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EVELY LEETMA

Solution of smoothing problems with obstacles

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Introduction

Functions are important mathematical tools for describing and analyzing different real life, in particular, physical processes. Very often we have to construct an approximation based on limited information about the underlying process. There exist two major categories of approximation problems. The first one consists of problems where it is required to construct an approximation to an unknown function based on some finite amount of data (often measurements) of that function. These problems can be called data fitting problems. The second category arises from mathematical models for various physical processes. These operator-equation problems include, for example, boundary value problems for ordinary and partial differential equations, eigenvalue problems, integral equations, integro-differential equations, optimal control problems, and so on. Our field of interest – smoothing problems – belong to the class of data fitting problems.

In approximation theory one has to choose a reasonable class of functions in which to look for an approximation. The functions in this class should be relatively smooth, they should be easy to store and manipulate on a computer, they should be easy to evaluate on a computer, along with their derivatives and integrals. The class should be large enough so that arbitrary smooth function can be well approximated by the elements of this function class. For many years polynomials have played a central role in approximation theory. The space of polynomials satisfies all the previous conditions, it is finite dimensional (provided polynomials of limited degree are considered), the derivatives and antiderivatives of polynomials are again polynomials and according to Weierstrass approximation theorem every continuous function on a bounded closed interval can be approximated uniformly to any prescribed accuracy by a polynomial. But the class of polynomials is quite inflexible: higher order polynomials on large intervals tend to oscillate widely.

More flexible are piecewise polynomials or polynomial splines. Piecewise polynomials were used in approximation theory already in the early 1900s but the terminology *spline function* was first introduced by Schoenberg [55] in 1946. Polynomial splines of order m (or degree $m-1$) are piecewise polynomials and usually defined in such a way that they are $m-2$ times continuously differentiable over the domain. The space of splines is finite dimensional and every continuous function on a closed interval can be approximated arbitrarily well by polynomial splines with the order m fixed, provided a sufficient number of knots are allowed. This makes splines very attractive tools for approximation. There are several specific polynomial splines used for approximation: B-splines (basis splines) as appropriately scaled divided differences of the truncated power function, periodic splines satisfying periodicity conditions, natural splines with order $m = 2k$ and natural boundary conditions (derivatives of order $k, \ldots, 2k-2$ at the boundary vanish to zero), g-splines (generalized polynomial splines) and so on. The works by Stechkin and Subbotin [59], Schumaker [57] and de Boor [13] present a comprehensive treatment of the theory and numerical analysis of polynomial spline functions.

The most simple way to reconstruct a function according to discrete data is the interpolation. Suppose we have n distinct datapoints $a = x_1 < \ldots < x_n = b$, called knots or nodes, and values $y_1, \ldots, y_n$, we are looking for a continuous function f satisfying $f(x_i) = y_i$, $i = 1, \ldots, n$. Usually some amount of smoothness is assumed for f. The minimum curvature property for the cubic splines was discovered by Holladay [31] in 1957. He considered the problem

$$\min_{\substack{f \in C^2[a,b] \\ f(x_i)=y_i,\, i=1,\ldots,n}} \int_a^b |f''(x)|^2 dx$$

and showed that the solution of this problem is a cubic spline S with natural boundary conditions $S''(a) = S''(b) = 0$. This result was generalized by Walsh, Ahlberg and Nilson [67] (see also de Boor [12]) to the case where the integral was taken from the square of the kth derivative of function f – the minimization problem which possesses a solution among splines of degree $2k-1$ and with natural boundary conditions $S^{(k)}(a) = S^{(k)}(b) = \ldots = S^{(2k-2)}(a) = S^{(2k-2)}(b) = 0$. The idea of minimizing an integral from the square of some derivative produces a solution with minimum oscillation. The term *smooth* in approximation theory is used mostly to denote the function without big oscillations, it does not necessarily mean the differentiability.

If the values of the ordinates are given only approximately, for example, if we are working with measured or experimental data, then the strict interpolation should be replaced by some kind of smoothing. In 1964 Schoenberg [56] formulated the smoothing problem

$$\min_{f \in W_2^k(a,b)} \left(\varepsilon \int_a^b |f^{(k)}(x)|^2 dx + \sum_{i=1}^n (f(x_i) - y_i)^2 \right),$$

where $\varepsilon > 0$ is the smoothing parameter which determines the balance between the smoothness of solution, as represented by the integral from the square of the kth derivative, and fidelity to the data, as represented by the residual sum of squares. The solution of this problem is a natural spline of degree $2k-1$ and under the assumption $k < n$ this solution is unique. Reinsch [50] has shown that in case of $k = 2$ this problem reduces to the solution of a linear system of equations with a five-diagonal matrix. In later works the sum of squares was replaced by the weighted sum of squares and the problem obtained the form

$$\min_{f \in W_2^k(a,b)} \left(p \int_a^b |f^{(k)}(x)|^2 dx + \sum_{i=1}^{n} p_i (f(x_i) - y_i)^2 \right), \tag{A}$$

with weights $p_i > 0$, $i = 1, \ldots, n$, and smoothing parameter $p > 0$.

Another approach to construct a smoothing function is analyzed by Reinsch in [50, 51]. He considered the problem

$$\min_{\substack{f \in W_2^k(a,b) \\ \sum\limits_{i=1}^{n} \left(\frac{f(x_i) - y_i}{\delta y_i} \right)^2 \leqslant S}} \int_a^b |f^{(k)}(x)|^2 dx, \tag{B}$$

with $S \geqslant 0$, $\delta y_i > 0$ as given parameters, and proposed an algorithm for solution of this problem by minimizing the functional (A) with $p_i = 1/(\delta y_i)^2$ and smoothing parameter p depending on S. The solution of problem (B) is also a natural spline of degree $2k-1$ and under the assumption $k < n$ it is unique. Disadvantage of both problems (A) and (B) is the fact that in practice we usually do not have any information about the weights p_i and in case of equal weights the knot values y_i do not influence the result equally, i.e., the influence of exceptionally big deviations is pushed down compared to average deviations. But we may have information about the error bounds at knots which leads us to the third approach to smoothing problems

$$\min_{\substack{f \in W_2^k(a,b) \\ |f(x_i) - y_i| \leqslant \varepsilon_i,\ i=1,\ldots,n}} \int_a^b |f^{(k)}(x)|^2 dx. \tag{C}$$

This problem was formulated by Atteia [8] in 1967 (see also [22, 47] and [62] for multidimensional case). The solution of problem (C) is a natural spline of degree $2k-1$.

Exhaustive treatment of problem (A) is given in [59] by Steckin and Subbotin. They also generalize problem (A) to the two-dimensional case where the integral is taken from the sum of the squares of first order partial derivatives. For solution they consider a spline on rectangular mesh, linear with respect to both variables separately.

The method of Reinsch is generalized to multivariate case in [32].

There have been many articles on the topic of how to choose a smoothing parameter p in (A) or S in (B), see, e.g., [63, 65, 69]. Methods suggested include cross-validation [66], generalized cross-validation [23, 60, 62] and generalized maximum likelihood [64].

The definition of the spline can be generalized in two directions. Firstly as the solution of certain minimization problem in Hilbert spaces, secondly as regular piecewise polynomial or rational multidimensional function. In univariate case splines have both properties at the same time but in multivariate case these two properties cannot be preserved simultaneously. The general definition of splines in Hilbert spaces, existence, uniqueness and characterization theorems were obtained in the 1960s by Atteia [7, 9], Anselone and Laurent [2]. Jerome and Schumaker [35] showed that the classical spline functions fit into the abstract framework developed by Anselone and Laurent. Nielson [48] generalized the results of Anselone and Laurent to the bivariate case where data need not lie on a regular grid. In subject of the variational theory of splines in Hilbert spaces we refer the reader to [11, 33, 43, 61]. In following we compare the main assumptions made for solvability of the generalized smoothing problem with weights in [11, 43, 61] and also in [41].

Let X, Y, Z be real Hilbert spaces, $T : X \to Y$, $\Lambda : X \to Z$ bounded linear operators and $z \in Z$ an arbitrary element. Laurent [43] and Vershinin, Zav'yalov, Pavlov [61] considered the problem

$$\min_{x\in X} \left(\|Tx\|_Y^2 + \rho\|\Lambda x - z\|_Z^2 \right), \tag{A'}$$

where $\rho > 0$. They assumed that $\operatorname{ran} T = Y$, $\operatorname{ran} A = Z$ and proved the next two assertions. Problem (A') has a solution for every $z \in Z$ if (and only if [43]) $\ker T + \ker \Lambda$ is closed in X. For the uniqueness it is sufficient that $\ker T \cap \ker \Lambda = \{0\}$. Bezhaev and Vasilenko [11] assume X, Y, Z to be real separable Hilbert spaces and consider also problem (A'). They introduce Hilbert space $H = Y \times Z$ with inner product $\langle \cdot, \cdot \rangle_H = \langle \cdot, \cdot \rangle_Y + \rho \langle \cdot, \cdot \rangle_Z$ and linear bounded operator $A : X \to H$, $Ax = (Tx, \Lambda x)$. For the existence of the solution of problem (A') they assume that $\operatorname{ran} A$ is closed in H. Bezhaev and Vasilenko also consider the mixed case of interpolating-smoothing splines. In this situation the operator $\Lambda : X \to Z$ is split up into two operators $\Lambda_0 : X \to Z_0$, $\Lambda_1 : X \to Z_1$, with Z_0, Z_1 as Hilbert spaces and $Z = Z_0 \times Z_1$. In case of problem

$$\min_{x\in\Lambda_0^{-1}(\{z_0\})} \left(\|Tx\|_Y^2 + \rho\|\Lambda_1 x - z_1\|_Z^2 \right) \tag{A''}$$

the data $z_0 \in Z_0$ will be interpolated and the data $z_1 \in Z_1$ will be smoothened. For the existence of the solution of problem (A'') they assume that $A_1(\ker \Lambda_0)$ is closed in $Y \times Z_1$, here $A_1 : X \to Y \times Z_1$ is defined as $A_1 x = (Tx, \Lambda_1 x)$. Bezhaev and Vasilenko also note that the solution of problem exists if $\dim \ker T < \infty$ and ranges $\operatorname{ran} T$, $\operatorname{ran} \Lambda_0$, $\operatorname{ran} \Lambda_1$ are closed in Y, Z_0, Z_1, respectively. Kersey [41] tries to generalize the results of Bezhaev and Vasilenko. He introduces $\pi : Z_1 \to Z_1$ as bounded linear operator and replaces the problem (A″) with the problem

$$\min_{x \in \Lambda_0^{-1}(\{z_0\})} \left(\|Tx\|_Y^2 + \rho \|\pi(\Lambda_1 x - z_1)\|_Z^2 \right).$$

For the existence of solution Kersey assumes that $\operatorname{ran} T = Y$, $z_0 \in \operatorname{ran} \Lambda_0$ and $\dim Z_1 < \infty$. But, as shown in [45], these assumptions do not guarantee the existence of solution.

Atteia [9] generalized problem (C) to Hilbert spaces as problem

$$\min_{x \in \Lambda^{-1}(C)} \frac{1}{2} \|Tx\|_Y^2, \tag{C′}$$

where $C \subset \operatorname{ran} \Lambda$ is closed convex set in Z (as in previous, X, Y, Z are real Hilbert spaces and $T : X \to Y$, $\Lambda : X \to Z$ bounded linear operators). In subject of problem (C′) we refer also to [42, 43].

The theory of (m, s)-splines is situated in the similar framework but instead of Hilbert spaces semi-Hilbert spaces have been considered [4].

We note also the papers [5, 16, 18, 30] about particular cases of smoothing problems where the spaces and operators are specified and some methods of solution are analyzed.

The second approach of generalizing the spline definition, keeping the polynomial character of splines, leads us to B-splines (see [13, 57]). Ahlberg, Nilson and Walsh [1] have generalized one-dimensional spline theory to higher dimensions in a manner which preserves the extremal, orthogonality and convergence properties. The results depend highly on the mesh, thus several later works have been written on optimizing the knot positions for multidimensional B-spline models, in particular, in the framework of the theory of box splines [14].

In [68] the meshless scattered data methods are considered for constructing multivariate approximations, amongst them radial basis functions, or, more generally, approximation by (conditionally) positive definite kernels, the moving least squares approximation and partition-of-unity methods.

Our technique uses the expansion of natural splines by certain radial basis functions. We refer the reader to [19, 34, 68] for a systematic treatment of radial basis functions and scattered data modelling using radial basis functions. The convergence of radial polynomials, stability of interpolation by smooth radial basis functions and other properties are analysed in [52, 53, 54].

The main topic of this thesis is the solution of smoothing problems with obstacles. We consider the smoothing problem with obstacles in the general setting for several variables. It is known that the solution of the problem is a natural spline and that under some additional assumptions the solution is unique. In our opinion there are not yet any satisfactory methods for finding the solution to this problem. In [33] it has been proposed a method of adding-removing knots which is based on the use of certain necessary and sufficient conditions imposed on the coefficients in a natural spline expansion. But this method can lead to a cycle as shown in [44]. An attempt to use a modified Wolfe's method (see [24]) to treat the problem in univariate case as a quadratic programming problem is made in [17]. The effectiveness of such an approach is not clear because the number of unknowns increases several times and the complexity of the method may become very high.

Note also the paper [49] about the use of the penalty method for the solution of smoothing problems.

Another very natural idea is to reduce the smoothing problem with obstacles to an equivalent problem with weights. For the univariate case the connection between obstacle parameters and weights in equivalent problems is studied in [39, 40]. Therein an iterative algorithm for the determination of the weights by obstacle parameters is proposed. The problem setting in [39, 40] does not allow any interpolation knots. A problem with interpolation knots and only one obstacle knot in the one variable case is studied in [15]. In the several variable case a nonlinear system connecting weights and deviation limits is given in [6]. Therein the obstacles can take zero values and thus the problem with obstacles may have also interpolation knots. But in [6] the special case of problem with weights has been considered where all the weights are positive. The problem with obstacles has an equivalent problem with positive weights only in exceptional case: when all the knots in the solution of smoothing problem with obstacles are active. Under this restriction an equation connecting deviations of the solution from given values and weights has been derived in [6]. No attempts have been made in order to solve this equation. In [46] we have derived an equation connecting weights and deviation limits in situation where the equivalence between smoothing problems with weights and obstacles always exists.

For proving the equivalence of smoothing problems with obstacles and weights we use the saddle point theory for certain Lagrange functions. It is known that, if the Lagrangian associated to the smoothing problem with obstacles has a saddle point, then its first component is a solution of this problem and the second component consists of weights for the equivalent problem. For the definiteness, we prove such a principle in a general case. Although in convex programming problems the saddle point may not exist, an encouraging fact is that the problem of linear programming has always a saddle point (see, e.g., [38]). Another important fact for us is that the simplex method for solving the problems of linear programming actually finds a saddle point. In [15, 17], the Wolfe's method being a modification of simplex method for the problems of quadratic programming, is adapted to particular smoothing problems in one variable case. Several methods for finding saddle points are proposed and studied in [21, 26, 70]. Their effectiveness in case of smoothing problems is not yet clear. In [45] we proved that, for problems with obstacles in Hilbert spaces and also in classical case, especially, in several variable problems, the associated Lagrangian has a saddle point. This implies the existence of equivalent problems with weights.

The pair $(x_0, y_0) \in X \times Y$ is said to be a saddle point for the function $f : X \times Y \to \mathbb{R}$ if

$$f(x_0, y) \leqslant f(x_0, y_0) \leqslant f(x, y_0) \quad \forall x \in X, \forall y \in Y.$$

The necessary and sufficient condition for f to have a saddle point is

$$\min_{x\in X} \sup_{y\in Y} f(x, y) = \max_{y\in Y} \inf_{x\in X} f(x, y).$$

In subject of the minimax theory we refer the reader to [10, 25]. In [37] one can find a general result about the existence of saddle points in case of X, Y being compact convex sets in Banach spaces, the proof of this result uses Kakutani's theorem, the last one is a fixed-point type theorem.

We are sure that an important class of adequate methods for solving smoothing problems with obstacles will be saddle point methods.

The thesis is organized as follows.

In Chapter 1 we consider smoothing problems in the most general situation and give some preliminary results concerning the equivalence of smoothing problems with obstacles and weights. We also introduce the concept of stability in weight reduction being used for proving the equivalence between these problems and note that in general the problem with weights may not have this property.

In Chapter 2 we present some known results about variational theory of splines. As a new result we give a correct characterization theorem for smoothing problem proposed by Kersey in [41] and also point out a mistake made in [41]. As the main result, we show that the Lagrangian associated to the smoothing problem with obstacles in Hilbert space has a saddle point. This result implies at once that the problems with obstacles have equivalent problems with weights. To prove the equivalence in opposite direction that any problem with weights has an equivalent problem with obstacles, we prove that the smoothing problems with weights in Hilbert spaces are stable in weight reduction.

In Chapter 3 we consider the classical multivariate smoothing problems in Beppo Levi spaces, being the most important practical case of smoothing problems. In the literature the classical problem with weights is proposed with nonzero weights. Having in mind the equivalence of problems with weights and obstacles it is important to us to allow zero weights. For that reason we propose the classical problem with weights in a slightly more general situation and give a new characterization theorem for the solution. As in previous chapter, we prove the equivalence between the problems with obstacles and weights by proving the saddle point theorem for the problem with obstacles and also the stability of weight reduction for the problem with weights.

The solution of the smoothing problem with obstacles can be characterized by certain necessary and sufficient conditions imposed on the coefficients in a natural spline expansion. This leads to a quite natural method of adding-removing knots as described in the book [33]. In Chapter 4 we give a detailed description of this algorithm with natural extension to some cases arising in practice. The proof of the finiteness of the method is proposed in [33] but this proof is based on a false lemma. We give a counterexample to this lemma and also an example of cycling in the algorithm. In the last section of this chapter we give some sufficient conditions implying the finiteness of the method.

In Chapter 5 we derive an equation connecting deviations and weights in the case where the weights can take zero values. Note that similar equation in the case of strictly positive weights and on the assumption that all the knots in the solution of smoothing problem with obstacles are active is derived in [6]. In practice the assumption made in [6] often does not hold. We propose a method for solving the equation connecting deviations and weights. The effectiveness of the method has not yet been studied, but as our first example about this topic shows, the problem from Chapter 4, where the method of adding-removing knots is cycling, can be solved successfully by this method.

The results of Chapter 4 have been published in [44]. The other results of this thesis have been submitted for publication, the results of Chapters 1-3 in [45] and those of Chapter 5 in [46].

CHAPTER 1

General smoothing problems

In this chapter we consider smoothing problems in the most general situation and present some well known results about saddle points of Lagrangian associated to smoothing problems. We also introduce the concept of stability in weight reduction which will be one of the fundamental questions in our theory concerning the equivalence of smoothing problems with obstacles and weights.

1.1. Problem setting

For arbitrary set X, objective function $f : X \to \mathbb{R}$ and constraint functions $f_i : X \to \mathbb{R}$, $i = 1, \ldots, n$, define the feasible set

$$\Omega = \{x \in X \mid f_i(x) \leqslant 0, i = 1, \ldots, n\}$$

and consider the generalized smoothing problem with obstacles as the minimization problem

$$\min_{x \in \Omega} f(x). \tag{1.1}$$

Let

$$L(x, y) = f(x) + \sum_{i=1}^{n} y_i f_i(x), \quad x \in X, y \in \mathbb{R}^n_+,$$

denote the Lagrangian associated to (1.1). Here $\mathbb{R}^n_+$ is the set of real-valued n-dimensional vectors with non-negative components.

The next saddle point result may be adapted from any source treating the connection between the problem of convex programming and saddle points, e.g., [10]. Nevertheless, to be self-contained, we present it here with the proof.

Lemma 1.1. *If* $(x^*, y^*) \in X \times \mathbb{R}^n_+$ *is a saddle point of Lagrangian associated to* (1.1), *i.e.,*

$$L(x^*, y) \leqslant L(x^*, y^*) \leqslant L(x, y^*) \quad \forall x \in X,\ \forall y \in \mathbb{R}^n_+,$$

then x^* is a solution of problem (1.1).

Proof. From the left-hand side of the saddle point inequality we get

$$\sum_{i=1}^{n} y_i f_i(x^*) \leqslant \sum_{i=1}^{n} y_i^* f_i(x^*) = \text{const} \quad \forall y \in \mathbb{R}_+^n. \tag{1.2}$$

For any $k \in \{1, \dots, n\}$ take $y_k = c$ and $y_i = 0$, $i \neq k$. Now $c f_k(x^*) \leqslant \text{const}$ for all $c \geqslant 0$, which implies that $f_k(x^*) \leqslant 0$. Thus $f_i(x^*) \leqslant 0$, $i = 1, \dots, n$, and $x^* \in \Omega$.

From the fact that $y^* \in \mathbb{R}_+^n$ and $f_i(x^*) \leqslant 0$, $i = 1, \dots, n$, we immediately get $\sum_{i=1}^{n} y_i^* f_i(x^*) \leqslant 0$. On the other hand, by taking $y = 0$ in (1.2), we have $\sum_{i=1}^{n} y_i^* f_i(x^*) \geqslant 0$ and all together $\sum_{i=1}^{n} y_i^* f_i(x^*) = 0$.

Let us take $x \in \Omega$, then $\sum_{i=1}^{n} y_i^* f_i(x) \leqslant 0$. From the right-hand side of the saddle point inequality we get

$$f(x^*) = f(x^*) + \sum_{i=1}^{n} y_i^* f_i(x^*) \leqslant f(x) + \sum_{i=1}^{n} y_i^* f_i(x) \leqslant f(x),$$

which implies that x^* is a solution of problem (1.1). $\square$

It is well known that, if problem (1.1) has a solution, then the saddle point of the corresponding Lagrangian does not necessarily exist. The next example is a slight modification of the example presented, e.g., in [36].

