The Application of Reproducing Kernel Based Spline Approximation to Seismic Surface and Body Wave Tomography: Theoretical Aspects and Numerical Results

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Vom Fachbereich Mathematik
der Universität Kaiserslautern
zur Erlangung des akademischen Grades
Doktor der Naturwissenschaften
(Doktor rerum naturalium, Dr. rer. nat.)
genehmigte Dissertation

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Vollzug der Promotion: 16. April 2007
D386

To my parents

Acknowledgements

First of all, I want to express my deep gratitude to my advisor, HDoz. Dr. Volker Michel for giving me the opportunity to work on this topic and for his great support concerning all the problems that have come up during my work. I would also like to thank Prof. Dr. Willi Freeden for making possible my study in Geomathematics Group, University of Kaiserslautern and for helpful advices.

I want to express my appreciation to Dr. Frederik J. Simons for very valuable discussions and suggestions, and to Prof. Dr. Jeannot Trampert for providing me with the phase data for surface waves.

I am grateful to all former and present members of the Geomathematics Group for valuable discussions.

I thank Dr. Falk Triebsch and Arthur Harutyunyan for their great assistance given to me during my study period in Kaiserslautern.

The financial support of the German Academic Exchange Service (DAAD), the Forschungsschwerpunkt "Mathematik und Praxis", University of Kaiserslautern and the International School for Graduate Studies (ISGS), University of Kaiserslautern is gratefully acknowledged.

Finally, I wish to thank my family for the warm encouragement and continuous support.

Introduction

The main task of geophysics is to study the internal structure of the Earth using surface and subsurface observational data. However, since direct measurements of the Earth's physical parameters can be done only on the Earth's surface or within an extremely narrow subsurface layer, the only method of studying the Earth's internal structure is based on solving inverse problems. One of such inverse problems is the so-called seismic traveltime tomography, whose task is to determine the velocity of seismic waves inside the Earth using the data about the time that the seismic wave takes to travel from one point to another or so-called traveltimes of seismic waves. The term tomography was coined from the Greek words tomos meaning slice and graphos meaning image, and is carried out in seismology from an analogous problem in medicine known as X-Ray tomography. Three types of seismic waves are commonly identified: body waves, surface waves, and free oscillations (for details see for example [1], [57]). Body waves travel through the interior of the Earth and are divided into two types: longitudinal or primary (P-waves) and transverse or secondary (S-waves). Longitudinal waves, which are compression and rarefaction waves, are connected with the oscillation of particles in the direction of propagation of the wave front; transverse waves are connected with the oscillation of particles in a direction orthogonal to the propagation direction of the wave front and characterize the resistance of the elastic substance to shear. Surface waves are analogous to water waves and travel over the Earth's surface. There are two types of surface waves: Rayleigh waves and Love waves. Due to this, in seismology, one distinguishes seismic body wave tomography, where the domain of the unknown velocity function and the ray paths are lying in the Earth's interior; and the seismic surface wave tomography, where the domain of the unknown velocity function and the ray paths are lying on the Earth's surface. However, it should be mentioned that surface wave tomography can be used to study the deeper structure of the Earth as well (see e.g. [67], [68]). The mechanical parameters of an isotropic elastic substance can be completely characterized by the elastic Lamé parameters λ, μ, and the material's density ρ. The propagation speeds of P-waves and S-waves (in geophysics they are usually denoted by v_{P} and v_{S}, respectively) are related with the Lamé parameters λ, μ, and the density ρ by the formulas

$$v_{\mathrm{P}} = \sqrt{\frac{\lambda + 2\mu}{\rho}}, \quad v_{\mathrm{S}} = \sqrt{\frac{\mu}{\rho}}. \tag{1}$$

Although the speeds of seismic waves v_P and v_S cannot completely characterize the mechanical parameters of an isotropic elastic substance but if they are known, then, as formulas (1) show, they provide two relations between the three parameters λ, μ, ρ and thus contain considerable information regarding the substance of the Earth. Therefore, one of the most important problems of seismology consists in finding the propagation speeds of seismic waves, which, as already mentioned is one of the main problems of seismic tomography. It is an inverse problem and may mathematically be represented as follows:

Given traveltimes $T_q; q = 1, ..., N$ of seismic waves between epicenters E_q and receivers R_q. Find a (slowness) function S, such that

$$\int_{\gamma_q} S(x) d\sigma(x) = T_q, \quad q = 1, ..., N, \tag{2}$$

where integrals are path integrals over $\gamma_q; q = 1, ..., N$, which, in general, are raypaths of seismic waves between E_q and R_q according to the slowness model S. In general (2) is non-linear. However, as it is shown e.g. in [1], [11], [41], [61] this problem can be solved approximately with the help of a linearization of (2), by taking seismic ray paths between E_q and R_q according to some reference slowness model as γ_q. In this thesis we only discuss the linear variant of the seismic traveltime tomography problem.

At present there basically exist two concepts used to solve this problem. One concept, which will be called here the "block concept" subdivides the invested region into small areas (blocks) where the velocity of the waves is assumed to be of a simple structure (e.g. constant [13], [85], or cubic B-spline [80], [81]). This method has some advantages in its practical implementation but has a natural limit in the obtainable resolution (as any other method has).

The second concept develops a spherical harmonic expansion of the velocity or its deviation from a given model (see e.g. [17], [73], [74], [75], [82]). Its advantages are based on the fact that the properties of spherical harmonics have been studied intensively in the past and many theorems and numerical tools are already available for its application. The drawback of this approach is that the used basis functions are polynomials and therefore, have a global character. However, since seismic events strongly agglomerate in certain regions and the density of recording stations extremely varies over the planet the available seismic data are by far not uniformly distributed over the Earth's surface. Due to this the structure of the Earth can only coarsely be resolved in some areas, whereas detailed models could be obtained elsewhere. This hampers the determination of local models and the local variation of the resolution of global models.
In this thesis we demonstrate that the concept of approximating/interpolating splines in reproducing kernel Sobolev spaces can be another alternative. Since such splines are constructed via reproducing kernel functions that, in contrast to spherical harmonics, are localizing (see also Section 3.2.2) we do not have the drawback of the spherical harmonics.
In several geoscientific applications such as gravity data analysis (see e.g. [20], [25]), modelling of the (anharmonic) density distribution inside the Earth ([45]), modelling of seismic wave front propagation ([37], [38]) and deformation analysis ([25], [77]) the splines or related spline methods derived from the harmonic version on the sphere have already been applied successfully. In this thesis we derive a theoretical basis for the applications of such splines to surface as well as body wave tomography, which includes in particular the construction of a corresponding spline method for the 3-dimensional ball. Moreover, we run numerous numerical tests that justify the theoretical considerations.

