$\begin{aligned}
(\grave{g}_j)'_-(\tau_{j-1}^{(3)}) &= -\frac{g(\tau_{j-1}^{(2)}) - \frac{c_2^*}{K_n^{1+\gamma}} - h(\tau_{j-1}^{(3)}, \tau_j)}{\tau_{j-1}^{(3)} - \tau_{j-1}^{(2)}} \\
&= -\frac{g(\tau_{j-1}^{(2)}) - g(\tau_j) - g'(\tau_j)(\tau_{j-1}^{(2)} - \tau_j) - \frac{c_2^*}{K_n^{1+\gamma}}}{\tau_{j-1}^{(3)} - \tau_{j-1}^{(2)}} + g'(\tau_j) \\
&= -\frac{g(\tau_{j-1}^{(2)}) - h(\tau_{j-1}^{(2)}, \tau_j) - \frac{c_2^*}{K_n^{1+\gamma}}}{\tau_{j-1}^{(3)} - \tau_{j-1}^{(2)}} + g'(\tau_j) \le g'(\tau_j) = (\grave{g}_j)'_+(\tau_{j-1}^{(3)}).
\end{aligned}$$

We have established that $(\grave{g}_j)'_-(\kappa_i) \le (\grave{g}_j)'_+(\kappa_i)$ for each $\kappa_i = \tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}, \tau_{j-1}^{(3)}$, which completes the proof of this Lemma. □

Lemma A.3.2. *For all $j = 1, \ldots, N$, we have*

$$\int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t)\mathbf{1}_{[\grave{g}_j - g \ge 0]}(t)\, dt \le \frac{c_{\infty,3}}{K_n^{2+\gamma}} \tag{A.15}$$

and also,

$$\int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t)\, dt \le 0. \tag{A.16}$$

Proof. On $[\tau_{j-1}, \tau_{j-1}^{(1)}]$, we have that $\grave{g}_j(x) = h(x, \tau_{j-1}^{(1)}) \le g(x)$ by (A.3), so $(\grave{g}_j - g)(x) \le 0$ for all $x \in [\tau_{j-1}, \tau_{j-1}^{(1)}]$. Similarly, $(\grave{g}_j - g)(x) \le 0$ for all $x \in [\tau_{j-1}^{(3)}, \tau_j]$. Additionally, for any $x \in [\kappa_{i-1}, \kappa_i]$,

$$\begin{aligned}
0 \le \widehat{g}(x) - g(x) &= \min\left\{\int_{\kappa_{i-1}}^{x} (\widehat{g} - g)'(t)\, dt, \int_{x}^{\kappa_i} (\widehat{g} - g)'(t)\, dt\right\} \\
&\le (g'(\kappa_i) - g'(\kappa_{i-1}))\frac{\kappa_i - \kappa_{i-1}}{2} \le \frac{c_2^*}{K_n^{1+\gamma}},
\end{aligned}$$

so we have that for all $x \in [\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}]$,

$$\grave{g}_j(x) - g(x) = \widehat{g}(x) - g(x) - \frac{c_2^*}{K_n^{1+\gamma}} \leq 0.$$

Consider $(\grave{g}_j - \widehat{g})(t)$ on $[\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}]$. When restricted to $[\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}]$, $(\grave{g}_j - \widehat{g})(t)$ is linear, with

$$(\grave{g}_j - \widehat{g})(\tau_{j-1}^{(1)}) = h(\tau_{j-1}^{(1)}, \tau_{j-1}) - g(\tau_{j-1}^{(1)}) \in \left(-\frac{c_2^*}{K_n^{1+\gamma}}, 0 \right],$$

by (A.3) and the choice of $\tau_{j-1}^{(1)}$. Furthermore,

$$(\grave{g}_j - \widehat{g})(\widetilde{\tau}_{j-1}) = \widehat{g}(\widetilde{\tau}_{j-1}) - \frac{c_2^*}{K_n^{1+\gamma}} - \widehat{g}(\widetilde{\tau}_{j-1}) = -\frac{c_2^*}{K_n^{1+\gamma}}.$$

Hence, $|\grave{g}_j - \widehat{g}|(t) \leq \frac{c_2^*}{K_n^{1+\gamma}}$ on $[\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}]$, and by (A.13),

$$\begin{aligned} \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} |\grave{g}_j - g|(t)\, dt &\leq \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} |\grave{g}_j - \widehat{g}|(t)\, dt + \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} |\widehat{g} - g|(t)\, dt \\ &\leq \frac{c_{\kappa,2} c_2^*}{K_n^{2+\gamma}} + \frac{1}{6} \frac{c_{\infty,3}}{K_n^{2+\gamma}} < \frac{1}{2} \frac{c_{\infty,3}}{K_n^{2+\gamma}}. \end{aligned}$$