Example 1.1. Let us take $X = \mathbb{R}$, $f(x) = -x$ and $f_1(x) = x^2$, then $\Omega = \{x \in \mathbb{R} \mid x^2 \leqslant 0\} = \{0\}$. Problem (1.1) with corresponding Lagrangian

$$L(x, y) = -x + yx^2, \quad x \in \mathbb{R}, y \in \mathbb{R}_+,$$

has a solution $x^* = 0$ as the only feasible solution. Analysing the left-hand side of the saddle point inequalities

$$-x^* + y(x^*)^2 \leqslant -x^* + y^*(x^*)^2 \leqslant -x + y^* x^2 \quad \forall x \in \mathbb{R}, \forall y \in \mathbb{R}_+,$$

we see that $x^* = 0$, but now for any $y^* \in \mathbb{R}_+$ there exists $x \in \mathbb{R}$ such that the right-hand side inequality does not hold, thus the Lagrangian corresponding to this problem does not have a saddle point.

For given set X, functions $f : X \to \mathbb{R}$ and $\lambda_i : X \to \mathbb{R}$, $i = 1, \dots, n$, data $z_i \in \mathbb{R}$, $\varepsilon_i \geqslant 0$, $i = 1, \dots, n$, consider the feasible set

$$\Omega = \{x \in X \mid |\lambda_i(x) - z_i| \leqslant \varepsilon_i, i = 1, \dots, n\}$$

and the smoothing problem with obstacles as the minimization problem

$$\min_{x\in\Omega} f(x). \tag{1.3}$$

Taking $f_i(x) = |\lambda_i(x) - z_i|^2 - \varepsilon_i^2$, $i = 1, \dots, n$, we see that problem (1.3) is actually a particular case of problem (1.1). According to Lemma 1.1, if (x^*, w) is a saddle point of Lagrangian

$$L(x, v) = f(x) + \sum_{i=1}^{n} v_i(|\lambda_i(x) - z_i|^2 - \varepsilon_i^2), \quad x \in X, v \in \mathbb{R}_+^n, \tag{1.4}$$

then x^* is a solution of problem (1.3).

For given set X, functions $f : X \to \mathbb{R}$ and $\lambda_i : X \to \mathbb{R}$, $i = 1, \dots, n$, data $z_i \in \mathbb{R}$, $w_i \geqslant 0$, $i = 1, \dots, n$, form the functional

$$J(x) = f(x) + \sum_{i=1}^{n} w_i |\lambda_i(x) - z_i|^2, \quad x \in X,$$

and consider the smoothing problem with weights as the minimization problem

$$\min_{x\in X} J(x). \tag{1.5}$$

The next result gives the same assertion as Proposition 2.3 (i) from [39] in more general situation.

Lemma 1.2. *If (x^*, w) is a saddle point of Lagrangian* (1.4) *then x^* is a solution of problem* (1.5) *with weights w.*

Proof. According to saddle point inequality we have

$$J(x^*) = L(x^*, w) + \sum_{i=1}^{n} w_i \varepsilon_i^2 \leqslant L(x, w) + \sum_{i=1}^{n} w_i \varepsilon_i^2 = J(x) \quad \forall x \in X,$$

which means that x^* is a solution of problem (1.5). □

Lemmas 1.1 and 1.2 yield that, if the Lagrangian associated to the smoothing problem with obstacles has a saddle point, then its first component is a solution of this problem and its second component defines weights in an equivalent smoothing problem with weights. By the equivalence of these problems we mean that the initial data f, λ_i, z_i, $i = 1, \dots, n$, and the solutions of the problems coincide.

1.2. Equivalence of problems

In the previous section we saw that a saddle point of the Lagrangian associated to (1.1) may not exist although the problem has a solution. This fact leaves the question of equivalence between smoothing problems with obstacles (1.3) and weights (1.5) still open. In this section we show that, for given problem (1.5), it exists an equivalent problem (1.3), but not vice versa. For that reason we modify a little the setting of problems so that the equivalence in opposite direction remains possible.

In [39] the smoothing problems have been posed so that $w_i \geqslant 0$ and $\varepsilon_i > 0$, $i = 1, \dots, n$. In our treatment, both, the weights and obstacles, can take zero values. Besides that we do not pose any restriction about the set X and functions λ_i. In this sense the next result is a generalization of Proposition 2.3 (ii) in [39].

Proposition 1.3. *Let problem* (1.5) *with weights w have a solution x^*. Define obstacles $\varepsilon_i = |\lambda_i(x^*) - z_i|$, $i = 1, \dots, n$. Then (x^*, w) is a saddle point of Lagrangian* (1.4) *and x^* is a solution of problem* (1.3) *with obstacles ε.*

Proof. By the definition $|\lambda_i(x^*) - z_i|^2 - \varepsilon_i^2 = 0$, $i = 1, \dots, n$. Thus $L(x^*, v) = L(x^*, w)$ for all $v \in \mathbb{R}^n_+$. Since x^* minimizes functional J, it follows that

$$L(x^*, w) = J(x^*) - \sum_{i=1}^{n} w_i \varepsilon_i^2 \leqslant J(x) - \sum_{i=1}^{n} w_i \varepsilon_i^2 = L(x, w) \quad \forall x \in X.$$

Now

$$L(x^*, v) \leqslant L(x^*, w) \leqslant L(x, w) \quad \forall x \in X,\ \forall v \in \mathbb{R}^n_+,$$

which means that (x^*, w) is a saddle point of Lagrangian associated to (1.3). Finally, according to Lemma 1.1, x^* is a solution of problem (1.3). □

Corollary 1.4. *For any smoothing problem* (1.5) *with weights having a solution x^* there exists an equivalent problem* (1.3) *with obstacles so that x^* is also a solution of problem* (1.3).

In general, the smoothing problem (1.3) with obstacles does not have an equivalent problem (1.5) with weights. To this end we give the next

Example 1.2. Consider the set

$$X = \{f : \mathbb{R} \to \mathbb{R} \mid f' \in L_2(\mathbb{R}) \text{ (distributional derivative)}\},$$

$x_1 = 1$, $x_2 = 2$, $x_3 = 3$, $\lambda_i(f) = f(x_i)$, $i = 1, 2, 3$, $z_1 = z_3 = 0$, $z_2 = 3$, $\varepsilon_1 = \varepsilon_3 = 1$, $\varepsilon_2 = 0$, and

$$\Omega = \big\{f \in X \mid |f(1)| \leqslant 1, f(2) = 3, |f(3)| \leqslant 1\big\}.$$

The solution of the smoothing problem

$$\min_{f \in \Omega} \int_{\mathbb{R}} |f'(x)|^2 dx$$

is a linear natural spline f^* presented in Figure 1.1. (In Section 3.3 we explain why f^* is the solution of this problem.)

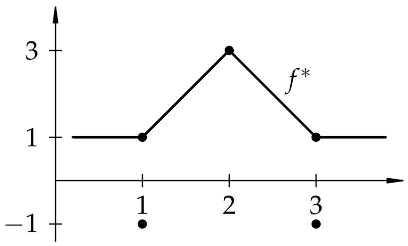

Figure 1.1. Solution of the problem

Suppose that there exists a smoothing problem

$$\min_{f \in X} J(f)$$

with the functional

$$J(f) = \int_{\mathbb{R}} |f'(x)|^2 dx + \sum_{i=1}^{3} w_i |f(x_i) - z_i|^2$$

and the solution f^*, then $J(f^*) \leqslant J(f)$ for all $f \in X$. Take the function f_δ as a linear natural spline with three knots and values $f_\delta(x_1) = f_\delta(x_3) = 1$, $f_\delta(x_2) = 3 - \delta$ (see Fig. 1.2).

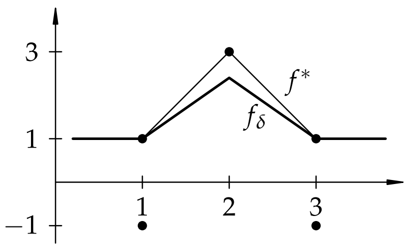

Figure 1.2. Splines f^* and f_δ

Clearly, $f_\delta \in X$. The straightforward calculation gives

$$\begin{aligned} J(f_\delta) &= \int_1^2 (2-\delta)^2 dx + \int_2^3 (\delta-2)^2 dx + \sum_{i=1}^{3} w_i |f_\delta(x_i) - z_i|^2 \\ &= 2(2-\delta)^2 + w_1|f^*(x_1) - z_1|^2 + w_2\delta^2 + w_3|f^*(x_3) - z_3|^2 \\ &= J(f^*) - 8\delta + (2+w_2)\delta^2 \end{aligned}$$

and, for any w_2, there is $\delta > 0$ such that $J(f_\delta) < J(f^*)$. This contradicts to the assumption that f^* is a solution of a smoothing problem with some weights.

The main idea arising from this example is that interpolation conditions, i.e., conditions $|\lambda_i(x) - z_i| \leqslant \varepsilon_i$, $\varepsilon_i = 0$, should be included to the feasible set of problem (1.5).

Consider index sets $I_0 = \{i \mid \varepsilon_i = 0\}$ and $I_1 = \{i \mid \varepsilon_i > 0\}$. Write problem (1.3) as

$$\min_{x \in \Omega} f(x), \tag{1.6}$$

where $\Omega = \{x \in X \mid \lambda_i(x) = z_i, i \in I_0,\ |\lambda_i(x) - z_i| \leqslant \varepsilon_i, i \in I_1\}$, and problem (1.5) as

$$\min_{x \in \Omega_0} \left(f(x) + \sum_{i \in I_1} w_i |\lambda_i(x) - z_i|^2 \right), \tag{1.7}$$

where $\Omega_0 = \{x \in X \mid \lambda_i(x) = z_i, i \in I_0\}$. According to Proposition 1.3, for any smoothing problem (1.7), there exists an equivalent problem (1.6) with obstacles $\varepsilon_i \geqslant 0$, $i \in I_1$. Some extra conditions must hold to obtain positive obstacles ε_i, $i \in I_1$.

Let the smoothing problem with weights w have a solution x^*. Define $\overline{w}_i = 0$ in case of $\lambda_i(x^*) = z_i$ and $\overline{w}_i = w_i$ in case of $\lambda_i(x^*) \neq z_i$. We say that the smoothing problem with weights w is stable in weight reduction if x^* is also a solution of the smoothing problem with weights $\overline{w}$.

Proposition 1.5. *Let problem* (1.5) *with weights w be stable in weight reduction and let x^* be a solution of this problem. Define*

$$\begin{aligned} &\overline{w}_i = w_i, \quad \varepsilon_i = |\lambda_i(x^*) - z_i|, \quad \text{if} \quad \lambda_i(x^*) \neq z_i, \\ &\overline{w}_i = 0, \quad \varepsilon_i \geqslant 0, \quad \text{if} \quad \lambda_i(x^*) = z_i. \end{aligned}$$

Then $(x^*, \overline{w})$ is a saddle point of Lagrangian (1.4) *associated to problem* (1.3) *and x^* is a solution of problem* (1.3) *with obstacles ε.*

Proof. According to the assumption, x^* is a solution of the smoothing problem with weights $\overline{w}$. Therefore,

$$\begin{aligned} L(x^*,\overline{w}) &= f(x^*) + \sum_{i=1}^{n} \overline{w}_i(|\lambda_i(x^*) - z_i|^2 - \varepsilon_i^2) \\ &\leqslant f(x) + \sum_{i=1}^{n} \overline{w}_i \left(|\lambda_i(x) - z_i|^2 - \varepsilon_i^2\right) = L(x,\overline{w}) \quad \forall x \in X. \end{aligned}$$

As $|\lambda_i(x^*) - z_i| = \varepsilon_i$ in case of $\lambda_i(x^*) \neq z_i$ and $\overline{w}_i = 0$ in case of $\lambda_i(x^*) = z_i$, we have

$$\overline{w}_i \left(|\lambda_i(x^*) - z_i|^2 - \varepsilon_i^2\right) = 0, \quad i = 1, \ldots, n.$$

In general, $v_i \geqslant 0$ and $|\lambda_i(x^*) - z_i| \leqslant \varepsilon_i$, hence, $v_i(|\lambda_i(x^*) - z_i|^2 - \varepsilon_i^2) \leqslant 0$, which gives

$$\begin{aligned} L(x^*,v) &= f(x^*) + \sum_{i=1}^{n} v_i(|\lambda_i(x^*) - z_i|^2 - \varepsilon_i^2) \\ &\leqslant f(x^*) + \sum_{i=1}^{n} \overline{w}_i \left(|\lambda_i(x^*) - z_i|^2 - \varepsilon_i^2\right) = L(x^*,\overline{w}) \quad \forall v \in \mathbb{R}^n_+. \end{aligned}$$

The saddle point inequalities hold and according to Lemma 1.1, x^* is a solution of problem (1.3). □

Corollary 1.6. *For any smoothing problem* (1.7)*, which is stable in weight reduction and has a solution x^*, there exists an equivalent problem* (1.6) *with obstacles so that x^* is also a solution of problem* (1.6).

In general the smoothing problem with weights is not stable in weight reduction.

Example 1.3. Let $X = \{x_1, x_2\}$, $f(x_1) = 1$, $f(x_2) = 2$, $\lambda_1(x_1) = 1$, $\lambda_1(x_2) = 1$, $\lambda_2(x_1) = 1$, $\lambda_2(x_2) = 0$, $z_1 = z_2 = 0$, $w_1 = w_2 = 2$. Consider the smoothing problem with weights

$$\min_{x \in X} \left(f(x) + \sum_{i=1}^{2} w_i |\lambda_i(x) - z_i|^2 \right).$$

Then

$$\begin{aligned} f(x_1) + w_1|\lambda_1(x_1) - z_1|^2 + w_2|\lambda_2(x_1) - z_2|^2 &= 5, \\ f(x_2) + w_1|\lambda_1(x_2) - z_1|^2 + w_2|\lambda_2(x_2) - z_2|^2 &= 4. \end{aligned}$$

Therefore, the solution of this problem is x_2. Since $\lambda_1(x_2) \neq z_1$ and $\lambda_2(x_2) = z_2$, we define $\overline{w}_1 = w_1 = 2$ and $\overline{w}_2 = 0$. Then

$$\begin{aligned} f(x_1) + \overline{w}_1|\lambda_1(x_1) - z_1|^2 + \overline{w}_2|\lambda_2(x_1) - z_2|^2 &= 3, \\ f(x_2) + \overline{w}_1|\lambda_1(x_2) - z_1|^2 + \overline{w}_2|\lambda_2(x_2) - z_2|^2 &= 4. \end{aligned}$$

We see that the solution of the problem with reduced weights $\overline{w}$ is x_1.

Note that the proof of Proposition 2.3 in [39] uses the stability in weight reduction but its validity is not proved there.

CHAPTER 2

Smoothing problems in Hilbert spaces

In this chapter we give the assertions about solvability and characterization of solutions for smoothing problems in Hilbert spaces. For better readability we present all the results here with the proof although several of them can be found in the literature, e.g., [11, 33, 43, 61].

In the first section we refer to an incorrect Theorem 1 in [41] and present the correct assertion about solvability of the problem considered there. In the second section we prove the theorems about stability in weight reduction and existence of a saddle point for the smoothing problems in Hilbert spaces.

2.1. Variational theory of splines

Let X, Y and Z be Hilbert spaces and let $T : X \to Y$, $\Lambda : X \to Z$ be bounded linear operators. The set

$$\mathcal{S} = \{s \in X \mid \langle Ts, Tx\rangle = 0 \quad \forall x \in \ker \Lambda\}$$

is called the space of splines. We use the notation $\langle \cdot, \cdot \rangle$ for inner product or semi-inner product depending on the context.

Let Y_0 be a linear subspace of Hilbert space Y and $y_0 \in Y$. According to Hilbert theorem for closed convex sets, the problem of finding an element with minimal norm from the shift $y_0 + Y_0$ possesses a unique solution if the subspace Y_0 is closed. The next Lemma characterizes the solution of this problem.

Lemma 2.1. *Let Y_0 be a linear subspace of Hilbert space Y and $y_0 \in Y$. An element $y^* \in y_0 + Y_0$ is the solution of problem*

$$\min_{y \in y_0 + Y_0} \|y\| \tag{2.1}$$

if and only if $\langle y^*, y\rangle = 0$ for all $y \in Y_0$.

Proof. If $y_0 \in Y_0$, then $y_0 + Y_0 = Y_0$ and the assertion holds trivially. Consider the case $y_0 \notin Y_0$. Let $\langle y^*, y - y^* \rangle = 0$ for all $y \in y_0 + Y_0$, then it holds $\|y\|^2 = \|y^*\|^2 + \|y - y^*\|^2$ and thus $\|y\| \geqslant \|y^*\|$ for all $y \in y_0 + Y_0$, which means that y^* is a solution of problem (2.1). If there exists $y_1 \in y_0 + Y_0$ such that $\langle y^*, y_1 - y^* \rangle = a \neq 0$, then we can construct an element $y = y^* + \delta(y_1 - y^*) = \delta y_1 + (1 - \delta) y^* \in y_0 + Y_0$, $\delta \in \mathbb{R}$, such that $\|y\|^2 = \|y^*\|^2 + 2\delta a + \delta^2 \|y_1 - y^*\|^2 < \|y^*\|^2$ and, consequently, y^* is not a solution of problem (2.1). All together, $y^* \in y_0 + Y_0$ is the solution of problem (2.1) if and only if $\langle y^*, y - y^* \rangle = 0$ for all $y \in y_0 + Y_0$. The last condition is equivalent to the condition $\langle y^*, y \rangle = 0$ for all $y \in Y_0$, since $y_0 - y^* + Y_0 = Y_0$. □

For given $z \in \operatorname{ran} \Lambda$ we consider the problem of finding an element with minimal seminorm

$$\min_{x \in \Omega} \|Tx\|, \tag{2.2}$$

where $\Omega = \Lambda^{-1}(\{z\}) = \{x \in X \mid \Lambda x = z\}$.

Proposition 2.2. *If $T(\ker \Lambda)$ is closed then a solution of problem* (2.2) *exists. The solution of problem* (2.2) *is unique if and only if* $\ker T \cap \ker \Lambda = \{0\}$. *An element $x^* \in \Omega$ is a solution of problem* (2.2) *if and only if $\langle Tx^*, Tx \rangle = 0$ for all $x \in \ker \Lambda$ or, equivalently, if x^* is a spline. If* $\operatorname{ran} \Lambda$ *is closed, then $x^* \in \Omega$ is a solution of problem* (2.2) *if and only if there exists an element $c \in Z$ such that $T^* T x^* = \Lambda^* c$.*

Proof. Let us take any element $x_0 \in \Omega$ and present the feasible set as $\Omega = x_0 + \ker \Lambda$. By our assumption $T(\ker \Lambda)$ is closed and thus $T(\Omega) = Tx_0 + T(\ker \Lambda)$ is closed. According to the projection theorem for closed convex sets in Hilbert spaces, the auxiliary problem

$$\min_{y \in T(\Omega)} \|y\|, \tag{2.3}$$

has the unique solution $y^* \in T(\Omega)$. Hereby there exists an element $x^* \in \Omega$, $Tx^* = y^*$, which is a solution of problem (2.2).

Suppose that there exists another solution $x^{**} \in \Omega$, $Tx^{**} = y^*$, of problem (2.2). Then $T(x^* - x^{**}) = y^* - y^* = 0$ and $\Lambda(x^* - x^{**}) = z - z = 0$, i.e., $x^* - x^{**} \in \ker T \cap \ker \Lambda = \{0\}$ which yields $x^* = x^{**}$. On the other hand, suppose that there exists $\overline{x} \in \ker T \cap \ker \Lambda$, $\overline{x} \neq 0$, then $x^* + \overline{x}$ is also a solution of problem (2.2) different from x^*.

According to Lemma 2.1, an element $y^* \in T(\Omega) = Tx_0 + T(\ker \Lambda)$ is the solution of problem (2.3) if and only if $\langle y^*, y \rangle = 0$ for all $y \in T(\ker \Lambda)$. Thus an element $x^* \in \Omega$ is a solution of problem (2.2) if and only if $\langle Tx^*, Tx \rangle = 0$ for all $x \in \ker \Lambda$.

The condition $\langle Tx^*, Tx \rangle = 0$ for all $x \in \ker \Lambda$ is equivalent to the orthogonality condition $T^*Tx^* \in (\ker \Lambda)^\perp$. According to the closedness of $\operatorname{ran} \Lambda$ it holds $(\ker \Lambda)^\perp = \operatorname{ran} \Lambda^*$, thus an element $x^* \in \Omega$ is a solution of problem (2.2) if and only if there exists $c \in Z$ such that $T^*Tx^* = \Lambda^* c$. □

With the next two remarks we give sufficient conditions for the closedness of $T(\ker \Lambda)$ and thus for the solvability of problem (2.2).

Remark 2.3. *Subspace* $T(\ker \Lambda)$ *is closed if* $\operatorname{ran} T$ *and* $\ker T + \ker \Lambda$ *are closed.*

Proof. Define an operator

$$\widetilde{T} = T\big|_{(\ker T)^\perp} : (\ker T)^\perp \to \operatorname{ran} T$$

as the restriction of the operator T to the closed subspace $(\ker T)^\perp$. It is easy to see that $\widetilde{T}$ is bijective. The closedness of $\operatorname{ran} T$ implies the completeness of $\operatorname{ran} T$. Thus $\widetilde{T}$ is a bounded linear bijective operator between complete spaces and according to Banach inverse mapping theorem its inverse $\widetilde{T}^{-1}$ is continuous.

Let us prove that for any set $E \subset X$ it holds

$$T(E) = \widetilde{T}\left((\ker T + E) \cap (\ker T)^\perp\right).$$

Take any element $y \in T(E)$. Then it exists $x \in E$ such that $Tx = y$. Since $X = \ker T \oplus (\ker T)^\perp$, we have the unique representation $x = x_1 + x_2$, $x_1 \in \ker T$, $x_2 \in (\ker T)^\perp$. In addition, $x_2 = -x_1 + x \in \ker T + E$ and thus $x_2 \in (\ker T + E) \cap (\ker T)^\perp$. It holds

$$y = Tx = Tx_1 + Tx_2 = Tx_2 = \widetilde{T}x_2 \in \widetilde{T}\left((\ker T + E) \cap (\ker T)^\perp\right).$$

To prove the opposite inclusion we take $y \in \widetilde{T}\left((\ker T + E) \cap (\ker T)^\perp\right)$, then it exists $x_2 \in (\ker T + E) \cap (\ker T)^\perp$ such that $\widetilde{T}x_2 = y$. According to $x_2 \in \ker T + E$ we have a representation $x_2 = x_1 + x$, $x_1 \in \ker T$, $x \in E$, and

$$y = \widetilde{T}x_2 = Tx_2 = Tx_1 + Tx = Tx \in T(E).$$

Now the set

$$T(\ker \Lambda) = \widetilde{T}\left((\ker T + \ker \Lambda) \cap (\ker T)^\perp\right),$$

as the inverse image of the closed set $(\ker T + \ker \Lambda) \cap (\ker T)^\perp$ with respect to the continuous operator $\widetilde{T}^{-1}$, is closed. □

Note that the sum of closed subspaces, e.g., $\ker T + \ker \Lambda$ is not necessarily closed. In normed spaces the closedness of the sum of two subspaces yields from the finite dimensionality of one addend. This justifies the next

Remark 2.4. *The condition* $\dim \ker T < \infty$ *implies the closedness of* $\ker T + \ker \Lambda$.