The outline of this thesis is as follows:

Chapter 1 presents the basic notations, concepts, definitions and theorems within the scope necessary for this study. In particular some orthogonal series of polynomials namely Legendre and Jacobi polynomials, as well as complete orthonormal systems on a sphere and a ball are presented.

In Chapter 2 we give a brief introduction to inverse ill-posed problems in the framework of linear problems in Banach spaces and in that context present (as far as we know) a new operator-form formulation of the seismic traveltime linear tomography problem. Furthermore, we discuss the question on uniqueness and obtain a new result on the instability of that inverse problem.

In Chapter 3 we introduce spline functions in a reproducing kernel Sobolev space to interpolate/approximate prescribed data. In order to be able to apply the spline approximation concept to surface wave as well as to body wave tomography problems, the spherical spline approximation concept, introduced by W. Freeden in [21] and [22], is extended for the case where the domain X of the function to be approximated is an arbitrary compact set in $\mathbb{R}^n$. This concept is discussed in details for the case of the unit ball and the unit sphere. In this context we also obtain some new results on convergence and error estimates of interpolating splines and demonstrate a method for construction of a regularization of inverse problems via splines.

In Chapter 4 we present an application of a spline approximation method to seismic surface wave traveltime tomography. We summarize briefly the results of Chapter 3 for the case where X is the unit sphere in $\mathbb{R}^3$. Some other theoretical aspects, including a new result on uniqueness and convergence, as well as numerical aspects of such an application are discussed. We also present results of numerical tests which include the reconstruction of the Rayleigh and Love wave phase velocity at 40, 50, 60, 80, 100, 130 and 150 seconds. Moreover, for comparison purposes (for some phases) we obtain the corresponding phase velocity maps using the well-known spherical harmonics approximation method. To verify our spline method some tests with synthetic data sets, namely the so-called checkerboard tests, a test by adding random noise to the initial traveltime data and a test with a so-called hidden object, have been done as well.

In Chapter 5 an application of the discussed spline approximation method to seismic body wave traveltime tomography is presented. Theoretical and numerical aspects of such an application are discussed and some results of numerical tests are demonstrated. Here numerical tests include a partial reconstruction of the

P-wave velocity function (according to PREM) and its perturbation with the use of synthetic data sets.

The results of this work are summarized in Chapter 6, some conclusions are made and an outlook is given.

Finally, Appendix A contains a brief overview of seismic ray theory within the framework of this thesis.

Contents

Chapter 1

Basic Fundamentals

In this chapter we present the basic notations, concepts, definitions and theorems within the scope necessary for this study. In particular some orthogonal series of polynomials namely Legendre and Jacobi polynomials, as well as complete orthonormal systems on a sphere and a ball are presented.

1.1 Preliminaries

The letters $\mathbb{N}, \mathbb{N}_0, \mathbb{Z}, \mathbb{R}$ and $\mathbb{C}$ denote the set of positive integers, non-negative integers, integers, real numbers and complex numbers, respectively. $\mathbb{R}^n, n \in \mathbb{N}$ denotes the n-dimensional Euclidean space. We consider $\mathbb{R}^n$ to be equipped with the canonical inner product $\cdot$ and associated norm $|\cdot|$. For $M \subset \mathbb{R}^n$ by $\text{int}M$, ∂M and $\bar{M}$ denote the set of all inner points of M, the boundary of M, and the closure of M, respectively. Throughout this work by Ω and B we will always denote the unit sphere and the closed unit ball in $\mathbb{R}^3$, respectively, i.e. $\Omega = \{x \in \mathbb{R}^3 : |x| = 1\}$ and $B = \{x \in \mathbb{R}^3 : |x| \leq 1\}$. We suppose that the reader is familiar with concepts of linear, topological, Banach, pre-Hilbert and Hilbert spaces.
A set S in a real linear space X is called *convex* if for any two distinct points $x_1, x_2 \in S$ and any real $0 \leq \alpha \leq 1$, the point $\alpha x_1 + (1-\alpha)x_2$ is in S.
A topological space is called *separable* if it contains a countable dense subset. Let V be a linear space and V_1 and V_2 be subspaces of V. We call V the *direct sum* of V_1 and V_2 and denote $V = V_1 \dot{+} V_2$, if any $v \in V$ can be uniquely decomposed as $v = v_1 + v_2$, where $v_1 \in V_1$ and $v_2 \in V_2$. Every direct sum induces a *projector*

of V onto V_1 along V_2, defined by $Pv := v_1$. Clearly P is a linear, idempotent (i.e. $P^2 = P$) operator, with the range V_1 and null space V_2. If the projector P is continuous, V is said to be a *topological direct sum* of V_1 and V_2, and written as $V = V_1 \oplus V_2$. In this case V_1 is called a *topological complement* of V_2 in V.
For $D \subset \mathbb{R}^n$ and $k \in \mathbb{N}$, we denote the set of all continuous functions $F : D \to \mathbb{R}$ such that every derivative of F of order $\leq k$ exists on int$D$ and is continuous by $\mathrm{C}^{(k)}(D)$. For $\mathrm{C}^{(0)}(D) =: \mathrm{C}(D)$ we define

$$\|F\|_{\mathrm{C}(D)} := \sup_{x\in D} |F(x)|, \quad F \in \mathrm{C}(D).$$

The functional $\|\cdot\|_{\mathrm{C}(D)}$ is a norm, if for instance D is compact. In this case $\mathrm{C}(D)$ becomes a Banach space.
Let $D \subset \mathbb{R}^n$ be a compact set. The space of all on D bounded functions is denoted by $\mathrm{B}(D)$. It is known that $\mathrm{B}(D)$ equipped with the (supremum) norm