By a similar argument, $\int_{\tau_{j-1}^{(2)}}^{\tau_{j-1}^{(3)}} |\grave{g}_j - g|(t)\, dt < \frac{1}{2} \frac{c_{\infty,3}}{K_n^{2+\gamma}}$. Combining the above arguments, we have that

$$\begin{aligned} &\int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \geq 0]}(t)\, dt \\ &\quad = \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \geq 0]}(t)\, dt + \int_{\tau_{j-1}^{(2)}}^{\tau_{j-1}^{(3)}} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \geq 0]}(t)\, dt \\ &\quad \leq \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} |\grave{g}_j - g|(t)\, dt + \int_{\tau_{j-1}^{(2)}}^{\tau_{j-1}^{(3)}} |\grave{g}_j - g|(t)\, dt < \frac{1}{2} \frac{c_{\infty,3}}{K_n^{2+\gamma}} + \frac{1}{2} \frac{c_{\infty,3}}{K_n^{2+\gamma}} = \frac{c_{\infty,3}}{K_n^{2+\gamma}}, \end{aligned}$$

giving us (A.15).

Recall from the above discussion that when restricted to $[\tau_{j-1}^{(1)}, \widetilde{\tau}_{j-1}]$, $(\grave{g}_j - \widehat{g})(t)$ is linear with $(\grave{g}_j - \widehat{g})(\tau_{j-1}^{(1)}) \leq 0$, and $(\grave{g}_j - \widehat{g})(\widetilde{\tau}_{j-1}) = -\frac{c_2^*}{K_n^{1+\gamma}}$. Thus,

$$\int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} (\grave{g}_j - \widehat{g})(t)\, dt = \left(\widetilde{\tau}_{j-1} - \tau_{j-1}^{(1)}\right) \frac{(\grave{g}_j - \widehat{g})(\tau_{j-1}^{(1)}) + (\grave{g}_j - \widehat{g})(\widetilde{\tau}_{j-1})}{2}$$
$$\leq -\frac{1}{2} \frac{c_{\kappa,2} c_2^*}{K_n^{2+\gamma}} = -\frac{1}{6} \frac{c_{\infty,3}}{K_n^{2+\gamma}},$$

which then gives us via (A.13) that

$$\int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} (\grave{g}_j - g)(t)\, dt = \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} (\grave{g}_j - \widehat{g})(t)\, dt + \int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} (\widehat{g} - g)(t)\, dt$$
$$\leq -\frac{1}{6} \frac{c_{\infty,3}}{K_n^{2+\gamma}} + \frac{1}{6} \frac{c_{\infty,3}}{K_n^{2+\gamma}} = 0$$

By a similar argument, $\int_{\tau_{j-1}^{(2)}}^{\tau_{j-1}^{(3)}} (\grave{g}_j - g)(t)\, dt \leq 0$. Hence, since both $\int_{\tau_{j-1}^{(1)}}^{\widetilde{\tau}_{j-1}} (\grave{g}_j - g)(t)\, dt \leq 0$, and $\int_{\tau_{j-1}^{(2)}}^{\tau_{j-1}^{(3)}} (\grave{g}_j - g)(t)\, dt \leq 0$, while $\grave{g}_j \leq g$ on $[\tau_{j-1}, \tau_{j-1}^{(1)}]$, $[\widetilde{\tau}_{j-1}, \tau_{j-1}^{(2)}]$, and $[\tau_{j-1}^{(3)}, \tau_j]$, we have (A.16). $\square$

Now that we have constructed the $\grave{g}_j$'s and established some properties of these functions via Lemmas A.3.1 and A.3.2, we will utilize these functions in the next section to construct $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$

A.4 Construction of $\widetilde{g}$ and f_B

We are now ready to construct $\widetilde{g}$. For each $j = 1, \ldots, N$, let $\phi_j : [0,1] \to \mathbb{R}$ be given by

$$\phi_j(r) := r \int_{\tau_{j-1}}^{\tau_j} (\widehat{g} - g)(t)\, dt + (1 - r) \int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t)\, dt. \tag{A.17}$$