Let X, Y, Z_0 and Z_1 be Hilbert spaces and let $T : X \to Y$, $\Lambda_0 : X \to Z_0$, $\Lambda_1 : X \to Z_1$, $\pi : Z_1 \to Z_1$ be bounded linear operators. For given $z_0 \in \operatorname{ran} \Lambda_0$ and $z_1 \in Z_1$ we consider the smoothing problem

$$\min_{x \in \Omega_0} \left(\|Tx\|^2 + \|\pi(\Lambda_1 x - z_1)\|^2 \right), \tag{2.4}$$

where $\Omega_0 = \Lambda_0^{-1}(\{z_0\}) = \{x \in X \mid \Lambda_0 x = z_0\}$.

Proposition 2.5. *If* $\{(Tx, \pi\Lambda_1 x) \mid x \in \ker \Lambda_0\}$ *is closed in* $Y \times Z_1$ *then problem* (2.4) *has a solution. The solution of problem* (2.4) *is unique if and only if* $\ker T \cap \ker \Lambda_0 \cap \ker(\pi\Lambda_1) = \{0\}$. *An element* $x^* \in \Omega_0$ *is a solution of problem* (2.4) *if and only if*

$$\langle Tx^*, Tx \rangle + \langle \pi\Lambda_1 x^* - \pi z_1, \pi\Lambda_1 x \rangle = 0 \quad \forall x \in \ker \Lambda_0.$$

If $\operatorname{ran} \Lambda_0$ *is closed, then* $x^* \in \Omega_0$ *is a solution of problem* (2.4) *if and only if there exists an element* $c \in Z_0$ *such that*

$$T^*Tx^* + \Lambda_1^*\pi^*\pi(\Lambda_1 x^* - z_1) = \Lambda_0^* c.$$

Proof. Consider Hilbert space $H = Y \times Z_1$ with the inner product $\langle \cdot, \cdot \rangle_H = \langle \cdot, \cdot \rangle_Y + \langle \cdot, \cdot \rangle_{Z_1}$. Problem (2.4) can be reformulated as

$$\min_{x \in \Omega_0} \|Ax - (0, \pi z_1)\|^2$$

where $A : X \to H$, $Ax = (Tx, \pi\Lambda_1 x)$. According to the assumption, the set $A(\Omega_0) = Ax_0 + A(\ker \Lambda_0)$, where $x_0 \in \Omega_0$, is closed and the auxiliary problem

$$\min_{(y,z) \in A(\Omega_0)} \|(y, z) - (0, \pi z_1)\|^2 \tag{2.5}$$

has the unique solution $(y^*, z^*) \in Y \times Z_1$. Thus, the solution of problem (2.4) $x^* \in A^{-1}(\{(y^*, z^*)\})$ exists.

Suppose that problem (2.4) has another solution $x^{**} \in A^{-1}(\{(y^*, z^*)\})$. As $(T(x^* - x^{**}), \pi\Lambda_1(x^* - x^{**})) = A(x^* - x^{**}) = 0$ and $\Lambda_0(x^* - x^{**}) = 0$, we have $x^* - x^{**} \in \ker T \cap \ker \Lambda_0 \cap \ker(\pi\Lambda_1) = \{0\}$ or $x^{**} = x^*$. On the other hand, if there exists $\overline{x} \in \ker T \cap \ker \Lambda_0 \cap \ker(\pi\Lambda_1)$, $\overline{x} \neq 0$, then $x^* + \overline{x} \in \Lambda_0^{-1}(\{z_0\}) = \Omega_0$, $A(x^* + \overline{x}) = Ax^*$, and $x^* + \overline{x}$ is a different from x^* solution of problem (2.4).

An element x^* is a solution of problem (2.4) or Ax^* is a solution of problem (2.5) if and only if

$$(Ax^* - (0, \pi z_1)) \perp A(\ker \Lambda_0)$$

or

$$(Tx^*, \pi\Lambda_1 x^* - \pi z_1) \perp (T(\ker \Lambda_0), \pi\Lambda_1(\ker \Lambda_0)),$$

i.e.,

$$\langle Tx^*, Tx\rangle + \langle \pi\Lambda_1 x^* - \pi z_1, \pi\Lambda_1 x\rangle = 0 \quad \forall x \in \ker \Lambda_0. \tag{2.6}$$

On passing to the adjoint operators, we obtain

$$\langle T^*Tx^*, x\rangle + \langle \Lambda_1^* \pi^* (\pi\Lambda_1 x^* - \pi z_1), x\rangle = 0 \quad \forall x \in \ker \Lambda_0,$$

i.e.,

$$T^*Tx^* + \Lambda_1^* \pi^* \pi(\Lambda_1 x^* - z_1) \in (\ker \Lambda_0)^\perp.$$

Due to the closedness of $\operatorname{ran} \Lambda_0$, $(\ker \Lambda_0)^\perp = \operatorname{ran} \Lambda_0^*$ and the last inclusion is equivalent to the existence of some $c \in Z_0$ such that

$$T^*Tx^* + \Lambda_1^* \pi^* \pi(\Lambda_1 x^* - z_1) = \Lambda_0^* c.$$

The proof is complete. □

Corollary 2.6. *Define* $\Lambda : X \to Z_0 \times Z_1$ *by* $\Lambda x = (\Lambda_0 x, \Lambda_1 x)$. *As for any* $x \in \ker \Lambda$, *according to* (2.6), *it holds* $\langle Tx^*, Tx\rangle = 0$, *any solution of problem* (2.4) *is a spline.*

Remark 2.7. *The assertion of Proposition 2.5 about the existence of solution is valid if* $T(\ker \Lambda_0)$ *is closed and* $\dim Z_1 < \infty$.

Proof. Denote

$$\widehat{T} = T\big|_{\ker \Lambda_0} : \ker \Lambda_0 \to Y, \quad \widehat{\pi\Lambda_1} = \pi\Lambda_1\big|_{\ker \Lambda_0} : \ker \Lambda_0 \to Z_1$$

and $\widehat{A}x = (\widehat{T}x, \widehat{\pi\Lambda_1}x)$, $x \in \ker \Lambda_0$. We show that $\operatorname{ran} \widehat{A}$ is closed. It holds $\operatorname{ran} \widehat{A}^* = \operatorname{ran} \widehat{T}^* + \operatorname{ran} (\widehat{\pi\Lambda_1})^*$. As $\operatorname{ran} \widehat{T} = T(\ker \Lambda_0)$ is closed, the equality $\operatorname{ran} \widehat{T}^* = (\ker \widehat{T})^\perp$ yields the closedness of $\operatorname{ran} \widehat{T}^*$. In addition, the assumption $\dim Z_1 < \infty$ gives $\dim \operatorname{ran} (\widehat{\pi\Lambda_1})^* < \infty$, thus, $\operatorname{ran} \widehat{A}^*$ is closed. This, in turn, implies that $\operatorname{ran} \widehat{A} = \operatorname{ran} (\widehat{A}^*)^* = (\ker \widehat{A}^*)^\perp$, i.e., $\operatorname{ran} \widehat{A}$ is closed. □

Basing on [28, 29], with the help of standard calculations it can be established the following

Proposition 2.8. *For any Hilbert spaces* X, Y *and* $T \in \mathcal{L}(X, Y)$, *having* $\dim \ker T = \infty$, $\dim(\ker T)^\perp = \infty$ *and* $\operatorname{ran} T$ *closed, there is a closed subspace* $X_0 \subset X$ *such that* $T(X_0)$ *is not closed.*

By this proposition we can take an operator $T \in \mathcal{L}(X, Y)$ satisfying $\dim \ker T = \infty$, $\dim(\ker T)^{\perp} = \infty$, $\operatorname{ran} T = Y$ and an operator $\Lambda_0 \in \mathcal{L}(X, Z_0)$ such that $T(\ker \Lambda_0)$ is not closed. We may assume that $\overline{T(\ker \Lambda_0)} \neq Y$. Now, choose the elements $\overline{y} \in \overline{T(\ker \Lambda_0)} \setminus T(\ker \Lambda_0)$ and $y' \in Y \setminus \overline{T(\ker \Lambda_0)}$ such that

$$\|y' + \overline{y}\|^2 = \min_{y \in y' + \overline{T(\ker \Lambda_0)}} \|y\|^2,$$

then the problem

$$\min_{y \in y' + T(\ker \Lambda_0)} \|y\|^2$$

does not have a solution. There exists $x' \in X$ such that $Tx' = y'$. Take $z_0 = \Lambda_0 x'$, then $\Omega_0 = \Lambda_0^{-1}(\{z_0\}) = x' + \ker \Lambda_0$. Choose any $\Lambda_1 \in \mathcal{L}(X, Z_1)$ with $\dim Z_1 < \infty$ and take $z_1 = \Lambda_1 x'$. Then it holds

$$\min_{z \in \Lambda_1 x' + \Lambda_1(\ker \Lambda_0)} \|z - z_1\|^2 = 0,$$

since $z_1 = \Lambda_1 x' \in \Lambda_1 x' + \Lambda_1(\ker \Lambda_0)$ is the solution of this problem. Finally, problem (2.5) with π as the identity operator

$$\min_{(y,z) \in A(\Omega_0)} \|(y, z) - (0, z_1)\|^2 = \min_{\substack{y \in T(\Omega_0),\, y = Tx, \\ z \in \Lambda_1(\Omega_0),\, z = \Lambda_1 x}} \left(\|y\|^2 + \|z - z_1\|^2 \right)$$

does not have a solution.

This proves that Theorem 1 in [41] is not correct. Thus, Proposition 2.5 is a right generalization of similar assertions from [11].

Let X, Y be Hilbert spaces and let $T : X \to Y$ be a bounded linear operator. For a closed convex set $C \subset X$ we consider the smoothing problem

$$\min_{x \in C} \|Tx\|. \tag{2.7}$$

Problem (2.2) is a special case of problem (2.7).

Proposition 2.9. *If $T(C)$ is closed then problem* (2.7) *has a solution. The solution $x^* \in C$ is unique if and only if $(x^* + \ker T) \cap C = \{x^*\}$. An element $x^* \in C$ is a solution of problem* (2.7) *if and only if $\langle Tx - Tx^*, Tx^* \rangle \geqslant 0$ for all $x \in C$.*

Proof. Consider the auxiliary problem

$$\min_{y \in T(C)} \|y\|. \tag{2.8}$$

The convexity and closedness of $T(C)$ implies that problem (2.8) has a unique solution $y^* \in T(C)$ and, consequently, problem (2.7) has a solution $x^* \in C$, $Tx^* = y^*$.

Suppose that there exists another solution $x^{**} \in C$ of problem (2.7). Due to the uniqueness of the solution of problem (2.8) it holds $Tx^{**} = Tx^*$ or $x^{**} \in x^* + \ker T$. But $(x^* + \ker T) \cap C = \{x^*\}$ which implies $x^* = x^{**}$. On the other hand, suppose that there exists $\overline{x} \in (x^* + \ker T) \cap C$, $\overline{x} \neq x^*$, then $\overline{x}$ is also a solution of problem (2.7). Thus, for problem (2.7), the uniqueness of solution $x^* \in C$ and the condition $(x^* + \ker T) \cap C = \{x^*\}$ are equivalent.

If $\langle y - y^*, y^* \rangle \geqslant 0$ for all $y \in T(C)$, then by the equality

$$\|y\|^2 = \|y - y^*\|^2 + 2\langle y - y^*, y^* \rangle + \|y^*\|^2$$

we have $\|y\| \geqslant \|y^*\|$ for all $y \in T(C)$ or, equivalently, y^* is a solution of problem (2.8). Suppose that there exists an element $y_1 \in T(C)$ with $\langle y_1 - y^*, y^* \rangle = a < 0$, then we can choose $\delta \in (0, 1)$ such that for $y = y^* + \delta(y_1 - y^*) = \delta y_1 + (1 - \delta) y^* \in C$ it holds

$$\begin{aligned} \|y\|^2 &= \|y - y^*\|^2 + 2\langle y - y^*, y^* \rangle + \|y^*\|^2 \\ &= \delta^2 \|y_1 - y^*\|^2 + 2\delta a + \|y^*\|^2 < \|y^*\|^2. \end{aligned}$$

We have proven that $y^* \in T(C)$ is a solution of problem (2.8) if and only if $\langle y - y^*, y^* \rangle \geqslant 0$ for all $y \in T(C)$. Thus, an element $x^* \in C$ is a solution of problem (2.7) if and only if $\langle Tx - Tx^*, Tx^* \rangle \geqslant 0$ for all $x \in C$. □

Note, in addition, following the argument of Remark 2.3, that $T(C)$ is closed provided $\operatorname{ran} T$ and $\ker T + C$ are closed.

Consider a particular case of problem (2.7). For Hilbert spaces X, Y, Z, operators $T \in \mathcal{L}(X, Y)$, $\Lambda \in \mathcal{L}(X, Z)$ and a nonempty closed convex set $C_Z \subset \operatorname{ran} \Lambda$, define $C = \Lambda^{-1}(C_Z)$. Then $C \subset X$ is a closed convex set.

The following result gives a characterization of the solution of problem (2.7) in this particular case.

Proposition 2.10. *Let* $\operatorname{ran} \Lambda$ *be closed in* Z*. An element* $x^* \in C$ *is a solution of problem* (2.7) *if and only if there exists* $z^* \in Z$ *such that* $T^*Tx^* = \Lambda^* z^*$ *(i.e.,* x^* *is a spline) and* $\langle z^*, z - \Lambda x^* \rangle \geqslant 0$ *for all* $z \in C_Z$*.*

Proof. Let $x^* \in C$ be a solution of problem (2.7). Take an arbitrary $z \in C_Z \subset \operatorname{ran} \Lambda$, then $z - \Lambda x^* \in \operatorname{ran} \Lambda$ and it exists $x \in X$ such that $\Lambda x = z - \Lambda x^*$. For any $\delta \in [0, 1]$, it holds $x^* + \delta x \in C$ since

$$\Lambda(x^* + \delta x) = \Lambda x^* + \delta \Lambda x = \Lambda x^* + \delta(z - \Lambda x^*) = \delta z + (1 - \delta)\Lambda x^* \in C_Z.$$

As x^* is the solution, we have

$$\langle T(x^* + \delta x), T(x^* + \delta x) \rangle \geqslant \langle Tx^*, Tx^* \rangle$$

or

$$2\delta\langle Tx^*, Tx\rangle + \delta^2\langle Tx, Tx\rangle \geqslant 0.$$

The assumption $\langle Tx^*, Tx\rangle < 0$ and sufficiently small $\delta > 0$ give a contradiction, thus, $\langle Tx^*, Tx\rangle \geqslant 0$. In particular, for $z = \Lambda x^*$ we may take as corresponding x any element of $\ker \Lambda$ and get $\langle Tx^*, Tx\rangle = 0$ or $\langle T^*Tx^*, x\rangle = 0$ for all $x \in \ker \Lambda$. This means that $T^*Tx^* \in (\ker \Lambda)^\perp = \operatorname{ran} \Lambda^*$ (due to the closedness of $\operatorname{ran} \Lambda$) and there is $z^* \in Z$ such that $T^*Tx^* = \Lambda^* z^*$. For any $z \in C_Z$ and $x \in X$ such that $\Lambda x = z - \Lambda x^*$, it holds

$$0 \leqslant \langle Tx^*, Tx\rangle = \langle T^*Tx^*, x\rangle = \langle \Lambda^* z^*, x\rangle = \langle z^*, \Lambda x\rangle = \langle z^*, z - \Lambda x^*\rangle.$$

Thus, $\langle z^*, z - \Lambda x^*\rangle \geqslant 0$ for all $z \in C_Z$.

Let there be $z^* \in Z$ such that $T^*Tx^* = \Lambda^* z^*$ and $\langle z^*, z - \Lambda x^*\rangle \geqslant 0$ for all $z \in C_Z$. As

$$\|Tx\|^2 - \|Tx^*\|^2 = \|Tx - Tx^*\|^2 + 2\langle Tx^*, T(x - x^*)\rangle$$

and for all $x \in C$

$$\langle Tx^*, T(x - x^*)\rangle = \langle T^*Tx^*, x - x^*\rangle = \langle \Lambda^* z^*, x - x^*\rangle = \langle z^*, \Lambda x - \Lambda x^*\rangle \geqslant 0,$$

we see that $\|Tx\|^2 \geqslant \|Tx^*\|^2$ for all $x \in C$, i.e., x^* is a solution of problem (2.7). $\square$

2.2. Problems in Hilbert spaces

Let us consider a particular case of problem (2.4). For finite index sets I_0 and I_1, with $I_0 \cap I_1 = \emptyset$, denote $I = I_0 \cup I_1$, take $Z_0 = \mathbb{R}^{|I_0|}$, $Z_1 = \mathbb{R}^{|I_1|}$, $\Lambda_0 = (\lambda_i)_{i \in I_0} \in \mathcal{L}(X, \mathbb{R}^{|I_0|})$, $\Lambda_1 = (\lambda_i)_{i \in I_1} \in \mathcal{L}(X, \mathbb{R}^{|I_1|})$, $\pi = \operatorname{diag}\{\sqrt{w_i}\}$, $w_i \geqslant 0$, $i \in I_1$, then $\pi : \mathbb{R}^{|I_1|} \to \mathbb{R}^{|I_1|}$. Problem (2.4) can be reformulated as

$$\min_{x \in \Omega_0} \left(\|Tx\|^2 + \sum_{i \in I_1} w_i |\lambda_i x - \zeta_i|^2 \right), \tag{2.9}$$

with given $z_0 = (\zeta_i)_{i \in I_0} \in \operatorname{ran} \Lambda_0$, $z_1 = (\zeta_i)_{i \in I_1}$ and the feasible set $\Omega_0 = \Lambda_0^{-1}(\{z_0\}) = \{x \in X \mid \lambda_i x = \zeta_i, i \in I_0\}$. We call (2.9) the smoothing problem with weights in Hilbert space. By Remark 2.7, problem (2.9) has a solution if $T(\ker \Lambda_0)$ is closed and by Corollary 2.6 this solution is a spline.

Let s_i, $i \in I$, be solutions of the problems

$$\min_{\substack{\lambda_i x = 1, \\ \lambda_j x = 0,\ j \in I \setminus \{i\}}} \|Tx\|.$$

Note that s_i, $i \in I$, are splines. For the existence of these splines, it is sufficient that $T(\ker \Lambda)$, $\Lambda = (\lambda_i)_{i\in I}$, is closed in Y. Any linear combination of these splines

$$s = \sum_{i\in I_1} \alpha_i s_i + \sum_{i\in I_0} \beta_i s_i \tag{2.10}$$

is also a spline. Let us take an element $\bar{s} \in \mathcal{S}$, define $z = (z_i)_{i\in I} = (\lambda_i \bar{s})_{i\in I}$ and $\Omega = \{x \in X \mid \Lambda x = z\}$. Then $\bar{s} \in \Omega$. For the spline $s_z = \sum_{i\in I} z_i s_i$ the equations $\Lambda s_z = z$ hold, thus $s_z \in \Omega$. Both, $\bar{s}$ and s_z as splines are the solutions of problem (2.2) with chosen z. If the solution of problem (2.2) is unique, i.e., $\ker T \cap \ker \Lambda = \{0\}$, then $\bar{s} = s_z = \sum_{i\in I} z_i s_i$. If the solution of problem (2.2) is not unique, then $\bar{s} - s_z \in \ker T \cap \ker \Lambda$ and $\bar{s} = s_z + s_0$, where $s_0 \in \ker T \cap \ker \Lambda$. We have proven that if the fundamental splines s_i, $i \in I$, do exist, then any spline can be written as $s + s_0$, where s has the form (2.10) and $s_0 \in \ker T \cap \ker \Lambda$. Consequently, if the fundamental splines s_i, $i \in I$, exist and problem (2.9) has a solution, then it has a solution of the form (2.10).

From now on we assume that s_i, $i \in I$, exist. Use notations $\alpha = (\alpha_i)_{i\in I_1}$, $\beta = (\beta_i)_{i\in I_0}$, $g_{ij} = \langle Ts_i, Ts_j \rangle$, $i, j \in I$, $G_1 = (g_{ij})_{i,j\in I_1}$, $G_0 = (g_{ij})_{i,j\in I_0}$, $G_{01} = (g_{ij})_{i\in I_1, j\in I_0}$, $W = \operatorname{diag}\{w_i\}$.

Proposition 2.11. *The spline*

$$s = \sum_{i\in I_1} \alpha_i s_i + \sum_{i\in I_0} \beta_i s_i$$

is a solution of problem (2.9) *if and only if the coefficients* α_i, $i \in I_1$, *satisfy the equations*

$$[G_1\alpha]_i = w_i(\zeta_i - \alpha_i) - [G_{01}\beta]_i, \quad i \in I_1, \tag{2.11}$$

with $\beta = (\zeta_i)_{i\in I_0}$.