$$\|F\|_\infty := \sup_{x\in D} |F(x)|, \quad F \in \mathrm{B}(D),$$

is a Banach space (see e.g. [62]). Clearly, $\mathrm{C}(D) \subset \mathrm{B}(D)$.
Let $D \subset \mathbb{R}^n$ be a compact set and $\Theta \subset D$ be a set of finitely many points of D. We denote the set of all functions which are bounded on D and continuous on $D \setminus \Theta$ by $\mathrm{C}_\Theta(D)$, i.e. every function in $\mathrm{C}_\Theta(D)$ is bounded and piecewise continuous on D. Clearly, for any set $\Theta \subset D$ of finitely many points, $\mathrm{C}(D) \subset \mathrm{C}_\Theta(D) \subset \mathrm{B}(D)$. It can be shown that $\mathrm{C}_\Theta(D)$ equipped with the supremum norm is a Banach space. In fact, since $\mathrm{C}_\Theta(D) \subset \mathrm{B}(D)$ and $B(D)$ is complete, if $\{F_n\}_{n\in\mathbb{N}} \subset \mathrm{C}_\Theta(D)$ is a Cauchy sequence then there exists $F \in \mathrm{B}(D)$ such that

$$\|F - F_n\|_\infty \to 0, \quad \text{as} \quad n \to \infty.$$

This implies that if for any $n \in \mathbb{N}$, F_n is continuous at $x \in D$, then F is continuous at $x \in D$, too. Hence F is continuous on $D \setminus \Theta$, and therefore $F \in \mathrm{C}_\Theta(D)$. Thus, $\mathrm{C}_\Theta(D)$ is a Banach space.
Let $D \subset \mathbb{R}^n$ be an arbitrary measurable set. By $\mathrm{L}^2(D)$ we denote the space of all real and square-Lebesgue-integrable functions defined on D, where the elements of $\mathrm{L}^2(D)$ are, more precisely, equivalence classes of almost everywhere identical functions. $\mathrm{L}^2(D)$ equipped with the inner product

$$(F, G)_{\mathrm{L}^2(D)} := \int_D F(x)G(x)dx, \quad F, G \in \mathrm{L}^2(D),$$

is a Hilbert space.

Lemma 1.1.1 *([62]) Let $D \subset \mathbb{R}^n$ be an arbitrary compact set. Then for any $F \in \mathrm{B}(D) \cap \mathrm{L}^2(D)$*

$$\|F\|_{\mathrm{L}^2(D)} \le \sqrt{\mathrm{measure}(D)}\, \|F\|_\infty.$$

Definition 1.1.2 *Let X be a normed linear space and $\{x_k\}_{k\in\mathbb{N}_0}$ be a sequence of elements of X.*
(i) $\{x_k\}_{k\in\mathbb{N}_0}$ is called complete in X if for any linear bounded functional $\mathcal{F}$ on X, $\mathcal{F}(x_k) = 0$, $k = 0, 1, 2, ...$ implies $\mathcal{F} = 0$.
(ii) $\{x_k\}_{k\in\mathbb{N}_0}$ is called closed in X if any $y \in X$ can be arbitrarily well approximated by a finite linear combination of $\{x_k\}_{k\in\mathbb{N}_0}$, i.e. for any $y \in X$ and real $\varepsilon > 0$ there exists $n \in \mathbb{N}_0$ and $a_1, ..., a_n \in \mathbb{R}$ such that

$$\left\| y - \sum_{i=0}^{n} a_i x_i \right\| \le \varepsilon.$$

Theorem 1.1.3 *([15]) A sequence of elements $\{x_k\}$ of a normed linear space X is closed if and only if it is complete.*

Theorem 1.1.4 *([15]) Let $\{x_n\}_{n\in\mathbb{N}_0}$ be an orthonormal system in a real Hilbert space $(X, (\cdot,\cdot))$. Then the following statements are equivalent:*

(A) $\{x_n\}_{n\in\mathbb{N}_0}$ is closed (in sense the of the approximation theory) in X, i.e.

$$X = \overline{\mathrm{span}\{x_n | n \in \mathbb{N}_0\}}^{(\cdot,\cdot)}.$$

(B) $\{x_n\}_{n\in\mathbb{N}_0}$ is complete in X. That is $y \in X$ and $(y, x_i) = 0$, $i \in \mathbb{N}_0$ implies $y = 0$.

(C) The Fourier series of any element $y \in X$ converges in the norm to y, i.e.

$$\lim_{N\to\infty} \left\| y - \sum_{i=0}^{N} (y, x_i) x_i \right\| = 0.$$

(D) Any element of X is uniquely determined by its Fourier coefficients: That is, if $(y, x_i) = (z, x_i)$, for all $i \in \mathbb{N}_0$, then $y = z$.

(E) Parseval's identity holds. That is for all $y, z \in X$,

$$(y, z) = \sum_{i=0}^{N} (y, x_i)(z, x_i).$$

Theorem 1.1.5 *([15]) The powers* $1, x, x^2, \ldots,$ *defined on* $[a, b]$ *are complete in* $\mathrm{L}^2([a, b])$.

Corollary 1.1.6 *([15]) A sequence* $\{p_n\}_{n\in\mathbb{N}_0}$, *where* p_n *is a polynomial of degree* n *defined in* $[a, b]$, *is complete in* $\mathrm{L}^2([a, b])$.

Theorem 1.1.7 *(Weierstraß, [62]) A sequence* $\{p_n\}_{n\in\mathbb{N}_0}$, *where* p_n *is a polynomial of degree* n *defined in* $[a, b]$, *is closed in* $\mathrm{C}([a, b])$.