For each j, we have that $\phi_j(0) = \int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t)\,dt \le 0$ by (A.16) and $\phi_j(1) = \int_{\tau_{j-1}}^{\tau_j} (\widehat{g} - g)(t)\,dt \ge 0$, since $\widehat{g} \ge g$ is the linear interpolant of g, a convex function. Additionally, ϕ_j is continuous on $[0,1]$. By the Intermediate Value Theorem, there exists $r_j \in [0,1]$ satisfying $\phi_j(r_j) = 0$. Define $\widetilde{g} : [0,1] \to \mathbb{R}$ such that

$$\widetilde{g}(t) := \begin{cases} \widetilde{g}_j(t) := r_j \widehat{g}(t) + (1-r_j)\grave{g}_j(t) & \text{for all } t \in [\tau_{j-1}, \tau_j),\ j = 1, \ldots, N \\ \widehat{g}(t) & \text{for all } t \in [\tau_N, 1]. \end{cases} \tag{A.18}$$

The following lemma will allow us to establish Proposition 4.2.1.

Lemma A.4.1. *The function $\widetilde{g}$ is continuous and convex on $[0,1]$. Also, $\widetilde{g}$ is a piecewise linear function with knot sequence T_κ. Hence, $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$. Finally, for all $x \in [0,1]$,*

$$\left| \int_0^x (\widetilde{g} - g)(t)\,dt \right| \le \frac{c_{\infty,3}}{K_n^{2+\gamma}}. \tag{A.19}$$

Proof. To see that $\widetilde{g}$ is continuous on $[0,1]$, first note that $\widetilde{g}$ is continuous on $[\tau_0, \tau_1)$ as well as (τ_{j-1}, τ_j) for each $j = 2, \ldots, N$, and on $(\tau_N, 1]$. Define $r_{N+1} := 1$ and $\widetilde{g}_{N+1}(x) := \widehat{g}(x)$ for all $x \in [\tau_N, 1]$, if $\tau_N \ne 1$. To see that $\widetilde{g}$ is continuous at each τ_j, $j = 1, \ldots, N$, observe that (i) $\widehat{g}$ is continuous at each τ_j, with $\widehat{g}(\tau_j) = g(\tau_j)$, (ii) each $\grave{g}_j$ is left continuous at τ_j, with $\grave{g}_j(\tau_j) = g(\tau_j)$, and (iii) each $\grave{g}_{j+1}$ is right continuous at τ_j, with $\grave{g}_{j+1}(\tau_j) = g(\tau_j)$. Hence, $\widetilde{g}$ is continuous on all of $[0,1]$, as

$$\begin{aligned} \lim_{t \to \tau_j^-} \widetilde{g}(t) &= \lim_{t \to \tau_j^-} \left(r_j\, \widehat{g}(t) + (1-r_j)\grave{g}_j(t) \right) = g(\tau_j) \\ &= \lim_{t \to \tau_j^+} \left(r_{j+1}\, \widehat{g}(t) + (1-r_{j+1})\, \grave{g}_{j+1}(t) \right) = \lim_{t \to \tau_j^+} \widetilde{g}(t). \end{aligned}$$

By construction, on each $[\tau_{j-1}, \tau_j]$ and on $[\tau_N, 1]$, $\widetilde{g}$ is a convex (and thus linear) combination of the piecewise linear functions $\widehat{g}$ and $\grave{g}_j$, each with knot sequence T_κ. Therefore, $\widetilde{g}$ is a piecewise linear function with knot sequence T_κ.

Next, we will show that $\widetilde{g}$ is convex on $[0, 1]$. Note that $\widetilde{g}$ is convex on each $[\tau_{j-1}, \tau_j]$ and on $[\tau_N, 1]$, since (i) $\widehat{g}$ is convex, (ii) each $\grave{g}_j$ is convex on $[\tau_{j-1}, \tau_j]$ by Lemma A.3.1, and (iii) any convex (and thus, conic) combination of convex functions is convex. Since $\widetilde{g}$ is a continuous piecewise linear function, the convexity of $\widetilde{g}$ is equivalent to the line segments forming $\widetilde{g}$ having increasing slopes when moving from left to right on $[0, 1]$. Since we already have that $\widetilde{g}$ is convex on each $[\tau_{j-1}, \tau_j]$ and on $[\tau_N, 1]$, it is sufficient to show that the slope of the line segment immediately to the left of each τ_j is less than or equal to the slope of the corresponding line segment immediately to the right of that τ_j for each $j = 1, \ldots, N$, i.e., we must show that $\widetilde{g}'_-(\tau_j) \le \widetilde{g}'_+(\tau_j)$, for $j = 1, \ldots, N$. Fix $j \in \{1, \ldots, N-1\}$. Let $\kappa_{i^*} = \tau_j$, so that κ_{i^*-1} is the knot immediately to the left of κ_{i^*} and κ_{i^*+1} is the knot immediately to the right of κ_{i^*}. Using (A.8) and the fact that g' is an increasing function, we have that