Proof. The condition $\Lambda_0 s = z_0$ is satisfied if $\beta_i = \zeta_i$, $i \in I_0$. The functional to minimize in (2.9) can be written in the form

$$\begin{aligned}
&\|Ts\|^2 + \sum_{i\in I_1} w_i |\lambda_i s - \zeta_i|^2 \\
&\quad = \left\langle \sum_{i\in I_1} \alpha_i Ts_i + \sum_{i\in I_0} \beta_i Ts_i, \sum_{j\in I_1} \alpha_j Ts_j + \sum_{j\in I_0} \beta_j Ts_j \right\rangle + \sum_{i\in I_1} w_i |\alpha_i - \zeta_i|^2 \\
&\quad = \langle G_1\alpha, \alpha\rangle + 2\langle G_{01}\beta, \alpha\rangle + \langle G_0\beta, \beta\rangle + \langle W\alpha, \alpha\rangle - 2\langle Wz_1, \alpha\rangle + \langle Wz_1, z_1\rangle
\end{aligned}$$

and the minimization of the last expression with respect to α is equivalent to the following minimization problem of quadratic functional

$$\min_{\alpha\in\mathbb{R}^{|I_1|}} \Big(\big\langle (G_1+W)\alpha,\alpha\big\rangle - 2\big\langle Wz_1 - G_{01}\beta,\alpha\big\rangle\Big). \tag{2.12}$$

The matrix G_1 as the Gram matrix is symmetric and positive semidefinite, the same holds for the matrix W since $w_i \geqslant 0$, $i\in I_1$. Therefore, the matrix G_1+W is symmetric and positive semidefinite and an element $\alpha\in\mathbb{R}^{|I_1|}$ is a solution of problem (2.12) if and only if $(G_1+W)\alpha = Wz_1 - G_{01}\beta$.

The proof is complete. □

With the help of this proposition we prove that problem (2.9) as particular case of problem (1.7) is stable in weight reduction, which is needed to complete the proof of Proposition 2.3 in [39].

Theorem 2.12. *Smoothing problem* (2.9) *is stable in weight reduction.*

Proof. Let s be a solution of problem (2.9). Note that $\lambda_i s = \alpha_i$ for $i\in I_1$. In case of $\lambda_i s = \alpha_i \neq \zeta_i$ we have $\overline{w}_i = w_i$ and in case of $\lambda_i s = \alpha_i = \zeta_i$ we have $\overline{w}_i = 0$. If equations (2.11) hold for w_i then they also hold for $\overline{w}_i$ and the spline s is a solution of smoothing problem with reduced weights $\overline{w}$. □

Let us consider a particular case of problem (2.7). For finite index sets I_0, I_1, $I_0\cap I_1=\emptyset$, $I=I_0\cup I_1$, take $Z=\mathbb{R}^{|I|}$, $\Lambda=(\lambda_i)_{i\in I}\in\mathcal{L}(X,\mathbb{R}^{|I|})$,

$$C_Z = \prod_{i\in I_0}\{\zeta_i\}\times\prod_{i\in I_1}[\zeta_i-\varepsilon_i,\zeta_i+\varepsilon_i]\subset \operatorname{ran}\Lambda,$$

with $\varepsilon_i>0$, $i\in I_1$. The problem (2.7) in this case is

$$\min_{x\in C}\|Tx\|, \tag{2.13}$$

where

$$C=\{x\in X \mid \lambda_i x = \zeta_i, i\in I_0, \zeta_i-\varepsilon_i\leqslant\lambda_i x\leqslant\zeta_i+\varepsilon_i, i\in I_1\}.$$

We call (2.13) the smoothing problem with obstacles in Hilbert space.

Proposition 2.13. *An element $x^*\in C$ is a solution of problem* (2.13) *if and only if there exists $z^*=(z_i^*)_{i\in I}$ such that $T^*Tx^*=\sum_{i\in I} z_i^*\lambda_i$ (i.e., x^* is a spline) and*

$$\begin{aligned} z_i^* &\geqslant 0 \quad \text{if} \quad \lambda_i x^* = \zeta_i-\varepsilon_i,\ i\in I_1,\\ z_i^* &\leqslant 0 \quad \text{if} \quad \lambda_i x^* = \zeta_i+\varepsilon_i,\ i\in I_1,\\ z_i^* &= 0 \quad \text{if} \quad \zeta_i-\varepsilon_i<\lambda_i x^*<\zeta_i+\varepsilon_i,\ i\in I_1. \end{aligned} \tag{2.14}$$

Proof. According to Proposition 2.10, $x^* \in C$ is a solution of problem (2.13) if and only if there exists $z^* \in \mathbb{R}^{|I|}$ such that $T^*Tx^* = \Lambda^* z^*$ and $\langle z^*, z - \Lambda x^*\rangle \geqslant 0$ for all $z \in C_Z$. By the definition of adjoint operator

$$\langle \Lambda x, r\rangle = \sum_{i\in I}(\lambda_i x) r_i = \left(\sum_{i\in I} r_i \lambda_i\right)(x) = \langle x, \Lambda^* r\rangle,$$

thus, $\Lambda^* r = \sum_{i\in I} r_i\lambda_i$ and $T^*Tx^* = \sum_{i\in I} z_i^*\lambda_i$.

The condition $\langle z^*, z - \Lambda x^*\rangle \geqslant 0$ for all $z = (z_i)_{i\in I} \in C_Z$ means that

$$\sum_{i\in I} z_i^*(z_i - \lambda_i x^*) \geqslant 0 \quad \forall z \in C_Z = \prod_{i\in I_0}\{\zeta_i\} \times \prod_{i\in I_1}[\zeta_i - \varepsilon_i, \zeta_i + \varepsilon_i].$$

Suppose that it takes place. It is clear that $(\lambda_i x^*)_{i\in I} \in C_Z$. If $\lambda_i x^* = \zeta_i - \varepsilon_i$, $i \in I_1$, we take $z \in C_Z$ such that $z_i > \lambda_i x^*$, $z_j = \lambda_j x^*$, $j \in I \setminus \{i\}$, and from the inequality

$$0 \leqslant \sum_{j\in I} z_j^*(z_j - \lambda_j x^*) = z_i^*(z_i - \lambda_i x^*)$$

we obtain $z_i^* \geqslant 0$. Similarly, if $\lambda_i x^* = \zeta_i + \varepsilon_i$, $i \in I_1$, then $z_i^* \leqslant 0$. If $\zeta_i - \varepsilon_i < \lambda_i x^* < \zeta_i + \varepsilon_i$ for some $i \in I_1$ then we can choose $z \in C_Z$ such that $z_i > \lambda_i x^*$, $z_j = \lambda_j x^*$, $j \in I \setminus \{i\}$, and obtain $z_i^* \geqslant 0$, or such that $z_i < \lambda_i x^*$, $z_j = \lambda_j x^*$, $j \in I \setminus \{i\}$, and obtain $z_i^* \leqslant 0$, all together $z_i^* = 0$. Thus, conditions (2.14) are satisfied.

Suppose conditions (2.14) are fulfilled. For any $z \in C_Z$ it holds $z_i^*(z_i - \lambda_i x^*) \geqslant 0$ if $i \in I_1$, and $z_i - \lambda_i x^* = 0$ if $i \in I_0$. Thus $\sum_{i\in I} z_i^*(z_i - \lambda_i x^*) \geqslant 0$ for all $z \in C_Z$. □

Notice that there is no restriction about the signs of z_i^*, $i \in I_0$. In [61], p. 11-12, it is allowed that $I_0 \neq \emptyset$ but in that case according to Theorem 3, p. 12, we obtain $z_i^* = 0$, $i \in I_0$, which is not correct.

Consider again the fundamental splines s_i, $i \in I$.

Lemma 2.14. *The spline*

$$s = \sum_{i\in I_1}\alpha_i s_i + \sum_{i\in I_0}\zeta_i s_i$$

is a solution of problem (2.9) *if and only if there exists $c \in \mathbb{R}^{|I|}$ such that*

$$\langle Ts, Tx\rangle = \sum_{i\in I} c_i\lambda_i x \quad \forall x \in X$$

and

$$c_i = w_i(\zeta_i - \alpha_i), \quad i \in I_1. \tag{2.15}$$

Proof. Suppose that

$$s = \sum_{i \in I_1} \alpha_i s_i + \sum_{i \in I_0} \zeta_i s_i$$

is a solution of problem (2.9). Since s is a spline and $\operatorname{ran} \Lambda$ is closed, there exists $c \in \mathbb{R}^{|I|}$ such that

$$T^* T s = \sum_{i \in I} c_i \lambda_i$$

or, equivalently,

$$\langle Ts, Tx \rangle = \sum_{i \in I} c_i \lambda_i x \quad \forall x \in X.$$

Consequently, $\langle Ts, Ts_i \rangle = c_i$, $i \in I$. On the other hand,

$$\langle Ts, Ts_i \rangle = \sum_{j \in I_1} \alpha_j \langle Ts_j, Ts_i \rangle + \sum_{j \in I_0} \zeta_j \langle Ts_j, Ts_i \rangle = [G_1 \alpha]_i + [G_{01} z_0]_i, \quad i \in I_1,$$

and by Proposition 2.11

$$[G_1 \alpha]_i + [G_{01} z_0]_i = w_i(\zeta_i - \alpha_i), \quad i \in I_1.$$

We see that the equations (2.15) hold.

Suppose that there exists $c \in \mathbb{R}^{|I|}$ such that

$$\langle Ts, Tx \rangle = \sum_{i \in I} c_i \lambda_i x \quad \forall x \in X$$

and (2.15) holds. Then

$$w_i(\zeta_i - \alpha_i) = c_i = \langle Ts, Ts_i \rangle = [G_1 \alpha]_i + [G_{01} z_0]_i, \quad i \in I_1,$$

and by Proposition 2.11 the spline

$$s = \sum_{i \in I_1} \alpha_i s_i + \sum_{i \in I_0} \zeta_i s_i$$

is a solution of problem (2.9). □

Let us introduce the Lagrangian

$$L(x, v) = \|Tx\|^2 + \sum_{i \in I_1} v_i \left(|\lambda_i x - \zeta_i|^2 - \varepsilon_i^2 \right), \quad x \in \Omega_0, v \in \mathbb{R}_+^{|I_1|}, \tag{2.16}$$

associated to problem (2.13) with $\Omega_0 = \{x \in X \mid \lambda_i x = \zeta_i, i \in I_0\}$.

Theorem 2.15. *Suppose that $T(\ker \Lambda)$ is closed. For any solution x^* of problem (2.13), the Lagrangian (2.16) has a saddle point (x^*, w). Consequently, x^* is also a solution of problem (2.9) with the weights w (with the same given data I_0, I_1, λ_i, z_0 and z_1).*

Proof. The closedness of $T(\ker \Lambda)$ implies the existence of fundamental splines s_i, $i \in I$. Let x^* be a solution of smoothing problem with obstacles (2.13). The solution x^* as spline can be written in form $x^* = s^* + s_0$ where

$$s^* = \sum_{i \in I_1} \alpha_i s_i + \sum_{i \in I_0} \beta_i s_i$$

and $s_0 \in \ker T \cap \ker \Lambda$. Consequently, $Tx^* = Ts^*$ and $\lambda_i x^* = \lambda_i s^*$, $i \in I$, which means that s^* is also a solution of problem (2.13). According to Proposition 2.13, there exists z^* such that $T^*Ts^* = \sum_{i \in I} z_i^* \lambda_i$ and the conditions (2.14) hold. In case of $\lambda_i s^* = \alpha_i = \zeta_i - \varepsilon_i$, $i \in I_1$, we have $z_i^* \geqslant 0$ and $\zeta_i - \alpha_i = \varepsilon_i > 0$. Similarly, in case of $\lambda_i s^* = \alpha_i = \zeta_i + \varepsilon_i$, $i \in I_1$, we have $z_i^* \leqslant 0$ and $\zeta_i - \alpha_i = -\varepsilon_i < 0$. In both cases define $w_i = z_i^*/(\zeta_i - \alpha_i)$, then $w_i \geqslant 0$. If $\zeta_i - \varepsilon_i < \lambda_i s^* < \zeta_i + \varepsilon_i$, $i \in I_1$, then $z_i^* = 0$ and we take $w_i = 0$. We see that the conditions (2.15) hold for $c_i = z_i^*$, $i \in I_1$. Therefore, by Lemma 2.14, the spline s^* with $\beta_i = \zeta_i$, $i \in I_0$, is a solution of smoothing problem (2.9) with just defined weights w.

Define $\bar{\varepsilon}_i = |\lambda_i s^* - \zeta_i|$, $i \in I_1$, then, by Proposition 1.3, (s^*, w) is a saddle point of Lagrangian

$$L(x, v) = \|Tx\|^2 + \sum_{i \in I_1} v_i \left(|\lambda_i x - \zeta_i|^2 - \bar{\varepsilon}_i^2 \right), \quad x \in \Omega_0, v \in \mathbb{R}_+^{|I_1|},$$

i.e.,

$$\begin{aligned}
&\|Ts^*\|^2 + \sum_{i \in I_1} v_i \left(|\lambda_i s^* - \zeta_i|^2 - \bar{\varepsilon}_i^2 \right) \\
&\qquad \leqslant \quad \|Ts^*\|^2 + \sum_{i \in I_1} w_i \left(|\lambda_i s^* - \zeta_i|^2 - \bar{\varepsilon}_i^2 \right) \\
&\qquad \leqslant \quad \|Tx\|^2 + \sum_{i \in I_1} w_i \left(|\lambda_i x - \zeta_i|^2 - \bar{\varepsilon}_i^2 \right) \quad \forall x \in \Omega_0, \forall v \in \mathbb{R}_+^{|I_1|}.
\end{aligned}$$

By the definition $\bar{\varepsilon}_i \leqslant \varepsilon_i$ and if $\bar{\varepsilon}_i < \varepsilon_i$ then $w_i = 0$, $i \in I_1$. Consequently, for all $v \in \mathbb{R}_+^{|I_1|}$, $x \in \Omega_0$ and $i \in I_1$ it holds

$$\begin{aligned}
v_i \left(|\lambda_i s^* - \zeta_i|^2 - \varepsilon_i^2 \right) &\leqslant v_i \left(|\lambda_i s^* - \zeta_i|^2 - \bar{\varepsilon}_i^2 \right), \\
w_i \left(|\lambda_i x - \zeta_i|^2 - \bar{\varepsilon}_i^2 \right) &= w_i \left(|\lambda_i x - \zeta_i|^2 - \varepsilon_i^2 \right),
\end{aligned}$$

thus (s^*, w) is a saddle point of Lagrangian (2.16). Considering the equalities $Tx^* = Ts^*$ and $\lambda_i x^* = \lambda_i s^*$, $i \in I$, we see that (x^*, w) is also a saddle point of Lagrangian (2.16) and, by Lemma 1.2, x^* is a solution of problem (2.9) with weights w. $\square$

Finally, let us present some practical examples of smoothing problems in Hilbert spaces.

Example 2.1. Let $X = W_2^m(a,b)$ be the Sobolev space and $Y = L_2(a,b)$ the space of square integrable functions. Take $T = D^m$ as the operator of m-th order differentiation and for given mesh $a = t_1 < t_2 < \ldots < t_n = b$ define $\Lambda = (\lambda_i)_{i=1}^n$ as point functionals $\lambda_i x = x(t_i)$. Let $I = \{1, 2, \ldots, n\}$, $I_0, I_1 \subset I$, $I_0 \cap I_1 = \emptyset$, $I_0 \cup I_1 = I$. Then we have the smoothing problem with obstacles

$$\min_{x \in \Omega} \int_a^b \left(x^{(m)}(t)\right)^2 dt,$$

where $\Omega = \left\{x \in W_2^m(a,b) \bigm| x(t_i) = z_i, i \in I_0,\ |x(t_i) - z_i| \leqslant \varepsilon_i, i \in I_1\right\}$, and the smoothing problem with weights

$$\min_{x \in \Omega_0} \left(\int_a^b \left(x^{(m)}(t)\right)^2 dt + \sum_{i \in I} w_i |x(t_i) - z_i|^2 \right),$$

where $\Omega_0 = \left\{x \in W_2^m(a,b) \bigm| x(t_i) = z_i, i \in I_0\right\}$. The set $\ker T$ consists of polynomials of degree not exceeding $m-1$, therefore, $\dim \ker T = m$. In addition, $T(\ker \Lambda)$ and $T(\ker \Lambda_0)$ are closed which means that the corresponding assumptions in several Propositions of Sections 2.1 and 2.2 are satisfied.

Example 2.2. Let X, Y and T be as in previous example. For given mesh $a = t_1 \leqslant t_2 \leqslant \ldots \leqslant t_n = b$ with multiplicity of knots t_i at most m, i.e., $m_i = \left|\{t_k \mid k \leqslant i, t_k = t_i\}\right| \leqslant m$, $i = 1, \ldots, n$, define $\lambda_i x = x^{(m_i - 1)}(t_i)$. Note that in case of $m_i = 1$, $i = 1, \ldots, n$, this example coincides with the previous one. The smoothing problems with such data are the main objects of study in [39, 40, 41].

Example 2.3. Let X, Y and T be as in previous examples. For given mesh $a = t_0 < t_1 < \ldots < t_n = b$, define

$$\lambda_i x = \frac{1}{t_i - t_{i-1}} \int_{t_{i-1}}^{t_i} x(t)dt, \quad i = 1, \ldots, n.$$

The corresponding problems (2.9) and (2.13) are problems of smoothing histopolation.

CHAPTER 3

Classical smoothing problems in Beppo Levi space

In this chapter we consider classical smoothing problems for several variables where the values to be smoothened are the knot values of an unknown function. The solutions of these problems are natural splines – functions consisting of polynomial part and a linear combination of the shifts of certain radial basis functions. We refer the reader to [19] and [68] for a systematic treatment of radial basis functions.

For the solution of classical smoothing problem with weights one has to solve a linear system of equations given in Section 3.2. In case of the classical smoothing problem with obstacles necessary and sufficient conditions describing the solution are known (see Section 3.4) but finding an algorithm to solve this problem is still an open problem. One natural idea is to reduce the problem with obstacles to the problem with weights. In Section 3.4 we prove that this kind of reduction is possible – for any problem with obstacles there exists an equivalent problem with weights and vice versa.

3.1. Notation and preliminaries

For given integers r and n, $2r > n \geqslant 1$, let us denote by $L_2^{(r)}(\mathbb{R}^n)$ the space of functions defined on $\mathbb{R}^n$ having all partial (distributional) derivatives of order r in $L_2(\mathbb{R}^n)$, i.e.,

$$L_2^{(r)}(\mathbb{R}^n) = \{f : \mathbb{R}^n \to \mathbb{R} \mid D^\alpha f \in L_2(\mathbb{R}^n), |\alpha| = r\},$$

where $\alpha = (\alpha_1, \ldots, \alpha_n)$, $\alpha_i \geqslant 0$ and $|\alpha| = \alpha_1 + \ldots + \alpha_n$. The space $L_2^{(r)}(\mathbb{R}^n)$ is called Beppo Levi space. Comprehensive treatment of Beppo Levi spaces can be found in [27]. Define the operator

$$T : L_2^{(r)}(\mathbb{R}^n) \to L_2(\mathbb{R}^n) \times \ldots \times L_2(\mathbb{R}^n)$$

as

$$Tf = \left\{ \sqrt{\frac{r!}{\alpha!}} D^\alpha f \,\middle|\, |\alpha| = r \right\}$$

with $\alpha! = \alpha_1! \dots \alpha_n!$. We also need the semi-inner product

$$\langle Tf, Tg \rangle = \sum_{|\alpha|=r} \frac{r!}{\alpha!} \int_{\mathbb{R}^n} D^\alpha f \, D^\alpha g \, dX, \quad f, g \in L_2^{(r)}(\mathbb{R}^n),$$

and the corresponding seminorm $\|Tf\| = \sqrt{\langle Tf, Tf \rangle}$.

Let $\mathcal{P}_{r-1}$ be the space of polynomials of degree not exceeding $r-1$. From the theory of distributions it is known that if $\|Tf\| = 0$ or, equivalently, $D^\alpha f = 0$ for all α such that $|\alpha| = r$, then $f \in \mathcal{P}_{r-1}$ (see, e.g., [3]).

A function of the form

$$S(X) = P(X) + \sum_{i \in I} d_i G(X - X_i), X \in \mathbb{R}^n, \tag{3.1}$$

with $P \in \mathcal{P}_{r-1}$,

$$\sum_{i \in I} d_i Q(X_i) = 0 \quad \forall Q \in \mathcal{P}_{r-1}, \tag{3.2}$$

I a finite set and arbitrary $X_i \in \mathbb{R}^n$, $X_i \neq X_j$ for $i \neq j$, is called a natural spline. Here G is the fundamental solution of the operator Δ^r, where Δ is the n-dimensional Laplace operator. It is known that, for n odd, $G(X) = c_{nr}\|X\|^{2r-n}$ and, for n even, $G(X) = c_{nr}\|X\|^{2r-n} \log \|X\|$ with some constants $c_{nr} > 0$ and $\|X\| = \sqrt{x_1^2 + \ldots + x_n^2}$ (see [58], p. 521). It is also known that any natural spline belongs to $L_2^{(r)}(\mathbb{R}^n)$. Futhermore, for all $f \in L_2^{(r)}(\mathbb{R}^n)$ and any natural spline S, it holds

$$\langle TS, Tf \rangle = (-1)^r \sum_{i \in I} d_i f(X_i). \tag{3.3}$$

The proof of the last two assertions can be found in [33], p. 21-23.

Assume that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ in the knots X_i, $i \in I$, possesses a unique solution. This assumption is not very restrictive, for instance, in case of $n = 1$ it is satisfied if $|I| \geqslant r$ (the notation $|I|$ is used to represent the number of elements in an index set I). In case of $n = 2$ this assumption is satisfied if $|I| \geqslant r(1+r)/2$ and the knots X_i, $i \in I$, are not situated on the same $(r-1)$th order algebraic curve.