Theorem 1.1.8 *(Luzin, [62]) Let* $X \subset \mathbb{R}^n$, $n \in \mathbb{N}$ *be a compact set. Then for any measurable function* f *on* X *and any real number* $\varepsilon > 0$ *there exists* $g \in \mathrm{C}(X)$ *such that*

$$\text{measure}(\{x \in X : f(x) \neq g(x)\}) \leq \varepsilon.$$

Theorem 1.1.9 *([62]) Let* $X \subset \mathbb{R}^n$, $n \in \mathbb{N}$ *be a compact set. Then*

$$\overline{\mathrm{C}(X)}^{\|\cdot\|_{\mathrm{L}^2(X)}} = \mathrm{L}^2(X).$$

Taking into account that the measure of a compact set is always finite and using Lemma 1.1.1 and Corollary 1.1.9 one obtain the following theorem.

Theorem 1.1.10 *Let* $X \subset \mathbb{R}^n$, $n \in \mathbb{N}$ *be a compact set and* $\{f_i\}_{i\in\mathbb{N}}$ *be a sequence of continuous functions on* X . *If* $\{f_i\}_{i\in\mathbb{N}}$ *is closed in* $\mathrm{C}(X)$ *then it is closed in* $\mathrm{L}^2(X)$ *as well.*

Theorem 1.1.11 *(F. Riesz' representation theorem, [84]) Let* $(X, (\cdot, \cdot))$ *be a Hilbert space and* $\mathcal{F}$ *a bounded linear functional on* X. *Then there exists a uniquely determined element* $y_{\mathcal{F}}$ *of* X, *called the representer of* $\mathcal{F}$, *such that*

$$\mathcal{F}(x) = (x, y_{\mathcal{F}}) \quad \text{for all} \quad x \in X, \quad \text{and} \quad \|\mathcal{F}\| = \|y_{\mathcal{F}}\|.$$

Conversely, any element $y \in X$ *defines a bounded linear functional* $\mathcal{F}_y$ *on* X *such by*

$$\mathcal{F}_y(x) = (x, y) \quad \text{for all} \quad x \in X, \quad \text{and} \quad \|\mathcal{F}_y\| = \|y\|.$$

Theorem 1.1.12 *([83]) Let H be a dense and convex set in a normed linear space E, and let $\mathcal{F}_1, ..., \mathcal{F}_n$ be n linear functionals over E. Then for any element f in E and for every real $\varepsilon > 0$ there exists $g \in H$ such that $\|f - g\|_E \leq \varepsilon$ and*

$$\mathcal{F}_i f = \mathcal{F}_i g, \quad \textit{for all} \quad i = 1, ..., n.$$

1.2 Legendre Polynomials

The following introduction to the theory of Legendre polynomials is based on [24], where further details about this subject can be found.

Definition 1.2.1 *The Legendre Polynomials $\{P_n\}_{n\in\mathbb{N}_0}$ are polynomials, defined in the interval $[-1, 1]$ and given by Rodriguez's formula:*

$$P_n(t) = \frac{1}{2^n n!} \left(\frac{d}{dt}\right)^n (t^2 - 1)^n, \quad t \in [-1, 1], n \in \mathbb{N}_0.$$

Theorem 1.2.2 *If for every $n \in \mathbb{N}_0$:*

(i) P_n *is a polynomial of degree n, defined on $[-1, 1]$,*

(ii) $\int_{-1}^{1} P_n(t)P_m(t)dt = 0$ *for all $m \in \mathbb{N}_0 \backslash \{n\}$,*

(iii) $P_n(1) = 1$,

then $\{P_n\}_{n\in\mathbb{N}_0}$ is the system of Legendre Polynomials.

Theorem 1.2.3 *For any $n \in \mathbb{N}_0$*

$$\|P_n\|^2_{\mathrm{L}^2([-1,1])} = \frac{2}{2n + 1}.$$

Theorem 1.2.4 *The Legendre Polynomials $\{P_n\}_{n\in\mathbb{N}}$ and their derivatives have the following property:*

$$|P_n^{(k)}(t)| \leq |P_n^{(k)}(1)|$$

for all $k \in \mathbb{N}_0$ and all $t \in [-1, 1]$, in particular

$$|P_n(t)| \leq |P_n(1)|$$

for all $t \in [-1, 1]$.

Theorem 1.2.5 ***(recurrence formulae)***
The Legendre Polynomials $\{P_n\}_{n\in\mathbb{N}_0}$ satisfy the following identities:

$$\begin{aligned} P'_{n+1}(t) - tP'_n(t) &= (n+1)P_n(t), \\ (t^2-1)P'_n(t) &= ntP_n(t) - nP_{n-1}(t), \\ (n+1)P_{n+1}(t) + nP_{n-1}(t) &= (2n+1)tP_n(t). \end{aligned}$$

1.3 Jacobi Polynomials

For further constructions we also need a more general orthogonal system of polynomials namely Jacobi polynomials. We only present definitions and some properties of them. For further details and proofs we refer to [44] and [70].

Definition 1.3.1 *Let $b > 0$ and $a > b-1$ be given real numbers. The Jacobi polynomials are defined by the following Rodriguez's formula*

$$G_n(a,b;x) := \frac{(-1)^n\Gamma(n+a)}{\Gamma(2n+a)} x^{(1-b)}(1-x)^{(b-a)} \left(\frac{d}{dx}\right)^n \left(x^{(n+b-1)}(1-x)^{n+a-b}\right)$$

for $n \in \mathbb{N}_0$ and $x \in [0,1]$, where Γ is the Gamma function.

Theorem 1.3.2 *Let $b > 0$ and $a > b-1$ be given real numbers. The Jacobi polynomials $\{G_n(a,b;x)\}_{n\in\mathbb{N}_0}$ are the only polynomials to satisfy the following properties for all $n \in \mathbb{N}_0$:*

(*i*) $G_n(a,b;\cdot)$ *is a polynomial of degree n, defined on* $[0,1]$.

(*ii*) $G_n(a,b;0) = 1$.

(*iii*) $\int_0^1 x^{b-1}(1-x)^{a-b}G_n(a,b;x)G_m(a,b;x)dx = 0$ *for all* $m \in \mathbb{N}_0 \backslash \{n\}$.