$$\begin{aligned}
\widetilde{g}'_-(\tau_j) &= r_j \widehat{g}'_-(\tau_j) + (1 - r_j)(\grave{g}_j)'_-(\tau_j) = \frac{r_j}{\tau_j - \kappa_{i^*-1}} \int_{\kappa_{i^*-1}}^{\tau_j} g'(x)\,dx + (1 - r_j) g'(\tau_j) \\
&\le g'(\tau_j) \le \frac{r_{j+1}}{\kappa_{i^*+1} - \tau_j} \int_{\tau_j}^{\kappa_{i^*+1}} g'(x)\,dx + (1 - r_{j+1}) g'(\tau_j) \\
&= r_{j+1}\, \widehat{g}'_+(\tau_j) + (1 - r_{j+1})(\grave{g}_{j+1})'_+(\tau_j) = \widetilde{g}'_+(\tau_j).
\end{aligned}$$

Alternatively, if $j = N$ and $\tau_N < 1$, so that $\tau_N = \kappa_{i^*}$, then

$$\begin{aligned}
\widetilde{g}'_-(\tau_N) &= r_N\, \widehat{g}'_-(\tau_N) + (1 - r_N)(\grave{g}_N)'_-(\tau_N) \le r_N\, \widehat{g}'_+(\tau_N) + (1 - r_N) g'(\tau_N) \\
&\le r_N\, \widehat{g}'_+(\tau_N) + \frac{1 - r_N}{\kappa_{i^*+1} - \tau_N} \int_{\tau_N}^{\kappa_{i^*+1}} g'(x)\,dx = \widehat{g}'_+(\tau_N) = \widetilde{g}'_+(\tau_N).
\end{aligned}$$

Thus $\widetilde{g}'_-(\tau_j) \le \widetilde{g}'_+(\tau_j)$ for all $j = 1, \ldots, N$ and $\widetilde{g} \in \mathbb{S}^{T_\kappa}_{+,2}$ is convex on $[0, 1]$.

Finally, we show that (A.19) holds for all $x \in [0, 1]$. Let $x \in [0, 1]$. We have that $x \in [\tau_{j-1}, \tau_j)$ for some $j = 1, \ldots, N$, or $x \in [\tau_N, 1]$. Note that for any $j = 1, \ldots, N$,

$$
\begin{aligned}
0 &\le \left| \int_0^{\tau_j} (\widetilde{g}(t) - g(t))\, dt \right| \le \sum_{i=1}^{j} \left| \int_{\tau_{i-1}}^{\tau_i} (\widetilde{g}(t) - g(t))\, dt \right| \\
&= \sum_{i=1}^{j} \left| \int_{\tau_{i-1}}^{\tau_i} (r_i \widehat{g}(t) + (1 - r_i) \grave{g}_i(t) - g(t))\, dt \right| \\
&= \sum_{i=1}^{j} \left| r_i \int_{\tau_{i-1}}^{\tau_i} (\widehat{g}(t) - g(t))\, dt + (1 - r_i) \int_{\tau_{i-1}}^{\tau_i} (\grave{g}_i(t) - g(t))\, dt \right| = \sum_{i=1}^{j} |\phi_i(r_i)| = 0.
\end{aligned}
$$

Hence, if $x \in [\tau_{j-1}, \tau_j]$, for some $j = 1, \ldots, N$, then

$$
\begin{aligned}
&\left| \int_0^{x} (\widetilde{g}(t) - g(t))\, dt \right| = \left| \int_{\tau_{j-1}}^{x} (\widetilde{g}(t) - g(t))\, dt \right| \\
&\quad = \left| r_j \int_{\tau_{j-1}}^{x} (\widehat{g}(t) - g(t))\, dt + (1 - r_j) \int_{\tau_{j-1}}^{x} (\grave{g}_j(t) - g(t))\, dt \right| \\
&\quad = \Big| r_j \int_{\tau_{j-1}}^{x} (\widehat{g} - g)(t)\, dt + (1 - r_j) \int_{\tau_{j-1}}^{x} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \ge 0]}(t)\, dt \\
&\quad + (1 - r_j) \int_{\tau_{j-1}}^{x} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g < 0]}(t)\, dt \Big| \\
&\quad \le \max \Big\{ r_j \int_{\tau_{j-1}}^{x} (\widehat{g} - g)(t)\, dt + (1 - r_j) \int_{\tau_{j-1}}^{x} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \ge 0]}(t)\, dt, \\
&\qquad\qquad (1 - r_j) \int_{\tau_{j-1}}^{x} (g - \grave{g}_j)(t) \mathbf{1}_{[\grave{g}_j - g < 0]}(t)\, dt \Big\} \\
&\quad \le r_j \int_{\tau_{j-1}}^{\tau_j} (\widehat{g} - g)(t)\, dt + (1 - r_j) \int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \ge 0]}(t)\, dt \\
&\quad \le r_j \frac{c_{\infty,3}}{K_n^{2+\gamma}} + (1 - r_j) \frac{c_{\infty,3}}{K_n^{2+\gamma}} = \frac{c_{\infty,3}}{K_n^{2+\gamma}}.
\end{aligned}
$$