Lemma 3.1. *If $P \in \mathcal{P}_{r-1}$, $P(X_i) = 0$, $i \in I$, implies $P = 0$, then for given data z_i, $i \in I$, there exists a unique natural spline S satisfying $S(X_i) = z_i$, $i \in I$.*

Proof. Let Q_j, $j \in J$ be a basis in the space $\mathcal{P}_{r-1}$. Conditions $S(X_i) = z_i$, $i \in I$, and (3.2) generate $|I| + |J|$ linear equations

$$\begin{aligned} P(X_i) + \sum_{k \in I} d_k G(X_i - X_k) &= z_i, \quad i \in I, \\ \sum_{k \in I} d_k Q_j(X_k) &= 0, \quad j \in J. \end{aligned}$$

The number of coefficients to be determined in the representation of natural spine (3.1) is also $|I| + |J|$. It is sufficient to show that the corresponding homogeneous system has only trivial solution. Let S_0 with $S_0(X_i) = 0$, $i \in I$, and coefficients $d_i(S_0)$, $i \in I$, be the solution of the corresponding homogeneous system. Then, by (3.3), it holds

$$\langle TS_0, TS_0 \rangle = (-1)^r \sum_{i \in I} d_i(S_0)\, S_0(X_i) = 0$$

which means that $S_0 \in \mathcal{P}_{r-1}$. Our assumption about unique solvability of zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ implies $S_0 = 0$ and, consequently, corresponding homogeneous system possesses a unique solution. Thus the initial problem has a unique solution. □

3.2. Smoothing problems with weights

For given sets of indexes I_0, I_1, $I_0 \cap I_1 = \emptyset$, $I_0 \cup I_1 = I$, weights $w_i \geqslant 0$, $i \in I_1$, pairwise distinct points $X_i \in \mathbb{R}^n$, $i \in I$, and values $z_i \in \mathbb{R}$, $i \in I$, define

$$\Omega_0 = \{ f \in L_2^{(r)}(\mathbb{R}^n) \mid f(X_i) = z_i, i \in I_0 \}.$$

We consider the minimization problem

$$\min_{f \in \Omega_0} \left(\|Tf\|^2 + \sum_{i \in I_1} w_i |f(X_i) - z_i|^2 \right) \tag{3.4}$$

as the classical smoothing problem with weights.

Assume that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ in the knots X_i, $i \in I_0 \cup \{ j \in I_1 \mid w_j \neq 0 \}$, possesses a unique solution. According to the next proposition the solution of problem (3.4) exists and is a natural spline of the form (3.1).

Proposition 3.2. *If $P \in \mathcal{P}_{r-1}$, $P(X_i) = 0$, $i \in I_0 \cup \{ j \in I_1 \mid w_j \neq 0 \}$, implies $P = 0$, then there exists only one natural spline S of the form* (3.1) *satisfying*

$$\begin{aligned} (-1)^r d_i + w_i S(X_i) &= w_i z_i, \quad i \in I_1, \\ S(X_i) &= z_i, \quad\;\; i \in I_0, \end{aligned} \tag{3.5}$$

and this spline is the unique solution of the smoothing problem with weights.

Proof. The number of coefficients to determine in the representation (3.1) of a natural spline is equal to the number of linear equations (3.5) with (3.2). For the uniqueness of the solution of (3.5) it is sufficient to show that the corresponding homogeneous system has only trivial solution. Suppose S_0 is a natural spline such that

$$\begin{aligned}(-1)^r d_i(S_0) + w_i S_0(X_i) &= 0, \quad i \in I_1,\\ S_0(X_i) &= 0, \quad i \in I_0.\end{aligned}$$

If $d_i(S_0) \neq 0$, then $w_i \neq 0$ and $S_0(X_i) = -(-1)^r \dfrac{d_i(S_0)}{w_i}$. From (3.3) with $S = f = S_0$, we obtain

$$\begin{aligned}0 \leqslant \langle TS_0, TS_0\rangle &= (-1)^r \sum_{i\in I} d_i(S_0)\, S_0(X_i)\\ &= (-1)^r \sum_{i\in I_1,\, d_i(S_0)\neq 0} d_i(S_0)\, S_0(X_i)\\ &= -(-1)^{2r} \sum_{i\in I_1,\, d_i(S_0)\neq 0} \frac{d_i^2(S_0)}{w_i},\end{aligned}$$

which implies that $d_i(S_0) = 0$ for all $i \in I_1$ and $\|TS_0\| = 0$ or, equivalently, $S_0 \in \mathcal{P}_{r-1}$. Since

$$\begin{aligned}w_i S_0(X_i) &= 0, \quad i \in I_1,\\ S_0(X_i) &= 0, \quad i \in I_0,\end{aligned}$$

we have $S_0(X_i) = 0$, $i \in I_0 \cup \{j \in I_1 \,|\, w_j \neq 0\}$, and according to our assumption $S_0 = 0$.

Let S be the natural spline satisfying (3.5). Each element in Ω_0 may be represented in the form $S + h$, where $h \in L_2^{(r)}(\mathbb{R}^n)$ and $h(X_i) = 0$, $i \in I_0$. Denote by F the functional to minimize in the smoothing problem. Then, using also (3.3), we have

$$\begin{aligned}F(S+h) &= \|T(S+h)\|^2 + \sum_{i\in I_1} w_i |S(X_i) + h(X_i) - z_i|^2\\ &= \|TS\|^2 + 2\langle TS, Th\rangle + \|Th\|^2 + \sum_{i\in I_1} w_i |S(X_i) - z_i|^2\\ &\quad + 2\sum_{i\in I_1} w_i (S(X_i) - z_i) h(X_i) + \sum_{i\in I_1} w_i |h(X_i)|^2\end{aligned}$$

$$= \quad F(S) + 2\sum_{i\in I_1} \left((-1)^r d_i(S) + w_i S(X_i) - w_i z_i\right) h(X_i)$$
$$+ \|Th\|^2 + \sum_{i\in I_1} w_i |h(X_i)|^2.$$

Hence, according to (3.5), we see that $F(S+h) \geqslant F(S)$. Moreover, $F(S+h) = F(S)$ yields $\|Th\| = 0$, $h(X_i) = 0$, $i \in \{j \in I_1 \mid w_j \neq 0\}$, and this with $h(X_i) = 0$, $i \in I_0$, gives $h = 0$. □

Note that a natural spline satisfying (3.5) is the solution of problem (3.4) without any additional assumptions. Assumptions about unique solvability of interpolation problem with polynomials is used to prove the existence and uniqueness of the solution.

The proof of Proposition 3.2 is a slight modification of that of Proposition 1 in [6], where the case $w_i > 0$, $i \in I_1$, is treated.

3.3. Smoothing problems with obstacles

For given sets of indexes I_0, I_1, $I_0 \cap I_1 = \emptyset$, $I_0 \cup I_1 = I$, obstacles $\varepsilon_i > 0$, $i \in I_1$, pairwise distinct points $X_i \in \mathbb{R}^n$, $i \in I$, and values $z_i \in \mathbb{R}$, $i \in I$, define

$$\Omega = \{f \in L_2^{(r)}(\mathbb{R}^n) \mid f(X_i) = z_i, i \in I_0, |f(X_i) - z_i| \leqslant \varepsilon_i, i \in I_1\}.$$

We consider the minimization problem

$$\min_{f\in\Omega} \|Tf\|^2 \tag{3.6}$$

as the classical smoothing problem with obstacles.

Assume that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ in the knots X_i, $i \in I$, possesses a unique solution. The solution of smoothing problem (3.6) with obstacles exists and is a natural spline (see [33], p. 64-67). The next proposition (see [33], p. 66) characterizes the solution of the problem (3.6).

Proposition 3.3. *A natural spline S of the form* (3.1) *such that $S \in \Omega$ is a solution of the problem* (3.6) *if and only if the coefficients d_i, $i \in I_1$, of S satisfy the conditions*

$$\begin{aligned} d_i = 0, &\quad \textit{if} \quad |S(X_i) - z_i| < \varepsilon_i, \\ (-1)^r d_i \geqslant 0, &\quad \textit{if} \quad S(X_i) = z_i - \varepsilon_i, \\ (-1)^r d_i \leqslant 0, &\quad \textit{if} \quad S(X_i) = z_i + \varepsilon_i. \end{aligned} \tag{3.7}$$

For the uniqueness of the solution it is sufficient that the interpolation problem with polynomials

$$P(X_i) = 0, \quad i \in I_0,\ P \in \mathcal{P}_{r-1},$$

has only the solution $P = 0$.

In the next example we observe how to determine the signs of d_i, $i \in I$, in case of natural linear splines when the graph of the spline is given.

Example 3.1. Consider the case $n = r = 1$. A natural linear spline S with knots $x_1 < \ldots < x_m$ can be represented as

$$S(x) = c + \sum_{i=1}^{m} d_i \frac{|x - x_i|}{2}, \quad \sum_{i=1}^{m} d_i = 0.$$

For $x \leqslant x_1$ it holds

$$S(x) = c + \frac{1}{2}\sum_{i=1}^{m} d_i x_i - \frac{1}{2}\left(\sum_{i=1}^{m} d_i\right) x = c + \frac{1}{2}\sum_{i=1}^{m} d_i x_i = c_1$$

and for $x \geqslant x_m$ it holds

$$S(x) = c + \frac{1}{2}\left(\sum_{i=1}^{m} d_i\right) x - \frac{1}{2}\sum_{i=1}^{m} d_i x_i = c - \frac{1}{2}\sum_{i=1}^{m} d_i x_i = c_2.$$

On every subinterval $[x_i, x_{i+1}]$, $i = 1, \ldots, m-1$, the spline S is a linear function and at the knots x_i, $i = 1, \ldots, m$, it is continuous. Let us compute the first order divided differences for data points $(x_i, S(x_i))$, $i = 1, \ldots, m$,

$$\begin{aligned}
S(x_{i+1}) &= c + \frac{1}{2}\sum_{k=1}^{i} d_k (x_{i+1} - x_k) + \frac{1}{2}\sum_{k=i+1}^{m} d_k (x_k - x_{i+1}), \\
S(x_i) &= c + \frac{1}{2}\sum_{k=1}^{i} d_k (x_i - x_k) + \frac{1}{2}\sum_{k=i+1}^{m} d_k (x_k - x_i), \\
S(x_{i+1}) - S(x_i) &= \frac{1}{2}\sum_{k=1}^{i} d_k (x_{i+1} - x_i) - \frac{1}{2}\sum_{k=i+1}^{m} d_k (x_{i+1} - x_i) \\
&= \frac{1}{2}\left(\sum_{k=1}^{i} d_k - \sum_{k=i+1}^{m} d_k + \sum_{k=1}^{m} d_k\right)(x_{i+1} - x_i) \\
&= \sum_{k=1}^{i} d_k (x_{i+1} - x_i), \\
S'(x_i+) &= \sum_{k=1}^{i} d_k.
\end{aligned}$$

We see that the slope of the spline on the interval $[x_i, x_{i+1}]$ differs from the slope on the interval $[x_{i-1}, x_i]$ by d_i. It allows us to determine the signs of d_i, $i = 1, \ldots, m$, on the graph of the spline S by comparing the slopes $S'(x_i+)$ and $S'(x_i-)$ (see Fig. 3.1).

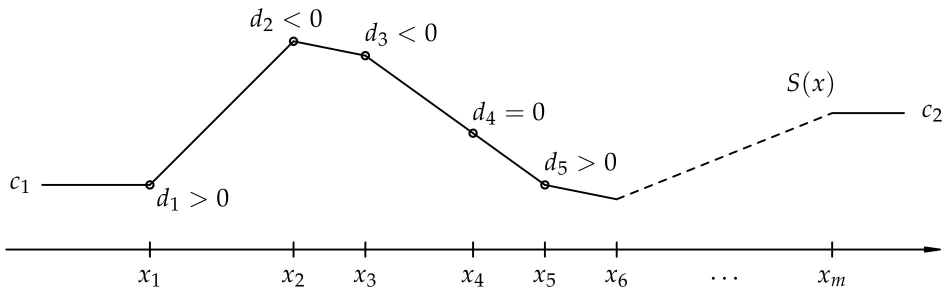

Figure 3.1. The signs of the coefficients d_i of the natural linear spline.

3.4. Equivalence of smoothing problems with obstacles and weights

Note that $L_2^{(r)}(\mathbb{R}^n)$ is not Hilbert space and we cannot treat problems (3.4) and (3.6) in the framework of Chapter 2.

The equivalence of problems (3.4) and (3.6) is based on next two theorems. In case of problem (3.4) with weights, we assume that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ in the knots X_i, $i \in I_0 \cup \{j \in I_1 \mid w_j \neq 0\}$, possesses a unique solution. In case of problem (3.6) with obstacles, for solvability we assume that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ in the knots X_i, $i \in I$, possesses a unique solution.

Theorem 3.4. *Classical smoothing problem* (3.4) *with weights is stable in weight reduction.*

Proof. Let S be a solution of problem (3.4) with weights w. According to Proposition 3.2, the conditions

$$(-1)^r d_i = w_i(z_i - S(X_i)), \quad i \in I_1,$$

hold. Define $\overline{w}_i = w_i$ in case of $S(X_i) \neq z_i$, $i \in I_1$, and $\overline{w}_i = 0$ in case of $S(X_i) = z_i$, $i \in I_1$. If previous equations hold for w_i then they also hold for $\overline{w}_i$ and S is a solution of problem with reduced weights $\overline{w}$. $\square$

By Corollary 1.6, for any smoothing problem (3.4) with weights there exists an equivalent smoothing problem (3.6) with obstacles such that I_0, I_1, X_i and z_i do not change and the solutions of problems coincide.

Now, consider the smoothing problem (3.6) with obstacles and let

$$L(f,v) = \|Tf\|^2 + \sum_{i\in I_1} v_i(|f(x_i) - z_i|^2 - \varepsilon_i^2), \quad f \in \Omega_0, v \in \mathbb{R}_+^{|I_1|}, \tag{3.8}$$

be the Lagrangian associated to problem (3.6).

Theorem 3.5. *The Lagrangian* (3.8) *has a saddle point and, consequently, there is a problem* (3.4) *such that the solutions of problems* (3.6) *and* (3.4) *coincide (at it I_0, I_1, X_i and z_i do not change).*

Proof. Let S be a solution of problem (3.6). We know that S has the form (3.1). According to Proposition 3.3, the solution S satisfies the conditions (3.7). Let us remove the knots X_i, $i \in I_1$, where $d_i = 0$. Define

$$\overline{I}_1 = \{i \in I_1 \mid d_i \neq 0\}$$

and consider the smoothing problem

$$\min_{f\in\overline{\Omega}} \|Tf\|^2,$$

where $\overline{\Omega} = \{f \in L_2^{(r)}(\mathbb{R}^n) \mid f(X_i) = z_i, i \in I_0, |f(X_i) - z_i| \leqslant \varepsilon_i, i \in \overline{I}_1\}$. Since $\Omega \subset \overline{\Omega}$, we have

$$\min_{f\in\overline{\Omega}} \|Tf\|^2 \leqslant \min_{f\in\Omega} \|Tf\|^2 = \|TS\|^2.$$

As in the knots of $\overline{I}_1$ the coefficients of the spline S satisfy the conditions (3.7), we have $\|TS\|^2 = \min\limits_{f\in\overline{\Omega}} \|Tf\|^2$.

Since $d_i \neq 0$, $i \in \overline{I}_1$, and according to (3.7), it also holds $S(X_i) \neq z_i$, $i \in \overline{I}_1$, determine the weights $\overline{w}_i > 0$, $i \in \overline{I}_1$, from equations

$$(-1)^r d_i = \overline{w}_i(z_i - S(X_i)), \quad i \in \overline{I}_1. \tag{3.9}$$

Consider the smoothing problem with obstacles

$$\min_{f\in\Omega_0} \left(\|Tf\|^2 + \sum_{i\in\overline{I}_1} \overline{w}_i |f(X_i) - z_i|^2 \right).$$

According to the conditions (3.9) and Proposition 3.2, the solution of this problem is S, i.e.,

$$\|TS\|^2 + \sum_{i\in\overline{I}_1} \overline{w}_i |S(X_i) - z_i|^2 \leqslant \|Tf\|^2 + \sum_{i\in\overline{I}_1} \overline{w}_i |f(X_i) - z_i|^2 \quad \forall f \in \Omega_0.$$

Define a new problem with weights $w_i = \overline{w}_i$, $i \in \overline{I}_1$, and $w_i = 0$, $i \in I_1 \setminus \overline{I}_1$. Then

$$\begin{aligned}
L(S,w) &= \|TS\|^2 + \sum_{i\in I_1} w_i(|S(X_i) - z_i|^2 - \varepsilon_i^2) \\
&= \|TS\|^2 + \sum_{i\in \overline{I}_1} \overline{w}_i(|S(X_i) - z_i|^2 - \varepsilon_i^2) \\
&\leqslant \|Tf\|^2 + \sum_{i\in \overline{I}_1} \overline{w}_i(|f(X_i) - z_i|^2 - \varepsilon_i^2) \\
&= L(f,w) \quad \forall f \in \Omega_0.
\end{aligned}$$

As $|S(X_i) - z_i| = \varepsilon_i$, $i \in \overline{I}_1$, and $w_i = 0$, $i \in I_1 \setminus \overline{I}_1$, it holds that $w_i(|S(X_i) - z_i|^2 - \varepsilon_i^2) = 0$, $i \in I_1$. In general, $|S(X_i) - z_i| \leqslant \varepsilon_i$, $i \in I_1$, since S is the solution of problem (3.6). Thus, $v_i(|S(X_i) - z_i|^2 - \varepsilon_i^2) \leqslant 0$ for all $v_i \geqslant 0$, $i \in I_1$. Therefore,

$$\begin{aligned}
L(S,v) &= \|TS\|^2 + \sum_{i\in I_1} v_i(|S(X_i) - z_i|^2 - \varepsilon_i^2) \\
&\leqslant \|TS\|^2 + \sum_{i\in I_1} w_i(|S(X_i) - z_i|^2 - \varepsilon_i^2) \\
&= L(S,w) \quad \forall v \in \mathbb{R}_+^{|I_1|}.
\end{aligned}$$

We have shown that (S,w) is a saddle point of Lagrangian (3.8). According to Lemma 1.2, the spline S is the solution of problem (3.4) with weights w.

□

CHAPTER 4

A method of adding-removing knots

In this chapter we study a method of adding-removing knots proposed in [33] for solving the smoothing problem with obstacles. A proof of the finiteness of the method in [33] is proposed but this proof is based on a false lemma (Lemma 10.3 in [33]). We give a counterexample to this lemma and also an example of cycling in the algorithm. The proof of the finiteness given in [33] uses the idea of monotonically increasing seminorms. One of our examples shows that even if the method provides the solution in a finite number of steps, the corresponding seminorms may in fact not be monotone. In the last section we give some sufficient conditions for finiteness of the method.

Each step of the method of adding-removing knots consists of the solution of an interpolation problem. Note that in the case of several variables the effect of the removal or addition of knots for interpolation, which uses radially symmetric functions, is analyzed in [20].

4.1. Algorithm

Smoothing problem (3.6) with obstacles can be reformulated as

$$\min_{f \in \Omega_{\alpha\beta}} \|Tf\|^2 \tag{4.1}$$

where $\Omega_{\alpha\beta} = \{f \in L_2^{(r)}(\mathbb{R}^n) \mid f(X_i) = z_i, i \in I_0,\ \alpha_i \leqslant f(X_i) \leqslant \beta_i, i \in I_1\}$ and $\alpha_i = z_i - \varepsilon_i$, $\beta_i = z_i + \varepsilon_i$, $i \in I_1$. According to Proposition 3.3, a natural spline $S \in \Omega_{\alpha\beta}$ is a solution of problem (4.1) if and only if the coefficients d_i, $i \in I_1$, of S satisfy the conditions

$$\begin{aligned} d_i = 0, \quad &\text{if} \quad \alpha_i < S(X_i) < \beta_i, \\ (-1)^r d_i \geqslant 0, \quad &\text{if} \quad S(X_i) = \alpha_i, \\ (-1)^r d_i \leqslant 0, \quad &\text{if} \quad S(X_i) = \beta_i. \end{aligned} \tag{4.2}$$

Hence, the solution of problem (4.1) is actually an interpolating natural spline. For the solution S it is sufficient to indicate the sets $M^\alpha, M^\beta \subset I_1$ of indices such that $S(X_i) = \alpha_i$, $i \in M^\alpha$, $S(X_i) = \beta_i$, $i \in M^\beta$, with $d_i \neq 0$, $i \in M^\alpha \cup M^\beta$, and $d_i = 0$, $i \in I_1 \setminus (M^\alpha \cup M^\beta)$. Then the knots X_i corresponding to $i \in M^\alpha \cup M^\beta$ can be called active. A method of adding-removing knots is in fact a procedure of finding the sets M^α and M^β of active knots for the solution. We present in the following a detailed description of the algorithm.

Step 1. Let Q_j, $j \in J$, be a basis in the space $\mathcal{P}_{r-1}$. Construct the natural spline

$$S_0(X) = \sum_{j\in J} c_j(S_0)Q_j(X) + \sum_{i\in I_0} d_i(S_0)G(X - X_i)$$

such that $S_0(X_k) = z_k$, $k \in I_0$. To find the coefficients $c_j(S_0)$ and $d_i(S_0)$ we have to solve the linear system of equations

$$\sum_{j\in J} c_j(S_0)Q_j(X_k) + \sum_{i\in I_0} d_i(S_0)G(X_k - X_i) = z_k, \quad k \in I_0,$$

$$\sum_{i\in I_0} d_i(S_0)Q_j(X_i) = 0, \quad j \in J.$$

Then we check the obstacle conditions

$$\alpha_i \leqslant S_0(X_i) \leqslant \beta_i, \quad i \in I_1. \tag{4.3}$$

If all the conditions (4.3) hold then S_0 is the solution of the initial problem, otherwise we define $M_0^\alpha = \emptyset$, $M_0^\beta = \emptyset$, $k = 1$, and we continue with step 2.