In case of $m = n$, we have (see [70] p. 212)

$$\int_0^1 x^{b-1}(1-x)^{a-b}G_n(a,b;x)G_n(a,b;x)dx = n!\frac{\Gamma(a+n)\Gamma(b+n)\Gamma(a-b+n+1)}{(2n+a)[\Gamma(a+2n)]^2}.$$

Hence, if we set

$$\tilde{G}_n(a,b;x) := \left[\frac{(2n+a)[\Gamma(a+2n)]^2}{n!\Gamma(a+n)\Gamma(b+n)\Gamma(a-b+n+1)}\right]^{1/2} G_n(a,b;x), \tag{1.1}$$

where $x \in [0,1]$, then the system $\{\tilde{G}_n(a,b;x)\}_{n\in\mathbb{N}_0}$ will be orthonormal in $\mathrm{L}^2[0,1]$ with the weight function $w(x) = x^{b-1}(1-x)^{a-b}$.
Since for any $b > 0$ and $a > b-1$, $G_n(a,b;\cdot)$ is a polynomial of degree n, defined on $[0,1]$, $\tilde{G}_n(a,b;\cdot)$ also is a polynomial of degree n, defined on $[0,1]$. Hence, Theorem 1.1.7 implies that the system $\{\tilde{G}_n(a,b;x)\}_{n\in\mathbb{N}_0}$ is closed in $\mathrm{C}[0,1]$.
Note that one finds an alternative definition in the literature (see e.g. [70]), where the functions $P_n^{(\alpha,\beta)}$, $n \in \mathbb{N}_0$, with $\alpha, \beta > -1$ fixed, are called Jacobi polynomials if they satisfy the following properties for all $n \in \mathbb{N}_0$:

(i) $P_n^{(\alpha,\beta)}$ is a polynomial of degree n, defined on $[-1,1]$.

(ii) $\int_0^1 (1-x)^\alpha (1+x)^\beta P_n^{(\alpha,\beta)}(x) P_m^{(\alpha,\beta)}(x)dx = 0 \quad \text{for all} \quad m \in \mathbb{N}_0 \backslash \{n\}.$

(ii) $P_n^{(\alpha,\beta)}(1) = \dfrac{\Gamma(n+\alpha+1)}{\Gamma(n+1)\Gamma(\alpha+1)}.$

The relation between $P_n^{(\alpha,\beta)}$ and $G_n(a,b;\cdot)$ is given by (see [70], p. 210)

$$G_n(a,b;x) = \frac{n!\Gamma(n+a)}{\Gamma(2n+a)} P_n^{(a-b,b-1)}(2x-1), \quad x \in [0,1]. \tag{1.2}$$

Note that the Legendre Polynomials represent the special case $P_n = P_n^{(0,0)}$.

Theorem 1.3.3 *For any $\alpha, \beta > -1$ the Jacobi Polynomials $P_n^{(\alpha,\beta)}$ have the following property (see [44], p. 217):*

$$\max_{x\in[-1,1]} |P_n^{(\alpha,\beta)}(x)| = \begin{cases} \mathcal{O}(n^q), & \textit{if} \quad q = \max(a,b) \geq -1/2 \\ \mathcal{O}(n^{-1/2}), & \textit{if} \quad q = \max(a,b) < -1/2 \end{cases} \tag{1.3}$$

as $n \to \infty$.

Theorem 1.3.4 ***(recurrence formula)***
For any $\alpha, \beta > -1$ and for all $x \in [-1,1]$ the Jacobi Polynomials $P_n^{(\alpha,\beta)}$ satisfy the following identities (see [44], p. 213):

$$P_0^{(\alpha,\beta)}(x) = 1, P_1^{(\alpha,\beta)}(x) = \frac{\alpha-\beta}{2} + \frac{1}{2}(\alpha+\beta+2)x,$$

and for $n \geq 2$,

$$\begin{aligned} & 2n(\alpha+\beta+n)(\alpha+\beta+2n-2)P_n^{(\alpha,\beta)}(x) \\ = & [(\alpha+\beta+2n-2)(\alpha+\beta+2n-1)(\alpha+\beta+2n)x + (\alpha^2-\beta^2)]P_{n-1}^{(\alpha,\beta)}(x) \\ & -2(\alpha+n-1)(\beta+n-1)(\alpha+\beta+2n)P_{n-2}^{(\alpha,\beta)}(x). \end{aligned}$$

1.4 Spherical Harmonics

Spherical harmonics are the functions most commonly used to represent scalar fields on a spherical surface. We will use constructions with spherical harmonics for approximations of seismic surface as well as body wave velocities. In this section we present definitions and some well-known facts from the theory of spherical harmonics. For the proofs of the theorems and further details we refer to [24] and references therein.

Definition 1.4.1 *Let $D \subset \mathbb{R}^3$ be open and connected. A function $F \in \mathrm{C}^{(2)}(D)$ is called harmonic if and only if*

$$\Delta_x F(x) = \sum_{i=1}^{3} \frac{\partial^2 F}{\partial x_i^2}(x) = 0, \quad \textit{for all} \quad x = (x_1, x_2, x_3)^{\mathrm{T}} \in D.$$

The set of all harmonic functions in $\mathrm{C}^{(2)}(D)$ is denoted by $\mathrm{Harm}(D)$.

Definition 1.4.2 *A polynomial P on $\mathbb{R}^3$ is called homogeneous of degree n if $P(\lambda x) = \lambda^n P(x)$ for all $\lambda \in \mathbb{R}$, and all $x \in \mathbb{R}^3$. The set of all homogeneous polynomials of degree n on $\mathbb{R}^3$ is denoted by $\mathrm{Hom}_n(\mathbb{R}^3)$.*

Theorem 1.4.3 *The dimension of $\mathrm{Hom}_n(\mathbb{R}^3)$ is given by*

$$\dim\left(\mathrm{Hom}_n(\mathbb{R}^3)\right) = \frac{(n+1)(n+2)}{2}, \quad n \in \mathbb{N}_0.$$

Definition 1.4.4 *The set of all homogeneous harmonic polynomials on $\mathbb{R}^3$ with degree $n \in \mathbb{N}_0$ is denoted by $\mathrm{Harm}_n(\mathbb{R}^3)$, i.e.*

$$\mathrm{Harm}_n(\mathbb{R}^3) := \left\{ P \in \mathrm{Hom}_n(\mathbb{R}^3) \mid \Delta P = 0 \right\}, \quad n \in \mathbb{N}_0.$$