The second inequality in the above display follows from the fact that

$$
r_j \int_{\tau_{j-1}}^{\tau_j} (\widehat{g} - g)(t)\, dt + (1 - r_j) \int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t) \mathbf{1}_{[\grave{g}_j - g \ge 0]}(t)\, dt
$$

$$= -(1-r_j)\int_{\tau_{j-1}}^{\tau_j} (\grave{g}_j - g)(t)\mathbf{1}_{[\grave{g}_j - g<0]}(t)\,dt,$$

which in turn follows from the choice of r_j and the inequality $\widehat{g}(x) \geq g(x)$ for all $x \in [0,1]$.

Finally, if $x \in [\tau_N, 1]$, then by (A.7),

$$\left|\int_0^x (\widetilde{g}(t) - g(t))\,dt\right| = \left|\int_{\tau_N}^x (\widehat{g}(t) - g(t))\,dt\right| \leq \int_{\tau_N}^1 (\widehat{g}(t) - g(t))\,dt \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}.$$

$\square$

Let $f_B : [0,1] \to \mathbb{R}$ be given by $f_B(x) := f(0) + \int_0^x \widetilde{g}(t)\,dt$. Since $f_B(x) := f(0) + \int_0^x \widetilde{g}(t)\,d$, and $\widetilde{g} \in \mathbb{S}_{+,2}^{T_\kappa}$, we must have that $f_B \in \mathbb{S}_{+,3}^{T_\kappa}$. Additionally,

$$|f_B(x) - f(x)| = \left|f_B(0) - f(0) + \int_0^x (f_B - f)'(t)\,dt\right| = \left|\int_0^x (\widetilde{g} - g)(t)\,dt\right| \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}},$$

for all $x \in [0,1]$ via Lemma A.4.1. Thus, $\|f - f_B\|_\infty \leq \frac{c_{\infty,3}}{K_n^{2+\gamma}}$, completing the proof of Proposition 4.2.1.

BIBLIOGRAPHY

[1] A. Auslender and M. Teboulle. *Asymptotic Cones and Functions in Optimization and Variational Inequalities*. Springer-Verlag, Heidelberg, 2002.

[2] F. Balabdaoui and J.A. Wellner. Estimation of a k-monotone density: characterizations, consistency and minimax lower bounds. *Statistica Neerlandica*, Vol. 64(1), pp. 45–70, 2010.

[3] A.V. Balakrishnan. *Introduction to Optimization in a Hilbert Space*. Lecture Notes in Operations Research and Mathematical Systems, Vol. 42, Springer-Verlag, 1971.

[4] R.G. Bartle. *The Elements of Integration and Lebesgue Measure*. John Wiley & Sons, Inc., 1995.

[5] R.K. Beatson. Convex approximation by splines. *SIAM Journal on Mathematical Analysis*, Vol. 12(4) pp. 549–559, 1981.

[6] R.K. Beatson. Monotone and convex approximation by splines: error estimates and a curve fitting algorithm. *SIAM Journal on Numerical Analysis*, Vol. 19(6) pp. 1278–1285, 1982.

[7] P. Bellec and A. Tsybakov. Sharp oracle bounds for monotone and convex regression through aggregation. *arXiv preprint arXiv:1506.08724*.

[8] M. Birke and J. Dette. Estimating a convex function in nonparametric regression. *Scandinavian Journal of Statistics*, Vol. 34, pp. 384–404, 2007.

[9] M.K. Çamlibel, J.S. Pang, and J. Shen. Conewise linear systems: non-Zenoness and observability. *SIAM Journal on Control and Optimization*, Vol. 45(5), pp. 1769–1800, 2006.