Step 2 (the step of adding knots). Suppose we have $M_{k-1}^\alpha, M_{k-1}^\beta \subset I_1$ and a natural spline

$$S_{k-1}(X) = \sum_{j\in J} c_j(S_{k-1})Q_j(X) + \sum_{i\in I_0\cup M_{k-1}^\alpha \cup M_{k-1}^\beta} d_i(S_{k-1})G(X - X_i)$$

such that

$$S_{k-1}(X_i) = z_i, \quad i \in I_0,$$

$$S_{k-1}(X_i) = \alpha_i,\ (-1)^r d_i(S_{k-1}) > 0, \quad i \in M_{k-1}^\alpha,$$

$$S_{k-1}(X_i) = \beta_i,\ (-1)^r d_i(S_{k-1}) < 0, \quad i \in M_{k-1}^\beta.$$

Note that by Proposition 3.3, S_{k-1} is the solution of the problem

$$\min_{f\in\Omega_{k-1}} \|Tf\|^2,$$

where

$$\Omega_{k-1} = \{f \in L_2^{(r)}\mathbb{R}^n \mid f(X_i) = z_i, i \in I_0,$$
$$\alpha_i \leqslant f(X_i) \leqslant \beta_i, i \in M_{k-1}^{\alpha} \cup M_{k-1}^{\beta}\}.$$

As $\Omega_{\alpha\beta} \subset \Omega_{k-1}$, it holds that

$$\min_{g \in \Omega_{k-1}} \|Tg\|^2 \leqslant \min_{g \in \Omega_{\alpha\beta}} \|Tg\|^2.$$

There may, however, be points X_i, $i \in I_1$, in which S_{k-1} does not satisfy the obstacle conditions (4.3). Define the sets $N_{k-1}^{\alpha}, N_{k-1}^{\beta} \subset I_1$ by the conditions

$$S_{k-1}(X_i) < \alpha_i \quad \text{for} \quad i \in N_{k-1}^{\alpha},$$
$$S_{k-1}(X_i) > \beta_i \quad \text{for} \quad i \in N_{k-1}^{\beta}.$$

In the case $N_{k-1}^{\alpha} \cup N_{k-1}^{\beta} = \emptyset$, the spline S_{k-1} is the solution of the initial problem, otherwise we construct the natural spline

$$S_k^0(X) = \sum_{j \in J} c_j(S_k^0) Q_j(X) + \sum_{\substack{i \in I_0 \cup M_{k-1}^{\alpha} \cup M_{k-1}^{\beta} \cup \\ \cup N_{k-1}^{\alpha} \cup N_{k-1}^{\beta}}} d_i(S_k^0) G(X - X_i),$$

such that

$$S_k^0(X_i) = z_i, \quad i \in I_0,$$
$$S_k^0(X_i) = \alpha_i, \quad i \in M_{k-1}^{\alpha} \cup N_{k-1}^{\alpha},$$
$$S_k^0(X_i) = \beta_i, \quad i \in M_{k-1}^{\beta} \cup N_{k-1}^{\beta}.$$

If the conditions

$$(-1)^r d_i(S_k^0) > 0, \quad i \in M_{k-1}^{\alpha} \cup N_{k-1}^{\alpha},$$
$$(-1)^r d_i(S_k^0) < 0, \quad i \in M_{k-1}^{\beta} \cup N_{k-1}^{\beta},$$

hold, we denote $M_k^{\alpha} = M_{k-1}^{\alpha} \cup N_{k-1}^{\alpha}$, $M_k^{\beta} = M_{k-1}^{\beta} \cup N_{k-1}^{\beta}$ and $S_k = S_k^0$. With the spline S_k we then continue again at the beginning of step 2. Otherwise we denote $L_{k,0}^{\alpha} = \emptyset$, $L_{k,0}^{\beta} = \emptyset$, and we proceed to step 3 with the spline S_k^0.

Step 3 (the step of removing knots). For the spline S_k^{j-1}, $j \geqslant 1$, define

$$L_{k,j}^{\alpha} = \{i \in M_{k-1}^{\alpha} \cup N_{k-1}^{\alpha} \mid (-1)^r d_i(S_k^{j-1}) \leqslant 0\},$$
$$L_{k,j}^{\beta} = \{i \in M_{k-1}^{\beta} \cup N_{k-1}^{\beta} \mid (-1)^r d_i(S_k^{j-1}) \geqslant 0\},$$

and solve the interpolation problem

$$S_k^j(X_i) = z_i, \quad i \in I_0,$$

$$S_k^j(X_i) = \alpha_i, \quad i \in (M_{k-1}^\alpha \cup N_{k-1}^\alpha) \setminus L_{k,j}^\alpha,$$

$$S_k^j(X_i) = \beta_i, \quad i \in (M_{k-1}^\beta \cup N_{k-1}^\beta) \setminus L_{k,j}^\beta.$$

Note that $L_{k,j-1}^\alpha \subset L_{k,j}^\alpha$ and $L_{k,j-1}^\beta \subset L_{k,j}^\beta$. If the conditions

$$(-1)^r d_i(S_k^j) > 0, \quad i \in (M_{k-1}^\alpha \cup N_{k-1}^\alpha) \setminus L_{k,j}^\alpha,$$

$$(-1)^r d_i(S_k^j) < 0, \quad i \in (M_{k-1}^\beta \cup N_{k-1}^\beta) \setminus L_{k,j}^\beta,$$

hold, denote $M_k^\alpha = (M_{k-1}^\alpha \cup N_{k-1}^\alpha) \setminus L_{k,j}^\alpha$, $M_k^\beta = (M_{k-1}^\beta \cup N_{k-1}^\beta) \setminus L_{k,j}^\beta$ and $S_k = S_k^j$. With the spline S_k we now continue at the beginning of step 2. Otherwise we start again step 3 with the spline S_k^j and still remove knots. It is clear that the consecutive construction of splines $S_k^0, S_k^1, \ldots$ during step 3 cannot be infinite and necessarily leads to $S_k = S_k^j$ for some j.

We will call the splines S_k, $k \geqslant 1$, self-optimal because they satisfy optimality conditions of type (4.2) on their own set of active knots.

Remark 4.1. *In practice we usually do not have any interpolation knots, thus it is necessary to make some natural extensions. In the case $I_0 = \emptyset$ we cannot construct the spline S_0 in step 1, thus we choose an interpolant $S_0 \in \mathcal{P}_{r-1}$ arbitrarily. Secondly, it may happen that in step 3 we may have to remove all knots of I_1, i.e., $L_{k,j}^\alpha = M_{k-1}^\alpha \cup N_{k-1}^\alpha$ and $L_{k,j}^\beta = M_{k-1}^\beta \cup N_{k-1}^\beta$ for some $j \geqslant 1$. While*

$$S_k^{j-1}(X) = \sum_{i \in J} c_i(S_k^{j-1}) Q_i(X) + \sum_{\substack{i \in \left((M_{k-1}^\alpha \cup N_{k-1}^\alpha) \setminus L_{k,j-1}^\alpha\right) \cup \\ \cup \left((M_{k-1}^\beta \cup N_{k-1}^\beta) \setminus L_{k,j-1}^\beta\right)}} d_i(S_k^{j-1}) G(X - X_i),$$

it is natural to set $S_k^j = S_k = \sum_{i \in J} c_i(S_k^{j-1}) Q_i(X)$ and continue at the beginning of step 2.

4.2. Examples

In this section we give a counterexample to the finiteness of this method in the case of cubic splines ($n = 1$, $r = 2$) (Example 4.1) and a counterexample to the extension of this algorithm in the case of linear splines ($n = 1$,

$r = 1$) without interpolation knots (Example 4.2). Examples 4.3 and 4.4 are counterexamples to Lemma 10.3 in [33] in the case of cubic and of linear splines, respectively. In Example 4.3 the seminorms of self-optimal splines do not increase monotonically.

Example 4.1. Let us take $n = 1$, $r = 2$ (cubic splines) and knots $x_1 = 1.5$, $x_2 = 2$, $x_3 = 3$, $x_4 = 4$, $x_5 = 6$, $x_6 = 7$. We pose obstacle conditions $1 \leqslant S(x_1) \leqslant 2.4$, $2 \leqslant S(x_2) \leqslant 3.4$, $3.5 \leqslant S(x_3) \leqslant 4.9$, $4.4 \leqslant S(x_4) \leqslant 5.8$ and interpolation conditions $S(x_5) = 4.7$, $S(x_6) = 4.8$. Therefore, $I_0 = \{5, 6\}$ and $I_1 = \{1, 2, 3, 4\}$.

In the first step of the algorithm we construct the interpolant S_0 with knots x_5 and x_6 (this spline and the following ones are plotted in Figures 4.1 and 4.2). For S_0 the obstacle conditions are not satisfied at knots x_1 and x_2, so we consider them in the next step as β-knots defining $N_0^\beta = \{1, 2\}$.

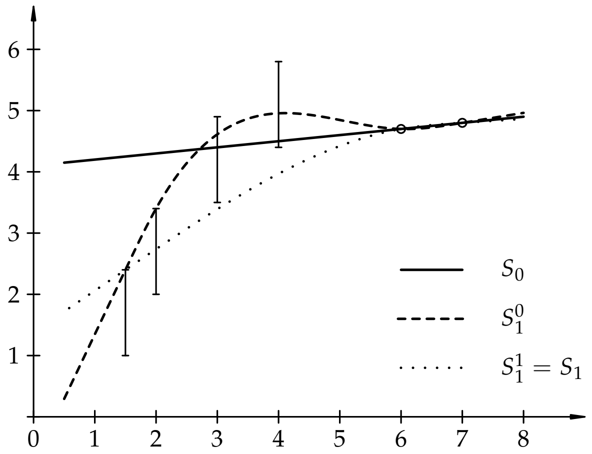

Figure 4.1. Splines generated by the algorithm

In the case of cubic splines, the conditions (3.7) require that the coefficients corresponding to α-knots are nonnegative and coefficients corresponding to β-knots are nonpositive. Now $d_2(S_1^0) > 0$, hence we define $L_{1,1}^\beta = \{2\}$. Removing the knot x_2 we get the spline $S_1^1 = S_1$ with $M_1^\alpha = \emptyset$ and $M_1^\beta = \{1\}$. For the spline S_1 the obstacle conditions do not hold at knots x_3 and x_4. We have to define $N_1^\alpha = \{3, 4\}$ and construct the spline S_2^0 with x_1 as α-knot, x_3, x_4 as β-knots and x_5, x_6 as interpolation knots (see Figure 4.2). Since $d_1(S_2^0) > 0$ and $d_3(S_2^0) < 0$, we define $L_{2,1}^\alpha = \{3\}$, $L_{2,1}^\beta = \{1\}$ and remove these two knots obtaining S_2^1. As $d_4(S_2^1) < 0$, we have to remove the last obstacle knot taking $L_{2,2}^\alpha = \{3, 4\}$ and $L_{2,2}^\beta = \{1\}$. The spline $S_2^2 = S_2$ with $M_2^\alpha = \emptyset$, $M_2^\beta = \emptyset$, and the spline S_0 coincide. We have there-

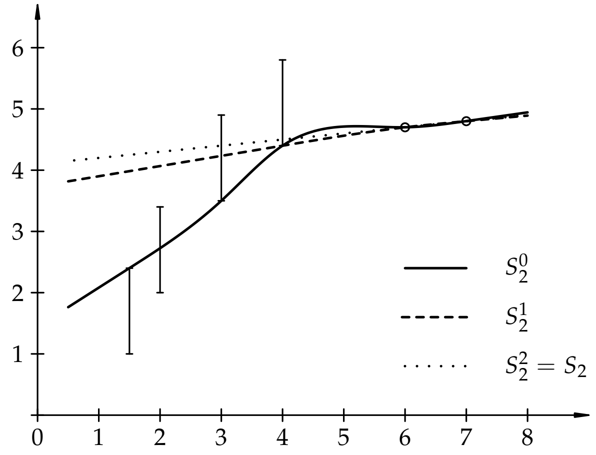

Figure 4.2. Splines generated by the algorithm

fore arrived at the initial state, thus the algorithm is cycling and does not provide the solution for this problem.

Let us note that the unique solution S with $M^\alpha = \{4\}$ and $M^\beta = \{1\}$ exists and is plotted in Figure 4.3.

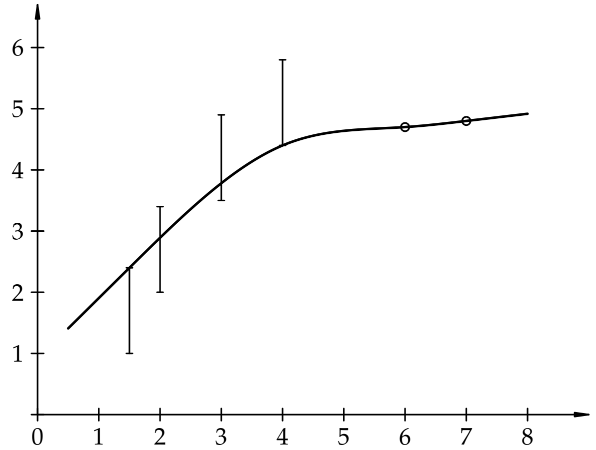

Figure 4.3. Solution of the problem

Example 4.1 proves that, in general, the method of adding-removing knots can generate a cycle. The next example shows that the natural extension of this algorithm to the case without interpolation knots can be infinite even in the case of linear splines.

Example 4.2. Consider the case $n = 1$, $r = 1$ (linear splines) and knots

$x_1 = 1$, $x_2 = 2$. Let us pose obstacle conditions $1 \leqslant S(x_1) \leqslant 1.5$ and $2 \leqslant S(x_2) \leqslant 2.5$. As $I_0 = \emptyset$, we have to choose $S_0 \in \mathcal{P}_0$ arbitrarily. Let us take $S_0(x) = 0.5$ for all x. Since $S_0(x_1) < \alpha_1$ and $S_0(x_2) < \alpha_2$, we have $N_0^\alpha = \{1, 2\}$ and obtain S_1^0 (this spline and the following ones are plotted in Figures 4.4 and 4.5). Next we remove the knot x_1 and get S_1^1. Since now

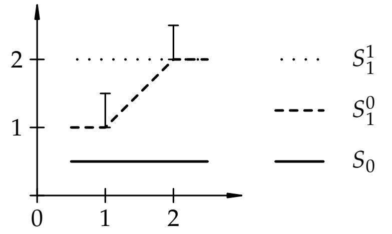

Figure 4.4. Splines generated by the algorithm

$d_2(S_1^1) = 0$, we have to remove the last knot x_2. As the polynomial part of S_1^1 is retained, we have $S_1^2(x) = 2$ for all x and $S_1 = S_1^2$. With the spline S_1 we go to step 2 and define $N_1^\beta = \{1\}$, obtaining S_2^0. Since $d_1(S_2^0) = 0$, we remove the knot x_1 and arrive at $S_2^1(x) = 1.5$ for all x. This means that $S_2 = S_2^1$. Continuing in this way, we see that $S_1 = S_3 = \ldots$ and $S_2 = S_4 = \ldots$.

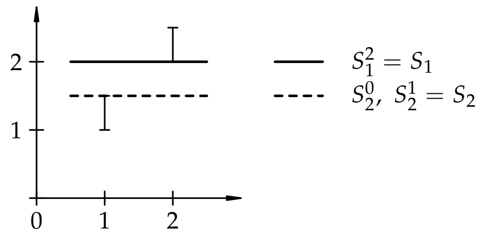

Figure 4.5. Splines generated by the algorithm

Example 4.3. Let us take $n = 1$, $r = 2$ (cubic splines) and knots $x_1 = 1$, $x_2 = 1.5$, $x_3 = 2.5$, $x_4 = 3$, $x_5 = 3.5$, $x_6 = 5$, $x_7 = 6.5$, $x_8 = 7$, $x_9 = 8$. Pose interpolation conditions $S(x_1) = -1.7$, $S(x_8) = 4.3$, $S(x_9) = 5.8$ and obstacle conditions $0.3 \leqslant S(x_2) \leqslant 1.7$, $2 \leqslant S(x_3) \leqslant 3.4$, $3 \leqslant S(x_4) \leqslant 4.4$, $4.6 \leqslant S(x_5) \leqslant 6$, $5.4 \leqslant S(x_6) \leqslant 6.8$, $5.4 \leqslant S(x_7) \leqslant 6.8$. Thus $I_0 = \{1, 8, 9\}$ and $I_1 = \{2, 3, 4, 5, 6, 7\}$.

In every step of the algorithm we construct an interpolant

$$S(x) = c_0 + c_1 x + \sum_{i \in I_0 \cup M^\alpha \cup M^\beta} d_i |x - x_i|^3,$$

where $M^\alpha, M^\beta \subset I_1$, $M^\alpha \cap M^\beta = \emptyset$, are the sets of indices corresponding to active knots, i.e., $S(x_i) = \alpha_i$ for $i \in M^\alpha$, $S(x_i) = \beta_i$ for $i \in M^\beta$ and $d_i \neq 0$ for $i \in M^\alpha \cup M^\beta$. Note that, for cubic splines, $G(x) = |x|^3/12$ and the coefficients of S in the representation (3.1) are multiples of the d_i used here. The process of finding suitable knots through the algorithm is summarised in Table 4.1. Here α or β in column x_i means that x_i is considered to be an active α-knot or β-knot for the spline S. The coefficients of the splines are presented in Tables 4.1 and 4.2.

Table 4.1. The status of the obstacle knots and the values of the corresponding coefficients

S	x_2	x_3	x_4	x_5	x_6	x_7	d_2	d_3	d_4	d_5	d_6	d_7
S_0	—	—	—	—	—	—	0	0	0	0	0	0
S_1^0	α	α	α	α	α	α	1.408	−0.055	−2.151	2.063	−0.813	2.627
S_1^1	α	—	—	α	—	α	0.481	0	0	−0.181	0	1.846
S_1	α	—	—	—	—	α	0.126	0	0	0	0	1.583
S_2^0	α	β	β	β	β	α	−0.023	1.560	−3.132	2.038	−0.502	2.034
S_2^1	—	—	β	—	β	α	0	0	0.056	0	−0.094	1.809
S_2	—	—	—	—	β	α	0	0	0	0	−0.029	1.751
S_3	α	—	—	—	β	α	0.214	0	0	0	−0.103	1.824
S_4^0	α	β	β	—	β	α	0.159	0.286	−0.280	0	−0.027	1.769
S_4	α	—	β	—	β	α	0.334	0	−0.077	0	−0.054	1.785

Table 4.2. The coefficients of the splines in the polynomial part and corresponding to the interpolation knots

S	c_0	c_1	d_1	d_8	d_9
S_0	−4.486	1.161	0.003	−0.021	0.018
S_1^0	−11.665	3.651	−0.853	−2.915	0.688
S_1^1	−11.283	3.500	−0.380	−2.421	0.655
S_1	−11.110	3.426	−0.140	−2.209	0.641
S_2^0	−11.262	3.445	−0.142	−2.493	0.660
S_2^1	−10.879	3.118	−0.048	−2.374	0.652
S_2	−10.657	2.910	−0.028	−2.344	0.650
S_3	−11.219	3.453	−0.205	−2.382	0.652
S_4^0	−11.202	3.451	−0.203	−2.353	0.650
S_4	−11.225	3.470	−0.277	−2.362	0.651

The graphs of the splines $S_0, \ldots, S_4$ (S_4 is the solution of the problem) are given in Figures 4.6 and 4.7.

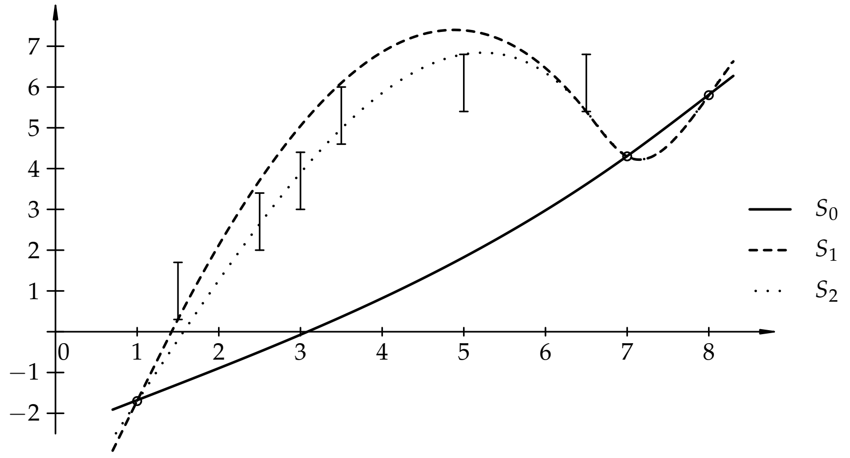

Figure 4.6. Splines S_0, S_1 and S_2, generated by the algorithm

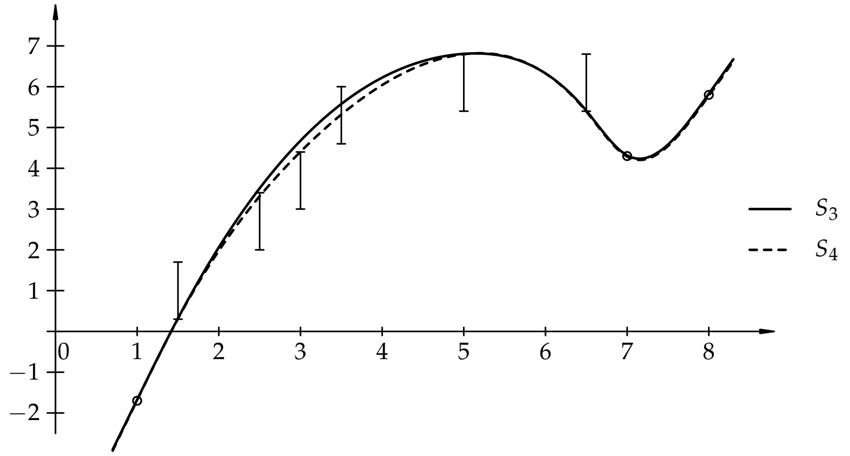

Figure 4.7. Splines S_3 and S_4, generated by the algorithm

This example provides a counterexample to Lemma 10.3 in [33] since $S_1(x_2) = \alpha_2$ but $S_2(x_2) < \alpha_2$. The main importance of this example lies in the fact that the seminorms $\|TS_i\|$ need not increase monotonically (Table 4.3) if the algorithm is finite.

Table 4.3. Squares of seminorms of the splines

i	0	1	2	3	4
$\|TS_i\|^2$	0.017	36.500	35.957	37.231	37.477

Example 4.4. Let us take $n = 1$, $r = 1$ (linear splines) and knots $x_1 = 1$, $x_2 = 2$, $x_3 = 4$, $x_4 = 5$, $x_5 = 7$, $x_6 = 8$, $x_7 = 9$. Pose the interpolation conditions $S(x_1) = 4$, $S(x_7) = 4$, and the obstacle conditions $6.2 \leqslant S(x_2) \leqslant 6.5$, $5 \leqslant S(x_3) \leqslant 6$, $4.2 \leqslant S(x_4) \leqslant 5.5$, $3.6 \leqslant S(x_5) \leqslant 3.8$, $0.3 \leqslant S(x_6) \leqslant 0.7$.