Furthermore, we define

$$\begin{aligned} \mathrm{Harm}_{0\ldots n}(\mathbb{R}^3) &:= \bigoplus_{i=0}^{n} \mathrm{Harm}_i(\mathbb{R}^3), \quad n \in \mathbb{N}_0, \\ \mathrm{Harm}_{0\ldots\infty}(\mathbb{R}^3) &:= \bigcup_{i=0}^{\infty} \mathrm{Harm}_{0\ldots i}(\mathbb{R}^3). \end{aligned}$$

Definition 1.4.5 *A spherical harmonic of degree n is the restriction of a homogeneous harmonic polynomial on $\mathbb{R}^3$ with degree $n \in \mathbb{N}_0$ to the unit sphere Ω. The collection of all spherical harmonics of degree n will be denoted by* $\mathrm{Harm}_n(\Omega)$*, i.e.*

$$\mathrm{Harm}_n(\Omega) = \left\{ F|_\Omega \mid F \in \mathrm{Harm}_n(\mathbb{R}^3) \right\}, \quad n \in \mathbb{N}_0.$$

Theorem 1.4.6 *If $m \neq n$ then* $\mathrm{Harm}_m(\Omega)$ *is orthogonal to* $\mathrm{Harm}_n(\Omega)$ *in the sense of* $\mathrm{L}^2(\Omega)$*, i.e. if $m \neq n$, then for all $Y_m \in \mathrm{Harm}_m(\Omega)$ and all $Y_n \in \mathrm{Harm}_n(\Omega)$*

$$(Y_m, Y_n)_{\mathrm{L}^2(\Omega)} = 0.$$

Hence, if we have orthonormal systems for every $\mathrm{Harm}_n(\Omega)$, $n \in \mathbb{N}_0$, we get an orthonormal system for the space $\mathrm{Harm}_{0\ldots\infty}(\Omega)$.

Theorem 1.4.7 *The dimension of* $\mathrm{Harm}_n(\Omega)$*, $n \in \mathbb{N}_0$ is equal to $2n+1$, i.e.*

$$\dim\left(\mathrm{Harm}_n(\Omega)\right) = 2n + 1, \quad n \in \mathbb{N}_0.$$

Therefore, a complete orthonormal system in $\mathrm{Harm}_n(\Omega)$ must have exactly $2n+1$ elements.

Definition 1.4.8 *By $\{Y_{n,j}\}_{n\in\mathbb{N}_0, j=-n,\ldots,n}$ we will always denote a complete* $\mathrm{L}^2(\Omega)$*-orthonormal system in* $\mathrm{Harm}_{0\ldots\infty}(\Omega)$*, such that $Y_{n,j} \in \mathrm{Harm}_n(\Omega)$ for all $j = -n, ..., n$. We call n the degree of $Y_{n,j}$, and j the order of $Y_{n,j}$.*

The evaluation of sums with spherical harmonics can be essentially simplified by the following theorem.

Theorem 1.4.9 ***(Addition Theorem for Spherical Harmonics)***
For all $\xi, \eta \in \Omega$ we have

$$\sum_{j=-n}^{n} Y_{n,j}(\xi) Y_{n,j}(\eta) = \frac{2n+1}{4\pi} P_n(\xi \cdot \eta),$$

where P_n is the Legendre Polynomial of degree n.

The following theorem implies that every function in $\mathrm{C}(\Omega)$ can be approximated arbitrarily well (in $\mathrm{C}(\Omega)$ sense) by the system $\{Y_{n,j}\}_{n\in\mathbb{N}_0, j=-n,\ldots,n}$.

Theorem 1.4.10 *The system* $\{Y_{n,j}\}_{n\in\mathbb{N}_0, j=-n,...,n}$ *is closed in* $\mathrm{C}(\Omega)$.

The fundamental importance of the spherical harmonics is demonstrated by the following theorem.

Theorem 1.4.11 *The system* $\{Y_{n,j}\}_{n\in\mathbb{N}_0, j=-n,...,n}$ *is complete in* $\mathrm{L}^2(\Omega)$.

Hence, Theorem 1.1.4 implies that the system $\{Y_{n,j}\}_{n\in\mathbb{N}_0, j=-n,...,n}$ is closed as well, i.e. every function in $\mathrm{L}^2(\Omega)$ can be approximated arbitrarily well (in $\mathrm{L}^2(\Omega)$ sense) by the system $\{Y_{n,j}\}_{n\in\mathbb{N}_0, j=-n,...,n}$.

In applications we will use a particular system of spherical harmonics given by

$$Y_{n,j}(\xi) = Y_{n,j}(\xi(\theta,\phi)) = \begin{cases} \sqrt{2}\, X_{n,|j|}(\theta)\cos(j\phi), & \text{if } \quad -n \le j < 0, \\ X_{n,0}(\theta), & \text{if } \quad j = 0, \\ \sqrt{2}\, X_{n,j}(\theta)\sin(j\phi), & \text{if } \quad 0 < j \le n, \end{cases} \tag{1.4}$$

$n \in \mathbb{N}_0$, $j \in \{-n, ..., n\}$; where

$$X_{n,j}(\theta) := (-1)^j \left(\frac{2n+1}{4\pi}\right)^{1/2} \left(\frac{(n-j)!}{(n+j)!}\right)^{1/2} P_{n,j}(\cos\theta), \tag{1.5}$$

$$P_{n,j}(t) := \frac{1}{2^n n!}\left(1-t^2\right)^{j/2} \left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^{n+j} \left(t^2-1\right)^n,$$

and $\theta \in [0,\pi]$ and $\phi \in [0, 2\pi)$ are the colatitude and the longitude corresponding to $\xi = (\xi_1, \xi_2, \xi_3) \in \Omega$ which can be calculated from the equations $\cos(\theta) = \xi_3$, $\tan(\phi) = \xi_2/\xi_3$. Usually $P_{n,j}$ is called associated Legendre function of degree n and order j.