[10] E. Cator. Adaptivity and optimality of the monotone least squares estimator. *Bernoulli*, Vol. 17(2), pp. 714–735, 2011.

[11] C.-S. Chee and Y. Wang. Least squares estimation of a k-monotone density function. *Computational Statistics and Data Analysis*, Vol. 74, pp. 209–216, 2014.

[12] R.W. Cottle, J.S. Pang, and R.E. Stone. *The Linear Complementarity Problem*, Academic Press Inc., (Cambridge 1992).

[13] T. Cover and J. Thomas. *Elements of Information Theory*. Wiley, 2005.

[14] C. de Boor. *A Practical Guide to Splines*. Springer, 2001.

[15] C. de Boor. The quasi–interpolant as a tool in elementary polynomial spline theory. *Approximation Theory*, pp. 269–276, 1973.

[16] R.A. DeVore. Monotone approximation by splines. *SIAM Journal on Mathematical Analysis*, Vol. 8 pp. 891–905, 1977.

[17] R.A. DeVore and G.G. Lorentz. *Constructive Approximation*. Springer, 1st edition, 1993.

[18] D. Donoho. Asymptotic minimax risk for sup-norm loss: solution via optimal recovery. *Probability Theory and Related Fields*, Vol. 99, pp. 145–170, 1994.

[19] A.L. Dontchev, H.-D. Qi, L. Qi, and H. Yin. A Newton method for shape-preserving spline interpolation. *SIAM Journal on Optimization*, Vol. 13(2), pp. 588–602, 2002.

[20] A.L. Dontchev, H.-D. Qi, and L. Qi. Quadratic convergence of Newton's method for convex interpolation and smoothing. *Constructive Approximation*, Vol. 19, pp. 123–143, 2003.

[21] L. Dümbgen, S. Freitag, and G. Jongbloed. Consistency of concave regression with an application to current-status data. *Mathematical Methods of Statistics*, Vol. 13(1), pp. 69–81, 2004.

[22] M. Egerstedt and C. Martin. *Control Theoretic Splines*. Princeton University Press, 2010.

[23] F. Facchinei and J.S. Pang. *Finite-Dimensional Variational Inequalities and Complementarity Problems*. Springer-Verlag, 2003.

[24] M. Gerdts and M. Kunkel. A nonsmooth Newton's method for discretized optimal control problems with state and control constraints. *Journal of Industrial and Management Optimization*, Vol. 4(2), pp. 247–280, 2008.

[25] A. Girard. Towards a multiresolution approach to linear control. *IEEE Trans. on Automatic Control*, Vol. 51(8), pp. 1261–1270, 2006.

[26] M.V. Golitschek. On the L_∞-norm of the orthogonal projector onto splines: A short proof of A. Shardin's theorem. *Journal of Approximation Theory*, Vol. 181, pp. 30–42, 2014.

[27] P. Groeneboom, F. Jongbloed, and J.A. Wellner. Estimation of a convex function: Characterizations and asymptotic theory. *Annals of Statistics*, Vol. 29(6), pp. 1653–1698, 2001.

[28] A. Guntuboyina and B. Sen. Covering numbers for convex functions. *IEEE Trans. on Information Theory*, Vol. 59(4), 1957–1965, 2013.

[29] A. Guntuboyina and B. Sen. Global risk bounds and adaptation in univariate convex regression. *Probability Theory and Related Fields*, Vol. 163(1-2), pp. 379–411, 2015.

[30] L. Han, M.K. Camlibel, J.-S. Pang, and W.P.M.H. Heemels. A unified numerical scheme for linear-quadratic optimal control problems with joint control and state constraints. *Optimization Methods and Software*, Vol. 27(4-5), pp. 761–799, 2012.

[31] P. Hanson and G. Pledger. Consistency in concave regression. *Annals of Statistics*, Vol. 4, pp.1038–1050, 1976.

[32] Y. Hu. Convexity preserving approximation by free knot splines. *SIAM Journal on Mathematical Analysis*, Vol. 22(4), pp. 1183–1191, 1991.

[33] A. Juditsky and A. Nazin. Information lower bounds for stochastic adaptive tracking problem under nonparametric uncertainty. *Proc. of the 36th IEEE Conf. Decision and Control*, pp. 3476–3477, San Diego, CA, 1997.

[34] A. Juditsky and A. Nazin. On minimax approach to non-parametric adaptive control. *International Journal of Adaptive Control and Signal Processing*, Vol. 15(2), pp. 153–168, 2001.

[35] H. Kano, M. Egerstedt, H. Nakata, and C.F. Martin. B-splines and control theory. *Applied Mathematics and Computation*, Vol. 145, pp. 265–288, 2003.