In the first step we construct an interpolant S_0 (this spline and the following ones are plotted in Figures 4.8 and 4.9). Adding knots x_2, x_3, x_4 to

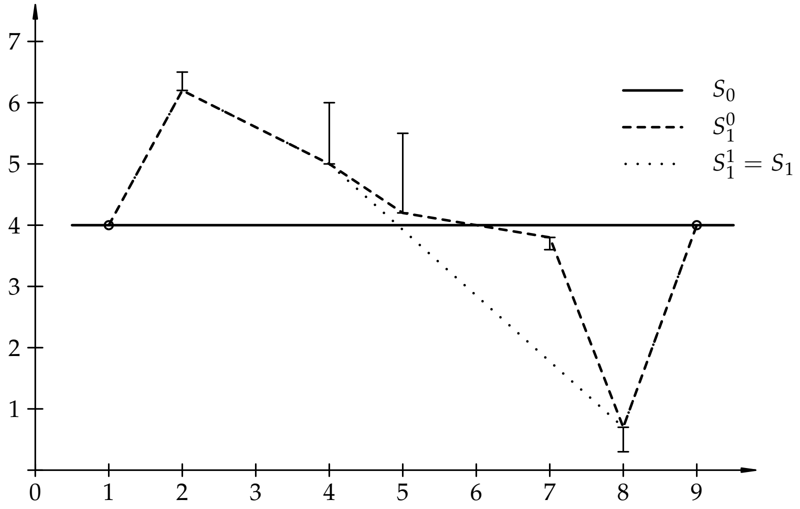

Figure 4.8. Splines S_0, S_1^0 and S_1, generated by the algorithm

the set of active α-knots and x_5, x_6 to the set of active β-knots yields the spline S_1^0. In the step of removing knots we obtain a self-optimal spline $S_1 = S_1^1$ with $M_1^\alpha = \{2, 3\}$ and $M_1^\beta = \{6\}$. From Figure 4.8 we can see that x_4 is an active α-knot for the spline S_1^0 but for the spline S_1 we get $S_1(x_4) < \alpha_4$. Therefore, this is also a counterexample to Lemma 10.3 in [33] in the case of linear splines.

For the spline S_1 the obstacle conditions do not hold at the knots x_4 and x_5. Adding these two knots to the set of active α-knots leads to the spline S_2^0. After removing at first the knot x_4 and then the knot x_3 we get splines S_2^1 and $S_2^2 = S_2$, respectively. The solution of the problem S_2 with $M_2^\alpha = \{2, 5\}$ and $M_2^\beta = \{6\}$ is presented in Figure 4.9.

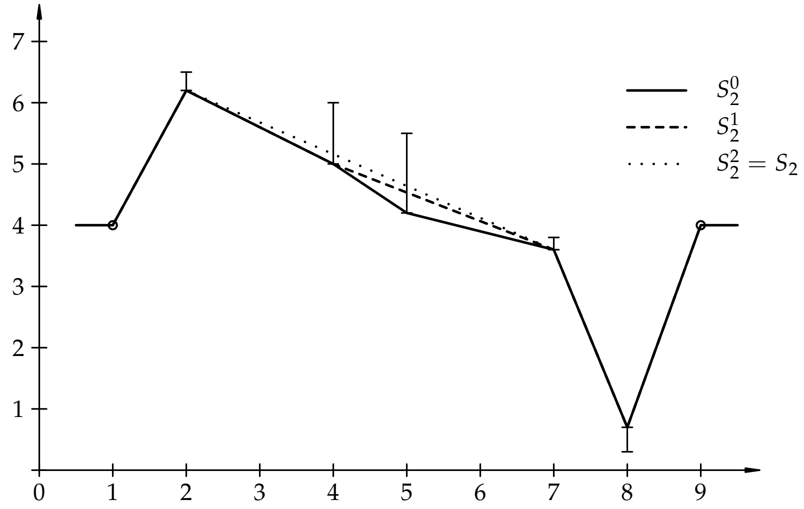

Figure 4.9. Splines S_2^0, S_2^1 and S_2, generated by the algorithm

4.3. Results about finiteness

We have seen in the previous section that in general the method of adding-removing knots may be infinite due to cycling. In this section we give some sufficient conditions guaranteeing the finiteness of the algorithm.

In the following lemma we consider the natural splines S_k and S_j of the form

$$\begin{aligned} S_k(X) &= \sum_{i \in J} c_i(S_k)\, Q_i(X) + \sum_{i \in I_0 \cup M_k^\alpha \cup M_k^\beta} d_i(S_k)\, G(X - X_i), \\ S_j(X) &= \sum_{i \in J} c_i(S_j)\, Q_i(X) + \sum_{i \in I_0 \cup M_j} d_i(S_j)\, G(X - X_i), \end{aligned}$$

satisfying the conditions

$$\begin{aligned} S_k(X_i) = z_i \quad &\text{if} \quad i \in I_0, \\ S_k(X_i) = \alpha_i \quad &\text{if} \quad i \in M_k^\alpha, \\ S_k(X_i) = \beta_i \quad &\text{if} \quad i \in M_k^\beta, \\ S_j(X_i) = z_i \quad &\text{if} \quad i \in I_0. \end{aligned}$$

Here M_j may be an arbitrary finite set of indices. Suppose that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ at the knots X_i, $i \in I_0 \cup M_k^\alpha \cup M_k^\beta$, has only the trivial solution.

Lemma 4.2. *If S_k is the solution of the problem*

$$\inf_{f \in \Omega_k} \|Tf\|^2,$$

where

$$\Omega_k = \{f \in L_2^{(r)}(\mathbb{R}^n) \mid f(X_i) = z_i, i \in I_0,\ \alpha_i \leqslant f(X_i) \leqslant \beta_i, i \in M_k^\alpha \cup M_k^\beta\},$$

with $d_i(S_k) \neq 0$ for $i \in M_k^\alpha \cup M_k^\beta$, and S_j, $S_j \neq S_k$, satisfies the conditions

$$\begin{aligned} S_j(X_i) &\geqslant \alpha_i \quad \text{for} \quad i \in M_k^\alpha, \\ S_j(X_i) &\leqslant \beta_i \quad \text{for} \quad i \in M_k^\beta, \end{aligned}$$

then $\|TS_j\| > \|TS_k\|$.

Proof. We will base on the equality

$$\|TS_j\|^2 - \|TS_k\|^2 = \|TS_j - TS_k\|^2 + 2\langle TS_k, TS_j - TS_k\rangle.$$

By (3.3) it holds that

$$\begin{aligned} \langle TS_k, TS_j - TS_k\rangle &= \sum_{i \in M_k^\alpha} (-1)^r d_i(S_k)(S_j(X_i) - S_k(X_i)) \\ &\quad + \sum_{i \in M_k^\beta} (-1)^r d_i(S_k)(S_j(X_i) - S_k(X_i)). \end{aligned}$$

Due to the optimality of the spline S_k, we have $(-1)^r d_i(S_k) \geqslant 0$ for $i \in M_k^\alpha$, and $(-1)^r d_i(S_k) \leqslant 0$ for $i \in M_k^\beta$. Since $S_j(X_i) \geqslant \alpha_i = S_k(X_i)$ for $i \in M_k^\alpha$, and $S_j(X_i) \leqslant \beta_i = S_k(X_i)$ for $i \in M_k^\beta$, it holds that $\langle TS_k, TS_j - TS_k\rangle \geqslant 0$ and $\|TS_j\| \geqslant \|TS_k\|$.

Suppose now that $\|TS_j\| = \|TS_k\|$. This implies $\|TS_j - TS_k\| = 0$ and $\langle TS_k, TS_j - TS_k\rangle = 0$. Then $S_j - S_k \in \mathcal{P}_{r-1}$ and for all $i \in M_k^\alpha \cup M_k^\beta$ it holds $d_i(S_k)(S_j(X_i) - S_k(X_i)) = 0$, thus $S_j(X_i) - S_k(X_i) = 0$, because of $d_i(S_k) \neq 0$ for $i \in M_k^\alpha \cup M_k^\beta$. The unique solvability of the polynomial interpolation at the knots X_i, $i \in I_0 \cup M_k^\alpha \cup M_k^\beta$, gives $S_j - S_k = 0$, which contradicts the assumption $S_j \neq S_k$. □

Lemma 4.3. *For the splines generated by the algorithm of adding-removing knots, it is not possible that $S_{k+1} = S_k$.*

Proof. By the algorithm, $S_{k+1} = S_{k+1}^j$ for some j. We may assume that $S_{k+1} \neq S_{k+1}^{j-1}$ and

$$(-1)^r d_i\left(S_{k+1}^{j-1}\right) < 0 \text{ for some } i \in L_{k+1,j}^\alpha$$

or

$$(-1)^r d_i\left(S_{k+1}^{j-1}\right) > 0 \text{ for some } i \in L_{k+1,j}^{\beta},$$

otherwise, if we remove only knots corresponding to zero valued coefficients when passing from S_{k+1}^{j-1} to S_{k+1}^{j}, we consider S_{k+1}^{j-2} instead of S_{k+1}^{j-1}.

Assume, contrary to the assertion of the lemma, that $S_{k+1} = S_k$. Then $M_{k+1}^{\alpha} = M_k^{\alpha}$ and $M_{k+1}^{\beta} = M_k^{\beta}$. We have

$$\|TS_{k+1}^{j-1} - TS_k\|^2 = \langle TS_{k+1}^{j-1}, TS_{k+1}^{j-1} - TS_k\rangle,$$

because

$$\langle TS_k, TS_{k+1}^{j-1} - TS_k\rangle = \sum_{i \in I_0 \cup M_k^{\alpha} \cup M_k^{\beta}} (-1)^r d_i(S_k)\left(S_{k+1}^{j-1}(X_i) - S_k(X_i)\right) = 0.$$

Using the index sets

$$\begin{aligned} M_{k+1,j-1}^{\alpha} &= \left\{i \in I_1 \mid S_{k+1}^{j-1}(X_i) = \alpha_i\right\}, \\ M_{k+1,j-1}^{\beta} &= \left\{i \in I_1 \mid S_{k+1}^{j-1}(X_i) = \beta_i\right\}, \end{aligned}$$

and taking into account that $M_k^{\alpha} \subset M_{k+1,j-1}^{\alpha}$, $M_k^{\beta} \subset M_{k+1,j-1}^{\beta}$ (due to $M_{k+1}^{\alpha} = M_k^{\alpha}$, $M_{k+1}^{\beta} = M_k^{\beta}$ and the removing steps), we can continue with

$$\begin{aligned} &\|TS_{k+1}^{j-1} - TS_k\|^2 \\ &\quad = \sum_{i \in M_{k+1,j-1}^{\alpha} \setminus M_k^{\alpha}} (-1)^r d_i(S_{k+1}^{j-1})\left(S_{k+1}^{j-1}(X_i) - S_k(X_i)\right) \\ &\qquad + \sum_{i \in M_{k+1,j-1}^{\beta} \setminus M_k^{\beta}} (-1)^r d_i(S_{k+1}^{j-1})\left(S_{k+1}^{j-1}(X_i) - S_k(X_i)\right) < 0, \end{aligned}$$

as

$$\begin{aligned} (-1)^r d_i(S_{k+1}^{j-1}) \leqslant 0,\ S_{k+1}^{j-1}(X_i) = \alpha_i,\ S_k(X_i) < \alpha_i \text{ for } i \in M_{k+1,j-1}^{\alpha} \setminus M_k^{\alpha}, \\ (-1)^r d_i(S_{k+1}^{j-1}) \geqslant 0,\ S_{k+1}^{j-1}(X_i) = \beta_i,\ S_k(X_i) > \beta_i \text{ for } i \in M_{k+1,j-1}^{\beta} \setminus M_k^{\beta}, \end{aligned}$$

and, by the assumption, at least one of the coefficients $d_i(S_{k+1}^{j-1})$ is different from zero. This contradiction proves the assertion. □

Note that in Lemma 4.3 we do not impose any assumptions about the unique solvability of the polynomial interpolation problem.

Theorem 4.4. *For the splines S_k and S_{k+1} generated by the algorithm and satisfying*

$$S_{k+1}(X_i) \geqslant \alpha_i, \quad i \in M_k^\alpha,$$
$$S_{k+1}(X_i) \leqslant \beta_i, \quad i \in M_k^\beta,$$

under the assumption that the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ at the knots X_i, $i \in I_0 \cup M_k^\alpha \cup M_k^\beta$, has only the trivial solution, it holds that

$$\|TS_{k+1}\| > \|TS_k\|.$$

Proof. By Lemma 4.3, $S_{k+1} \neq S_k$. It remains to apply Lemma 4.2. □

From Theorem 4.4 we obtain immediately

Corollary 4.5. *If the assumptions of the previous theorem are satisfied in every step of the algorithm of adding-removing knots then the algorithm is finite.*

Lemma 4.2 and its proof yield

Corollary 4.6. *For the solution S of the smoothing problem with obstacles, the interpolant S_0 and any self-optimal spline S_k generated by the algorithm, it holds that*

$$\|TS_0\| \leqslant \|TS_k\| \leqslant \|TS\|.$$

If $P(X_i) = 0$, $i \in I_0$, $P \in \mathcal{P}_{r-1}$, implies $P = 0$, then the first inequality is strict. Similarly, if $P(X_i) = 0$, $i \in I_0 \cup M_k^\alpha \cup M_k^\beta$, $P \in \mathcal{P}_{r-1}$, only for $P = 0$, and $S \neq S_k$, then the second inequality is strict.

Let us point out that the following result holds without any assumptions about the uniqueness of the solution for polynomial interpolation.

Theorem 4.7. *Suppose that $M_k^\alpha \subset M_{k+1}^\alpha$ and $M_k^\beta \subset M_{k+1}^\beta$ in every step of the algorithm. Then $\|TS_{k+1}\| > \|TS_k\|$ for all k. Consequently, the algorithm is finite under these assumptions.*

Proof. Here we use the equality

$$\|TS_{k+1}\|^2 - \|TS_k\|^2 = \|TS_{k+1} - TS_k\|^2 + 2\langle TS_k, TS_{k+1} - TS_k\rangle.$$

Since

$$\langle TS_k, TS_{k+1} - TS_k\rangle = \sum_{i \in I_0 \cup M_k^\alpha \cup M_k^\beta} (-1)^r d_i(S_k)\,(S_{k+1}(X_i) - S_k(X_i)) = 0,$$

it holds that

$$\|TS_{k+1}\|^2 - \|TS_k\|^2 = \|TS_{k+1} - TS_k\|^2. \tag{4.4}$$

On the other hand we have

$$\|TS_k\|^2 - \|TS_{k+1}\|^2 = \|TS_k - TS_{k+1}\|^2 + 2\langle TS_{k+1}, TS_k - TS_{k+1}\rangle. \quad (4.5)$$

According to Lemma 4.3, $M^{\alpha}_{k+1} \setminus M^{\alpha}_k \neq \emptyset$ or $M^{\beta}_{k+1} \setminus M^{\beta}_k \neq \emptyset$, whereas $(-1)^r d_i(S_{k+1}) > 0$, $S_k(X_i) < \alpha_i = S_{k+1}(X_i)$ for $i \in M^{\alpha}_{k+1} \setminus M^{\alpha}_k$ and $(-1)^r d_i(S_{k+1}) < 0$, $S_k(X_i) > \beta_i = S_{k+1}(X_i)$ for $i \in M^{\beta}_{k+1} \setminus M^{\beta}_k$. Thus

$$\begin{aligned}
&\langle TS_{k+1}, TS_k - TS_{k+1}\rangle \\
&\qquad = \sum_{i \in M^{\alpha}_{k+1} \setminus M^{\alpha}_k} (-1)^r d_i(S_{k+1}) \left(S_k(X_i) - S_{k+1}(X_i)\right) \\
&\qquad\quad + \sum_{i \in M^{\beta}_{k+1} \setminus M^{\beta}_k} (-1)^r d_i(S_{k+1}) \left(S_k(X_i) - S_{k+1}(X_i)\right) < 0.
\end{aligned}$$

Suppose now that $\|TS_{k+1} - TS_k\|^2 = 0$. Then, by (4.4) and (4.5),

$$0 = \|TS_k\|^2 - \|TS_{k+1}\|^2 = 2\langle TS_{k+1}, TS_k - TS_{k+1}\rangle < 0.$$

The contradiction proves that actually $\|TS_{k+1} - TS_k\|^2 > 0$ and (4.4) implies the inequality $\|TS_{k+1}\| > \|TS_k\|$. $\square$

Chapter 5

An equation connecting classical smoothing problems with obstacles and weights

Consider the smoothing problem (3.6) with obstacles $\varepsilon_i > 0$, $i \in I_1$. According to Theorem 3.5 there exists an equivalent smoothing problem (3.4) with weights. In the first section we will derive the equation connecting the deviations $z_i - S(X_i)$, $i \in I_1$, to the weights w_i, $i \in I_1$, both unknown. This equation will also contain the unknown coefficients d_i, $i \in I_0$, corresponding to the interpolation knots. In the following sections we will propose a method for solving this equation and illustrate it by examples. The effectiveness of the method has not yet been studied, but as our first example shows, the problem from Section 4.2, where the method of adding-removing knots is cycling, can be solved by this method.

5.1. The equation

Let us define the matrix $W = (w_{ij})_{i,j \in I}$ with $w_{ii} = w_i$ for $i \in I_1$, $w_{ii} = 1$ for $i \in I_0$, and $w_{ij} = 0$ for $i \neq j$. We also use the notations $z = (z_i)_{i \in I}$ and $s = (S(X_i))_{i \in I}$, then the equations (3.5) can be written as

$$(-1)^r d = W(z - s + (-1)^r \chi d), \tag{5.1}$$

$\chi : \mathbb{R}^{|I|} \to \mathbb{R}^{|I|}$ being the projection such that $(\chi d)_i = d_i$, $i \in I_0$, $(\chi d)_i = 0$, $i \in I_1$.

Let X^{β_j}, $j \in J$, be a basis in $\mathcal{P}_{r-1}$. Then the natural spline (3.1) may be presented as

$$S(X) = \sum_{j \in J} c_j X^{\beta_j} + \sum_{i \in I} d_i G(X - X_i).$$

By setting $V = (X_i^{\beta_j})_{i \in I, j \in J}$, $G = (G(X_i - X_j))_{i,j \in I}$, $c = (c_j)_{j \in J}$ and

$d = (d_i)_{i \in I}$, we get

$$s = Vc + Gd \tag{5.2}$$

with $d \in \ker V^T$ as an equivalent form for (3.3). From (5.1) and (5.2) we obtain

$$(-1)^r d + WVc + WGd = Wz + (-1)^r \chi d. \tag{5.3}$$

Take an arbitrary symmetric regular $|I| \times |I|$ matrix A and define $U = (WV)|_{(\ker(WV))^\perp}$ and $D = A^{-1}U$. Note that $WV : \mathbb{R}^{|J|} \to \mathbb{R}^{|I|}$ may not be injective but, according to $\mathbb{R}^{|J|} = \ker(WV) \oplus (\ker(WV))^\perp$, the operator $U : (\ker(WV))^\perp \to \mathbb{R}^{|I|}$ is injective. Define the operator $\Pi : \mathbb{R}^{|I|} \to \mathbb{R}^{|I|}$ with $\Pi = E - D(D^T D)^{-1} D^T$, where E is the identity operator. Using the ideas from [6], it can be shown that $\Pi^2 = \Pi$, $\operatorname{ran}\Pi = A \ker U^T$ and $\langle \Pi x, y\rangle = \langle x, \Pi y\rangle$ for all $x, y \in \mathbb{R}^{|I|}$, which means that Π is an orthogonal projection onto the subspace $A \ker U^T$.

Let us show that $\Pi A^{-1} WVc = 0$ for all $c \in \mathbb{R}^{|J|}$. It is sufficient to show that $\Pi A^{-1} WVc = 0$ for all $c \in (\ker(WV))^\perp$, which is equivalent to

$$A^{-1} WVc \in \ker \Pi = \ker \Pi^* = (\operatorname{ran}\Pi)^\perp = (A \ker U^T)^\perp \ \forall c \in (\ker(WV))^\perp.$$

But this holds since, for all $x \in \ker U^T$, we have

$$\langle A^{-1} WVc, Ax\rangle = \langle WVc, x\rangle = \langle Uc, x\rangle = \langle c, U^T x\rangle = 0.$$

Use the notation $\tilde\varepsilon = (\tilde\varepsilon_i)_{i \in I}$, where

$$\begin{aligned}
\tilde\varepsilon_i &= z_i - S(X_i), \quad i \in I_1, \\
\tilde\varepsilon_i &= (-1)^r d_i = (-1)^r d_i + z_i - S(X_i), \quad i \in I_0.
\end{aligned}$$

Then the equation (5.1) can be written as

$$(-1)^r d = W\tilde\varepsilon. \tag{5.4}$$

Now, applying ΠA^{-1} to (5.3) and taking (5.4) into account, we obtain

$$(\Pi A^{-1} + (-1)^r \Pi A^{-1} WG - \Pi A^{-1}\chi) W\tilde\varepsilon = \Pi A^{-1} Wz. \tag{5.5}$$

This equation connects the deviations $\tilde\varepsilon_i$, $i \in I_1$, and coefficients $\tilde\varepsilon_i$, $i \in I_0$, of the solution of smoothing problem with obstacles to the weights of equivalent smoothing problem with weights.

Note that the condition $\ker(WV) = \{0\}$ is equivalent to the unique solvability of the zero-valued interpolation problem with polynomials from $\mathcal{P}_{r-1}$ in the knots X_i, $i \in I_0 \cup \{j \in I_1 \mid w_j \neq 0\}$. In practice usually $\ker(WV) = \{0\}$ and thus $U = WV$. For example, in the case of cubic splines ($n = 1$, $r = 2$) it is sufficient that there is at least two non-zero weights for $\ker(WV)$ being trivial. Assuming $\ker(WV) = \{0\}$, we propose a method for finding the weights in the problem (3.4) equivalent to a given problem (3.6).