We will also use a system of complex valued spherical harmonics given by

$$\mathcal{Y}_{n,j}(\xi) = \mathcal{Y}_{n,j}(\xi(\theta,\phi)) := X_{n,j}(\theta)e^{ij\phi}; \quad n \in \mathbb{N}_0, j \in \{-n, ..., n\}, \tag{1.6}$$

where $X_{n,j}$ is defined in (1.5).
So, we see that, for $n \in \mathbb{N}_0$ and $j \in \{-n, ..., n\}$,

$$Y_{n,j}(\xi) = \begin{cases} \sqrt{2}\,\mathrm{Re}\mathcal{Y}_{n,|j|}(\xi), & \text{if } \quad -n \le j < 0, \\ \mathcal{Y}_{n,0}(\xi), & \text{if } \quad j = 0, \\ \sqrt{2}\,\mathrm{Im}\mathcal{Y}_{n,j}(\xi), & \text{if } \quad 0 < j \le n, \end{cases} \tag{1.7}$$

For details on the theory of complex spherical harmonics we refer to [14] and [52].

1.5 Complete Orthonormal System in $\mathrm{L}^2(B)$

Let $\{g_k(r)\}_{k\in\mathbb{N}_0}$, $r \in [0,1]$ be an orthonormal system in $\mathrm{L}^2[0,1]$ with the weight function $w(r) = r^2$ in $[0,1]$, i.e.

$$\int_0^1 r^2 g_k(r) g_l(r) dr = \delta_{k,l}, \quad k,l \in \mathbb{N}_0. \tag{1.8}$$

We define the sequence $\left\{W^B_{k,n,j}(x)\right\}_{k,n\in\mathbb{N}_0;j=-n,\dots,n}$ by

$$W^B_{k,n,j}(x) = W^B_{k,n,j}(r_x\xi_x) := \begin{cases} g_k(r_x)Y_{n,j}(\xi_x), & \text{if} \quad x \in B\setminus\{0\}, \\ 1, & \text{if} \quad x = 0, \end{cases} \tag{1.9}$$

where $r_x = |x|$, $\xi_x = x/|x|$ and $Y_{n,j}$ is the spherical harmonic of degree n and order j. Note that here any other real can be taken as $W^B_{k,n,j}(0)$, too. Throughout this work by r_x and ξ_x we will always denote the norm and the unit vector of $x \in \mathbb{R}^3 \setminus \{0\}$ respectively.
Next, we see that

$$\begin{aligned} \left(W^B_{k_1,n_1,j_1}, W^B_{k_2,n_2,j_2}\right)_{\mathrm{L}^2(B)} &= \int_B W^B_{k_1,n_1,j_1}(x) W^B_{k_2,n_2,j_2}(x) dx \\ &= \int_B (g_{k_1}(r_x)Y_{n_1,j_1}(\xi_x))(g_{k_2}(r_x)Y_{n_2,j_2}(\xi_x)) d(r_x\xi_x) \\ &= \int_0^1 r_x^2 g_{k_1}(r_x) g_{k_2}(r_x) \left(\int_\Omega Y_{n_1,j_1}(\xi_x)Y_{n_2,j_2}(\xi_x) d\omega(\xi_x)\right) dr_x \\ &= \left(\int_0^1 r_x^2 g_{k_1}(r_x) g_{k_2}(r_x) dr\right) \delta_{n_1,n_2}\delta_{j_1,j_2} \\ &= \delta_{k_1,k_2}\delta_{n_1,n_2}\delta_{j_1,j_2}, \end{aligned}$$

where (1.8) and the orthonormality of $\{Y_{n,j}\}_{n\in\mathbb{N}_0;j=-n,\dots,n}$ in $\mathrm{L}^2(\Omega)$ have been used. Hence, $\left\{W^B_{k,n,j}\right\}_{k,n\in\mathbb{N}_0;j=-n,\dots,n}$ is orthonormal in $\mathrm{L}^2(B)$. Moreover, it can be shown that if $\{g_k(r)\}_{k\in\mathbb{N}_0}$ is complete in $\mathrm{L}^2[0,1]$ then $\left\{W^B_{k,n,j}(x)\right\}_{k,n\in\mathbb{N}_0;j=-n,\dots,n}$ will be complete in $\mathrm{L}^2(B)$. In fact, $\left\{W^B_{k,n,j}\right\}_{k,n\in\mathbb{N}_0;j=-n,\dots,n}$ is complete in $\mathrm{L}^2(B)$ if for any $F \in \mathrm{L}^2(B)$,

$$\int_B F(x) W^B_{k,n,j}(x) dx = \int_0^1 g_k(r_x) r_x^2 \int_\Omega F(r_x\xi_x) Y_{n,j}(\xi_x) d\sigma(\xi_x) dr_x = 0, \tag{1.10}$$

for any $k, n \in \mathbb{N}_0, j = -n, ...n$, implies that $F = 0$ almost everywhere (a.e.) in B. Take any $F \in \mathrm{L}^2(B)$. We denote

$$U_{n,j}(r_x) := r_x^2 \int_\Omega F(r_x\xi_x)Y_{n,j}(\xi_x)d\sigma(\xi_x), \quad r_x \in [0,1].$$

Now, if $\{g_k(r)\}_{k\in\mathbb{N}_0}$ is complete in $\mathrm{L}^2[0,1]$ then from (1.10) follows that for any $n \in \mathbb{N}_0, j = -n, ..., n$, $U_{n,j} = 0$ a.e. in $[0,1]$. Hence,

$$\int_\Omega F(r_x\xi_x)Y_{n,j}(\xi_x)d\sigma(\xi_x) = 0$$

for almost all $r_x \in [0,1]$. However, since $\{Y_{n,j}\}_{n\in\mathbb{N}_0;j=-n,...,n}$ is complete in $\mathrm{L}^2(\Omega)$, $F(r_x\xi_x) = 0$ for almost all $r_x \in [0,1]$ and almost all $\xi_x \in \Omega$. Therefore, $F = 0$ a.e. in B.