[36] H. Kano, H. Fujioka, and C.F. Martin. Optimal smoothing spline with constraints on its derivatives. *Proc. of the 49nd IEEE Conf. on Decision and Control*, pp. 6785–6790, 2010.

[37] J. Kiefer. Optimum rates for non-parametric density and regression estimates under order restrictions. In: Kallianpur, G., Krishnaiah, P. R., Ghosh, J.K. (Eds.), *Statistics and Probability*. North–Holland, Amsterdam, pp.419–428 1982.

[38] V.N. Konovalov and D. Leviatan. Estimates on the approximation of 3-monotone functions by 3-monotone quadratic splines. *East J. Approx*, Vol. 7, pp. 333–349, 2001.

[39] V.N. Konovalov and D. Leviatan. Shape preserving widths of Sobolev-type classes of s-monotone functions on a finite interval. *Isreal J. Math.* Vol. 133 (2003), 239-268.

[40] A.P. Korostelev and O. Korosteleva. *Mathematical Statistics: Asymptotic Minimax Theory*. American Mathematical Soc., 2011.

[41] S. Kullback. A lower bound for discrimination information in terms of variation. *IEEE Trans. on Information Theory*, Vol. 13, pp. 126–127, 1967.

[42] S. Lang. *Real and Functional Analysis*. Springer-Verlag, 3rd Edition, 1993.

[43] O. Lepski and A. Tsybakov. Asymptotically exact nonparametric hypothesis testing in sup-norm and at a fixed point. *Probability Theory and Related Fields*, Vol. 117, pp. 17–48, 2000.

[44] D.G. Luenberger. *Optimization by Vector Space Methods*. John Wiley & Sons Inc., 1969.

[45] E. Mammen. Nonparametric regression under qualitative smoothness assumptions. *Annnals of Statistics*, Vol. 19, pp. 741–759, 1991.

[46] C.A. Micchelli and F.I. Utreras. Smoothing and interploation in a convex subset of a Hilbert space. *SIAM Journal on Scientific and Statistical Computing*, Vol. 9(4), pp. 728–746, 1988.

[47] M. Nagahara, C.F. Martin, and Y. Yamamoto. Quadratic programming for monotone control theoretical splines. *Proc. of the SICE 2010 Annual Conference*, pp. 531–534, 2010.

[48] A. Nazin and V. Katkovnik. Minimax lower bound for time-tarying frequency estimation of harmonic signal. *IEEE Trans. on Signal Processing*, Vol. 46(12), pp. 3235–3245, 1998.

[49] A. Nemirovski. *Topics in Non-parametric Statistics*. Lecture on Probability Theory and Statistics. Berlin, Germany: Springer-Verlag, Vol. 1738, Lecture Notes in Mathematics, 2000.

[50] A. Nemirovski, B. Polyak, and A. Tsybakov. Convergence rate of nonparametric estimates of maximum-likelihood type. *Problems of of Information Transmission*, Vol. 21(4), pp. 17–33, 1985.

[51] J.K. Pal. Spiking problem in monotone regression: Penalized residual sum of squares. *Statistics and Probability Letters*, Vol. 78(12), pp. 1548–1556, 2008.

[52] J.K. Pal and M. Woodroofe. Large sample properties of shape restricted regression estimators with smoothness adjustments. *Statistica Sinica*, Vol. 17(4), pp. 1601–1616, 2007.

[53] J.S. Pang. Newton's method for B-differentiable equations. *Mathematics of Operations Research*, Vol. 15, pp. 311–341, 1990.

[54] J.S. Pang and J. Shen. Strongly regular differential variational systems. *IEEE Trans. on Automatic Control*, Vol. 52(2), pp. 242–255, 2007.

[55] J.S. Pang and D. Stewart. Differential variational inequalities. *Mathematical Programming Series A*, Vol. 113, pp. 345–424, 2008.

[56] J.S. Pang and D. Stewart. Solution dependence on initial conditions in differential variational inequalities. *Mathematical Programming Series B*, Vol. 116, pp. 429–460, 2009.

[57] D. Papp, And F. Alizadeh. Shape constrained estimations using nonnegative splines. *Journal of Computational and Graphical Statistics*, Vol. 23(1), pp. 211–231, 2014.

[58] A.V. Prymak. Three-convex approximation by quadratic splines with arbitrary fixed knots. *East J. Approx*, Vol. 8(2), pp. 185–196, 2002.