5.2. An algorithm for finding weights

In the equation (5.5) both, W and $\tilde{\varepsilon}$, are unknown. For our method we take $w_i = 1, i \in I$, as guess values. Define $N = \{i \in I_1 \mid w_i = 0\}$ as the set of indexes corresponding to inactive obstacle knots. At the beginning we have $N = \emptyset$.

Step 1. (The step of finding $\tilde{\varepsilon}$.) Using (5.4), the equation (5.5) can be written as

$$(-1)^r(\Pi A^{-1} + (-1)^r \Pi A^{-1} W G - \Pi A^{-1}\chi)d = \Pi A^{-1} W z.$$

Adding the conditions $V^T d = 0$, we have a system of $|I| + |J|$ linear equations with $|I|$ unknowns d_i, $i \in I$. Let us solve this system by the standard least squares method. Even if we assume the sufficient uniqueness condition of solution for the interpolation problem with polynomials as in Prop. 3.3, it may happen that this system has more than one least squares solution. Then we take the solution with minimal Euclidean norm. Based on (5.4), determine

$$\tilde{\varepsilon}_i = \frac{(-1)^r d_i}{w_i}, \quad i \in I \setminus N.$$

If $N \neq \emptyset$, we proceed to step 2, otherwise to step 3.

Step 2. (The step of computing missing $\tilde{\varepsilon}$.) Solve the interpolation problem

$$\begin{aligned} S(X_i) &= z_i - \tilde{\varepsilon}_i, \quad i \in I_1 \setminus N, \\ S(X_i) &= z_i, \quad i \in I_0, \end{aligned}$$

or equivalently, the linear system

$$\begin{aligned} \sum_{j\in J} c_j X_k^{\beta_j} + \sum_{i \in I\setminus N} d_i G(X_k - X_i) &= z_k - \tilde{\varepsilon}_k, \quad k \in I_1 \setminus N, \\ \sum_{j\in J} c_j X_k^{\beta_j} + \sum_{i \in I\setminus N} d_i G(X_k - X_i) &= z_k, \quad k \in I_0, \\ \sum_{i \in I\setminus N} d_i X_i^{\beta_j} &= 0, \quad j \in J, \end{aligned}$$

with $(c_j)_{j\in J}$ and $(d_i)_{i \in I\setminus N}$ as unknowns. In the case of multiple solution we continue with that of minimal Euclidean norm. We also take $d_i = 0$, $i \in N$. The unknown deviations will be computed as

$$\tilde{\varepsilon}_k = z_k - S(X_k) = z_k - \sum_{j\in J} c_j X_k^{\beta_j} - \sum_{i\in I\setminus N} d_i G(X_k - X_i), \quad k \in N.$$

If the step preceding to this step was step 3, we also need to evaluate the coefficients

$$\tilde{\varepsilon}_i = (-1)^r d_i, \quad i \in I_0.$$

Proceed to step 3.

Step 3. (The step of correcting $\tilde{\varepsilon}$.) For the solution, any number $|\tilde{\varepsilon}_i|$ should not exceed the obstacle values ε_i, $i \in I_1$, and $|\tilde{\varepsilon}_i|$ corresponding to the active knots should not be less than ε_i, $i \in I_1 \setminus N$. Thus, define the set of indexes corresponding to the deviations that need to be corrected as

$$K = \{i \in I_1 \mid |\tilde{\varepsilon}_i| > \varepsilon_i\} \cup \{i \in I_1 \setminus N \mid |\tilde{\varepsilon}_i| < \varepsilon_i\}.$$

If $K = \emptyset$, we proceed to step 4. Otherwise, for $i \in K$, we take $\tilde{\varepsilon}_i = \operatorname{sign}(\tilde{\varepsilon}_i)\, \varepsilon_i$, if $\tilde{\varepsilon}_i \neq 0$. We include the knots with $\tilde{\varepsilon}_i = 0$, $i \in K$, to the set of inactive knots by defining the new set N as

$$N = (\{i \in I_1 \mid w_i = 0\} \setminus K) \cup \{i \in K \mid \tilde{\varepsilon}_i = 0\}.$$

If $N \cup I_0 \neq \emptyset$, we continue at the beginning of step 2, otherwise we proceed to step 4.

Step 4. (The step of finding the weights.) Since the equation (5.5) is nonlinear with respect to the weights w_i, $i \in I$, we compute the corresponding weights using the equations (3.5). For the interpolation knots take $w_i = 1$, $i \in I_0$. For the obstacle knots take

$$\begin{aligned} w_i &= \frac{(-1)^r d_i}{\tilde{\varepsilon}_i} \quad \text{if} \quad \tilde{\varepsilon}_i \neq 0,\ i \in I_1, \\ w_i &= 0 \quad \text{if} \quad \tilde{\varepsilon}_i = 0,\ i \in I_1. \end{aligned}$$

If all the weights are nonnegative, i.e., $w_i \geqslant 0$, $i \in I$, we have got the solution. Otherwise, define $N = \{i \in I_1 \mid w_i \leqslant 0\}$, take $w_i = 0$, $i \in N$, and continue at the beginning of step 1.

5.3. Examples

In Section 4.2 we presented a counterexample to the method of adding-removing knots (Example 4.1). In this section in the first example we use the same data and show how our method solves this problem. The implementation of the method goes via equation (5.5) and we take as A the identity matrix in both following examples.

Example 5.1. Let us take $n = 1$, $r = 2$ (cubic splines) and knots $x_1 = 1.5$, $x_2 = 2$, $x_3 = 3$, $x_4 = 4$, $x_5 = 6$, $x_6 = 7$. We pose obstacle conditions $|S(x_1) - 1.7| \leqslant 0.7$, $|S(x_2) - 2.7| \leqslant 0.7$, $|S(x_3) - 4.2| \leqslant 0.7$,

$|S(x_4) - 5.1| \leqslant 0.7$, interpolation conditions $S(x_5) = 4.7$, $S(x_6) = 4.8$ and look for the solution of problem (3.6).

The working process of our algorithm is presented in Table 5.1. The first line contains the guess values of weights. In step 1 we compute the values $\tilde{\varepsilon}_i$, $i \in I \setminus N$, given in second line. Since at the beginning $N = \emptyset$, we continue from step 3 and correct the deviations $\tilde{\varepsilon}_i$, $i \in K = \{1, 2, 3, 4\}$. In the end of step 3 the set of indexes corresponding to inactive knots is still empty, i.e. $N = \emptyset$, but since $I_0 \neq \emptyset$, we proceed from step 2. Compute the coefficients $\tilde{\varepsilon}_i$, $i \in I_0 = \{5, 6\}$. Now $K = \emptyset$ and we proceed to step 4. The computed weights and the corrected weights with indexes from $N = \{1, 2, 4\}$ are presented in Table 5.1 on lines 5-6. Line 7 contains values $\tilde{\varepsilon}_i$, $i \in I \setminus N$, computed in step 1 and so on.

Table 5.1. Values of $\tilde{\varepsilon}_i$ and w_i computed by the algorithm

	i	1	2	3	4	5	6
GV	w_i	1.000	1.000	1.000	1.000	1.000	1.000
Step 1	$\tilde{\varepsilon}_i$	−0.222	0.001	0.168	0.343	−0.482	0.193
Step 3	$\tilde{\varepsilon}_i$	−0.700	0.700	0.700	0.700	−0.482	0.193
Step 2	$\tilde{\varepsilon}_i$	−0.700	0.700	0.700	0.700	−0.176	0.046
Step 4	w_i	−7.581	−12.885	6.513	−1.023	1.000	1.000
	w_i	0.000	0.000	6.513	0.000	1.000	1.000
Step 1	$\tilde{\varepsilon}_i$			−0.001		0.033	−0.025
Step 2	$\tilde{\varepsilon}_i$	−2.215	−1.310	−0.001	0.710	0.033	−0.025
Step 3	$\tilde{\varepsilon}_i$	−0.700	−0.700	−0.700	0.700	0.033	−0.025
Step 2	$\tilde{\varepsilon}_i$	−0.700	−0.700	−0.700	0.700	0.729	−0.256
Step 4	w_i	−0.180	2.682	−5.902	−4.077	1.000	1.000
	w_i	0.000	2.682	0.000	0.000	1.000	1.000
Step 1	$\tilde{\varepsilon}_i$		−0.011			0.149	−0.119
Step 2	$\tilde{\varepsilon}_i$	−0.683	−0.011	0.843	1.156	0.149	−0.119
Step 3	$\tilde{\varepsilon}_i$	−0.683	−0.700	0.700	0.700	0.149	−0.119
Step 2	$\tilde{\varepsilon}_i$	−1.773	−0.700	0.700	0.700	−0.513	0.159
Step 3	$\tilde{\varepsilon}_i$	−0.700	−0.700	0.700	0.700	−0.513	0.159
Step 2	$\tilde{\varepsilon}_i$	−0.700	−0.700	0.700	0.700	−0.629	0.197
Step 4	w_i	6.719	−12.013	−8.181	3.504	1.000	1.000
	w_i	6.719	0.000	0.000	3.504	1.000	1.000
Step 1	$\tilde{\varepsilon}_i$	−0.031			0.175	−0.685	0.281
Step 2	$\tilde{\varepsilon}_i$	−0.031	0.120	0.132	0.175	−0.685	0.281
Step 3	$\tilde{\varepsilon}_i$	−0.700	0.120	0.132	0.700	−0.685	0.281
Step 2	$\tilde{\varepsilon}_i$	−0.700	−0.191	0.418	0.700	−0.191	0.051
Step 4	w_i	0.130	0.000	0.000	0.330	1.000	1.000

Take notice of lines 14-15. In step 3 the deviations $\tilde{\varepsilon}_3$ and $\tilde{\varepsilon}_4$ are corrected because they exceed the obstacle value 0.7, the deviation $\tilde{\varepsilon}_2$ is corrected because at this moment the point x_2 is an active knot. Only the deviation $\tilde{\varepsilon}_1$ is left unchanged and the index set corresponding to the inactive knots is defined as $N = \{1\}$. Despite that in the next steps the deviation $\tilde{\varepsilon}_1$ is corrected and the knot x_1 has been taken into the set of active knots.

By the end of the algorithm we have $w_2 = w_3 = 0$. Thus, the solution

$$S(x) = c_1 + c_2 x + \sum_{i=1}^{6} d_i |x - x_i|^3 \tag{5.6}$$

has two inactive knots, x_2 and x_3, with corresponding coefficients $d_i = 0$, $i = 2, 3$. The values of other coefficients are $c_1 = 2.448$, $c_2 = 0.554$, $d_1 = -0.015$, $d_4 = 0.038$, $d_5 = -0.032$, $d_6 = 0.009$. Note that, for cubic splines, $G(x) = |x|^3/12$ and the coefficients of S in the representation (3.1) are multiples of the d_i used in (5.6). In the next example the presented coefficients d_i also differ from these in the representation (3.1) by c_{nr} times.

Example 5.2. Let us take $n = 2$, $r = 2$, knots $X_1 = (1, 1)$, $X_2 = (1, 2)$, $X_3 = (1, 3)$, $X_4 = (2, 1)$, $X_5 = (2, 2)$, $X_6 = (2, 3)$, $X_7 = (3, 1)$, $X_8 = (3, 2)$, $X_9 = (3, 3)$ and values $z_1 = 1$, $z_2 = 1$, $z_3 = 2$, $z_4 = 3$, $z_5 = 4$, $z_6 = 4$, $z_7 = 3$, $z_8 = 1$, $z_9 = 4$. Pose obstacle conditions $|S(X_i) - z_i| \leqslant 0.5$, $i = 1, \ldots, n$, and look for the solution of problem (3.6).

The working process of our algorithm is described in Table 5.2.

Table 5.2. Values of $\tilde{\varepsilon}_i$ and w_i computed by the algorithm

	i	1	2	3	4	5	6	7	8	9
GV	w_i	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000	1.000
Step 1	$\tilde{\varepsilon}_i$	−0.122	−0.403	−0.122	0.263	0.768	0.263	0.260	−1.167	0.260
Step 3	$\tilde{\varepsilon}_i$	−0.500	−0.500	−0.500	0.500	0.500	0.500	0.500	−0.500	0.500
Step 4	w_i	−0.271	1.699	−0.271	−0.431	3.176	−0.431	1.167	3.491	1.167
	w_i	0.000	1.699	0.000	0.000	3.176	0.000	1.167	3.491	1.167
Step 1	$\tilde{\varepsilon}_i$		−0.426			0.456		0.447	−0.507	0.447
Step 2	$\tilde{\varepsilon}_i$	−0.307	−0.426	−0.307	0.306	0.456	0.306	0.447	−0.507	0.447
Step 3	$\tilde{\varepsilon}_i$	−0.307	−0.500	−0.307	0.306	0.500	0.306	0.500	−0.500	0.500
Step 2	$\tilde{\varepsilon}_i$	−0.369	−0.500	−0.369	0.331	0.500	0.331	0.500	−0.500	0.500
Step 4	w_i	0.000	1.393	0.000	0.000	2.786	0.000	1.014	3.421	1.014

The solution

$$\begin{aligned} S(x, y) &= c_1 + c_2 x + c_3 y \\ &\quad + \sum_{i=1}^{9} d_i \left((x - x_i)^2 + (y - y_i)^2 \right) \log \sqrt{(x - x_i)^2 + (y - y_i)^2} \end{aligned} \tag{5.7}$$

of this smoothing problem has four inactive knots with corresponding coefficients $d_1 = d_3 = d_4 = d_6 = 0$. The other coefficients in the representation (5.7) are $c_1 = 0.529$, $c_2 = 0.634$, $c_3 = 0.500$, $d_2 = -0.697$, $d_5 = 1.393$, $d_7 = 0.507$, $d_8 = -1.711$, $d_9 = 0.507$. Note that we used here the notations $X = (x, y)$ and $X_i = (x_i, y_i)$.

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Kokkuvõte

Tõketega silumisülesannete lahendamine

Sageli kerkivad praktikas esile probleemid, kus on vaja lõpliku koguse diskreetsete andmete põhjal taastada mingi funktsioon. Kõige lihtsam funktsiooni taastamise moodus on interpoleerimine: olgu antud sõlmed x_i, $i = 1, \ldots, n$, ning sõlmväärtused y_i, $i = 1, \ldots, n$, otsime funktsiooni f, mis interpoleeriks antud väärtusi, st. $f(x_i) = y_i$, $i = 1, \ldots, n$, ning oleks seejuures piisavalt heade omadustega (pidevus, diferentseeruvus, lihtsus jt.). Algandmed võivad sisaldada meetodist või mõõteseadmetest tulenevaid ebatäpsusi, sel juhul tuleks interpoleerimise asemel andmeid mingil moel siluda. Kaaludega silumisülesanne seisneb kahest liidetavast koosneva funktsionaali minimiseerimises: üks liidetavatest tagab funktsioonile teatavad head omadused (mingis mõttes optimaalsuse), teine liidetav tagab algandmete lähendamise. Mõlemad eesmärgid ühtviisi hästi enamasti saavutatavad ei ole, kahe eesmärgi vahekorra määrab ülesandes esinev silumisparameeter. Näiteks

$$\min_{f \in W_2^2(a,b)} \left(p \int_a^b |f''(x)|^2 dx + \sum_{i=1}^{n} p_i (f(x_i) - y_i)^2 \right),$$

kus $p > 0$ ja $p_i > 0$, $i = 1, \ldots, n$, on tüüpiline näide kaaludega silumisülesandest (p_i on kaalud ning p silumisparameeter). Selle ülesande lahendiks on kuupsplain nn. loomulike rajatingimustega $f''(a) = f''(b) = 0$, mille leidmine taandub viiediagonaalse süsteemi lahendamisele. Praktilistes ülesannetes sageli puudub informatsioon kaalude p_i väärtuste kohta, kuid olemas võib olla informatsioon mõõtmisvigade kohta. Tõketega silumisülesannete korral on nõutud, et iga sõlme korral erinevus ordinaadi väärtusest ei tohi ületada mingit etteantud väärtust. Näiteks ülesande

$$\min_{f \in \Omega} \int_a^b |f''(x)|^2 dx$$

puhul, kus

$$\Omega = \left\{ f \in W_2^2(a,b) \;\middle|\; |f(x_i) - y_i| \leqslant \varepsilon_i,\ \varepsilon_i \geqslant 0,\ i = 1, \ldots, n \right\},$$

on tegemist tõketega silumisülesandega, mille lahendiks on jällegi naturaalne kuupsplain.

Käesoleva töö põhiliseks uurimisobjektiks on tõketega silumisülesanne, kuna selle lahendamiseks ei ole veel leitud rahuldavaid meetodeid. Töö esimeses peatükis vaadeldakse tõketega ja kaaludega silumisülesandeid võimalikult üldisel kujul. On teada, et kui tõketega ülesande Lagrange'i funktsioonil on olemas sadulpunkt, siis selle sadulpunkti üks komponent on vastava ülesande lahend ning teine komponent defineerib kaalud ekvivalentses kaaludega ülesandes. Ekvivalentsete ülesannete all mõeldakse kaaludega ja tõketega ülesandeid, mille algandmed (va. kaalud ja tõkked) ning lahendid ühtivad. Üldiselt kumera planeerimise ülesannetele vastavatel Lagrange'i funktsioonidel ei pruugi sadulpunkti eksisteerida, isegi kui ülesanne ise on lahenduv.

Esimeses peatükis tuuakse sisse mõiste kaaludega ülesande stabiilsus kaalude redutseerimise suhtes ning näidatakse, et kui kaaludega ülesandel on vastav omadus, siis leidub temaga ekvivalentne tõketega ülesanne, milles tõkked saab valida positiivsed. Viimane tähendab seda, et kaaludega ülesandes silutavad väärtused jäävad ka tõketega ülesandes silutavateks väärtusteks, neist ei saa interpoleeritavaid väärtusi. Viimane on tarvilik selleks, et tõketega ülesande jaoks leiduks ekvivalentne kaaludega ülesanne – interpolatsioonitingimust ei saa tagada ühegi reaalarvulise kaaluga. Üldjuhul kaaludega ülesanne ei ole stabiilne kaalude redutseerimise suhtes.

Teises peatükis vaadeldakse silumisülesandeid Hilberti ruumide kontekstis. Esitatakse vajalikud tulemused splainide variatsioonteooriast. Näidatakse, et S. N. Kersey artiklis [41] toodud kaaludega ülesande lahendi olemasoluteoreem ei kehti ning esitatakse korrektne iseloomustusteoreem. Nii interpoleerimis- kui silumisülesannete iseloomustusteoreemide korral on ära toodud piisavad tingimused selleks, et vastavate teoreemide eeldused oleks täidetud. Põhitulemustena tõestatakse, et Hilberti ruumis tõketega ülesande Lagrange'i funktsioonil leidub sadulpunkt, mis tähendab ekvivalentse kaaludega ülesande olemasolu, ning et kaaludega ülesanne Hilberti ruumis on stabiilne kaalude redutseerimise suhtes, mis tähendab ekvivalentse tõketega ülesande olemasolu. Kersey artiklis [39] on vaikimisi kasutatud kaaludega ülesande stabiilsust kaalude redutseerimise suhtes, kuid vastava omaduse kehtimine on seal põhjendamata.

Kolmandas peatükis vaadeldakse klassikalisi mitme muutuja silumisülesandeid Beppo Levi ruumis ning tõestatakse ära nende ekvivalentsus. Kuna Beppo Levi ruum on poolskalaarkorrutisega ruum, siis ei ole vastavate ülesannete korral rakendatavad teise peatüki tulemused.

Klassikalise tõketega ülesande lahendiks on naturaalsplain – funktsioon, mis esitub teatavate radiaalsete baasfunktsioonide nihete lineaarkombinatsiooni ning mingi polünoomi summana. Lahendi näol on tegemist interpolandiga, milles aktiivsetele sõlmedele vastavad kordajad splaini esituses peavad olema õige märgiga, sõltuvalt sellest, kas interpolant läbib alumist või ülemist tõket. Aktiivsete sõlmede leidmist on kirjeldatud peatükis 4, kus on esitatud M. I. Ignatovi ja A. B. Pevnõi [33] poolt välja pakutud sõlmede lisamise ja eemaldamise algoritm. Monograafia [33] autorid väidavad, et on tõestanud ka algoritmi lõplikkuse, kuid see tõestus kasutab üht väära lemmat. Peatükis 4 esitatakse kontranäide sellele lemmale ning näide, kus algoritmi täitmise käigus tekib tsükkel ning lahend ei ole leitav. Esitatud on mitmed piisavad tingimused algoritmi lõplikkuseks.

Viiendas peatükis on tuletatud võrrand, mis seob tõketega ülesande lahendi hälbeid etteantud väärtustest sõlmedes ja ekvivalentse ülesande kaalusid. On välja pakutud iteratiivse iseloomuga algoritm ning esitatud kaks näidet ühe ja kahe muutuja juhul, kus lõpliku arvu sammudega õnnestub leida otsitavad kaalud ekvivalentses ülesandes ning ühtlasi algse tõkkeülesande lahend. Esimene nendest näidetest on sama, mille korral sõlmede lisamise ja eemaldamise meetodis tekib tsükkel.

Antud töö ei anna küll lõplikku vastust küsimusele kuidas alati efektiivselt lahendada tõketega silumisülesandeid, kuid näidatud on, et tõketega silumisülesande lahendamise saab taandada vastava Lagrange'i funktsiooni sadulpunkti leidmisele. Viimases peatükis väljapakutud algoritm on sisuliselt sadulpunkti leidmise meetod ning töö autori arvates adekvaatseid meetodeid tõketega ülesande lahendamiseks tuleks otsida just sadulpunkti leidmise meetodite seast.

Peatüki 4 tulemused on publitseeritud artiklis [44]. Dissertatsiooni ülejäänud tulemused on suunatud publitseerimisele, peatükkide 1-3 tulemused on esitatud artiklis [45] ja peatüki 5 tulemused artiklis [46].

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List of publications

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3. E. Leetma, P. Oja, Connection between smoothing problems with obstacles and weights (preprint).

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1. **Mati Heinloo.** The design of nonhomogeneous spherical vessels, cylindrical tubes and circular discs. Tartu, 1991, 23 p.
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