[59] C.V. Rao, J.B. Rawlings, and J.H. Lee. Constrained linear state estimation – a moving horizon approach. *Automatica*, Vol. 37(10), pp. 1619–1628, 2001.

[60] M. Renardy and R.C. Rogers. *An Introduction to Partial Differential Equations*. Springer, 2nd Edition, 2004.

[61] T. Robertson, F.T. Wright, and R.L. Dykstra. *Order Restricted Statistical Inference*. John Wiley & Sons Ltd., 1988.

[62] A.K. Sanyal, M. Chellappa, J.L. Valk, J. Ahmed, J. Shen, D.S. Berstien. Globally convergent adaptive tracking of spacecraft angular velocity with inertia identification and adaptive linearization. *Proceedings of the 42nd IEEE Conference on Decision and Control*, pp. 2704–2709, Hawaii, 2003.

[63] S. Scholtes. Introduction to piecewise differentiable equations. Habilitation thesis, Institut für Statistik und Mathematische Wirtschaftstheorie, Universität Karlsruhe, 1994.

[64] A.Y. Shardin. The L_∞-norm of the L_2-spline projector is bounded independently of the knot sequence: A proof of de Boor's conjecture. *Acta Mathematica*, Vol. 187(1), pp. 59–137, 2001.

[65] J. Shen. Observability analysis of conewise linear systems via directional derivative and positive invariance techniques. *Automatica*, Vol. 46(5), pp. 843–851, 2010.

[66] J. Shen. Robust non-Zenoness of piecewise analytic systems with applications to complementarity systems. *Proc. of 2010 American Control Conference*, pp. 148–153, Baltimore, MD, 2010.

[67] J. Shen and T.M. Lebair. Shape restricted smoothing splines via constrained optimal control and nonsmooth Newton's methods. *Automatica*, Vol. 53, pp. 216–224, 2015.

[68] J. Shen and J.S. Pang. Linear complementarity systems: Zeno states. *SIAM Journal on Control and Optimization*, Vol. 44, pp. 1040–1066, 2005.

[69] J. Shen and J.S. Pang. Linear complementarity systems with singleton properties: non-Zenoness. *Proc. of 2007 American Control Conference*, pp. 2769–2774, New York, 2007.

[70] J. Shen and X. Wang. A constrained optimal control approach to smoothing splines. *Proc. of the 50th IEEE Conf. on Decision and Control*, pp. 1729–1734, Orlando, FL, 2011.

[71] J. Shen and X. Wang. Convex regression via penalized splines: a complementarity approach. *Proc. of American Control Conference*, pp. 332–337, Montreal, Canada, 2012.

[72] J. Shen and X. Wang. Estimation of monotone functions via P-splines: A constrained dynamical optimization approach. *SIAM Journal on Control and Optimization*, Vol. 49(2), pp. 646–671, 2011.

[73] J. Shen and X. Wang. Estimation of shape constrained functions in dynamical systems and its application to genetic networks. *Proc. of American Control Conference*, pp. 5948–5953, 2010.

[74] C.J. Stone. Optimal rate of convergence for nonparametric regression. *Annals of Statistics*, Vol. 10, pp. 1040–1053, 1982.

[75] S. Sun, M. Egerstedt, and C.F. Martin. Control theoretic smoothing splines. *IEEE Trans. on Automatic Control*, Vol. 45(12), pp. 2271–2279, 2000.

[76] C. Tantiyaswasdikul and M. Woodroofe. Isotonic smoothing splines under sequential designs. *Journal of Statistical Planning and Inference*, Vol. 38, pp. 75-88, 1994.

[77] A.B. Tsybakov. *Introduction to Nonparametric Estimation*. Springer, 2010.

[78] G. Wahba. *Spline Models for Observational Data*. Philadelphia: SIAM, 1990.

[79] X. Wang and J. Shen. A class of grouped Brunk estimators and penalized spline estimators for monotone regression. *Biometrika*, Vol. 97(3), pp. 585–601, 2010.

[80] X. Wang and J. Shen. Uniform convergence and rate adaptive estimation of convex functions via constrained optimization. *SIAM Journal on Control and Optimization*, Vol. 51(4), pp. 2753–2787, 2013.

[81] M. Woodroofe and J. Sun. A penalized maximum likelihood estimate of $f(0_+)$ when f is nonincreasing. *Statistica Sinica*, Vol. 3, pp. 501–515, 1993.

[82] Y. Zhou, M. Egerstedt, and C.F. Martin. Hilbert space methods for control theoretic splines: a unified treatment. *Communication in Information and Systems*. Vol. 6(1), pp. 55–82, 2006.