Thus, in order to $\left\{W^B_{k,n,j}\right\}_{k,n\in\mathbb{N}_0;j=-n,...,n}$ be a complete orthonormal system in $\mathrm{L}^2(B)$, we need to choose the system $\{g_k(r)\}_{k\in\mathbb{N}_0}$ such that it is complete in $\mathrm{L}^2[0,1]$ and fulfils (1.8). However, in Section 1.3 we have seen that the system $\{\tilde{G}_k(3,3,r)\}_{k\in\mathbb{N}_0}$, $r \in [0,1]$ of normalized Jacobi polynomials is complete in $\mathrm{L}^2[0,1]$ and is orthonormal in $\mathrm{L}^2[0,1]$ with the weight function $w(r) = r^2$. Thus, by taking $g_k(r) := \tilde{G}_k(3,3,r)$, $\left\{W^B_{k,n,j}\right\}_{k,n\in\mathbb{N}_0;j=-n,...,n}$ will be a complete orthonormal system in $\mathrm{L}^2(B)$.

Using Equations (1.1) and (1.2), we can simplify $\tilde{G}_k(3,3,r_x)$.

$$\begin{aligned}
\tilde{G}_k(3,3,r_x) &= \left[\frac{(2k+3)[\Gamma(3+2k)]^2}{k!\Gamma(3+k)\Gamma(3+k)\Gamma(k+1)}\right]^{1/2} G_k(3,3,r_x) \\
&= \left[\frac{(2k+3)[\Gamma(3+2k)]^2}{k!\Gamma(3+k)\Gamma(3+k)\Gamma(k+1)}\right]^{1/2} \frac{k!\Gamma(k+3)}{\Gamma(2k+3)} P_k^{(0,2)}(2r_x-1) \\
&= \left[\frac{(2k+3)[2+2k)!]^2}{[k!]^2[(2+k)!]^2}\right]^{1/2} \frac{k!(k+2)!}{(2k+2)!} P_k^{(0,2)}(2r_x-1) \\
&= \sqrt{2k+3}P_k^{(0,2)}(2r_x-1).
\end{aligned}$$

Hence,

$$W^B_{k,n,j}(x) = W^B_{k,n,j}(r_x\xi_x) := \begin{cases} \sqrt{2k+3}P_k^{(0,2)}(2r_x-1)Y_{n,j}(\xi_x), & \text{if} \quad x \in B \setminus \{0\}, \\ 1, & \text{if} \quad x = 0, \end{cases} \tag{1.11}$$

with $k, n \in \mathbb{N}_0; j = -n, ..., n$.
The set $(0, 1] \times \Omega$ is isomorphic to $B \setminus \{0\}$, where e.g. the map $(r_x, \xi_x) \mapsto (r_x \xi_x)$, with $r_x \in (0, 1]$, $\xi_x \in \Omega$ can be taken as an isomorphism. Therefore, the continuity of $\tilde{G}_k(3, 3, \cdot)Y_{n,j}(\cdot)$ on $(0, 1] \times \Omega$ implies the continuity of $W^B_{k,n,j}(\cdot)$ on $B \setminus \{0\}$, where $k, n \in \mathbb{N}_0; j = -n, ..., n$. However, it can be shown that for all $k \in \mathbb{N}_0$, with $\tilde{G}_k(3, 3, 0) \neq 0$ and for all $n \in \mathbb{N}_0; j = -n, ..., n$, $W^B_{k,n,j}(\cdot)$ is not continuous at $0 \in B$. In fact, let $k \in \mathbb{N}_0$ such that $\tilde{G}_k(3, 3, 0) \neq 0$ and let $n \in \mathbb{N}_0; j = -n, ..., n$ be arbitrary, but fixed. Moreover, let $\xi_1, \xi_2 \in \Omega$ such that $Y_{n,j}(\xi_1) \neq Y_{n,j}(\xi_2)$ and let $\{r_m\}_{m\in\mathbb{N}}$ be a sequence in $[0, 1]$ with $r_m \to 0$ as $m \to \infty$. In this case,

$$\lim_{m\to\infty} x^1_m = \lim_{m\to\infty} x^2_m = 0,$$

where $x^1_m := r_m \xi_1$ and $x^2_m := r_m \xi_2$, $m \in \mathbb{N}$. However,

$$\tilde{G}_k(3, 3, 0)Y_{n,j}(\xi_1) = \lim_{m\to\infty} W^B_{k,n,j}(x^1_m) \neq \lim_{m\to\infty} W^B_{k,n,j}(x^2_m) = \tilde{G}_k(3, 3, 0)Y_{n,j}(\xi_2).$$

Hence, taking into account the fact that for any $k, n \in \mathbb{N}_0$ and $j = -n, ..., n$, $W^B_{k,n,j}$ is bounded on B we obtain that $\left\{W^B_{k,n,j}\right\}_{k,n\in\mathbb{N}_0;j=-n,...,n} \subset \mathrm{C}_\Theta(B)$, with $\Theta = \{0\}$.

Chapter 2

Seismic Tomography as an Inverse Problem

Here we give a brief introduction to inverse ill-posed problems in the framework of linear problems in Banach spaces (for more details see for example [10], [19], [53], [55], [59], [72]). In this context we discuss questions concerning the uniqueness, the stability and the existence of the solution of the seismic traveltime tomography problem.

2.1 Inverse Ill-posed Problems

Let $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ and $(\mathcal{K}, \|\cdot\|_{\mathcal{K}})$ be Banach spaces and $\Lambda : \mathcal{H} \to \mathcal{K}$ be a linear bounded operator.

Problem 2.1.1 *Given $G \in \mathcal{K}$, find $F \in \mathcal{H}$ such that*

$$\Lambda F = G. \tag{2.1}$$

Denote the domain, range and nullspace of Λ by $\mathcal{D}(\Lambda)$, $\mathcal{R}(\Lambda)$ and $\mathcal{N}(\Lambda)$, respectively.

Definition 2.1.2 *The inverse problem 2.1.1 is called well-posed in the sense of Hadamard (or in the classical sense), if the following conditions are satisfied:*

- *for each $G \in \mathcal{K}$ there exists $F \in \mathcal{H}$, such that $\Lambda F = G$,*
  (existence of a solution)

- *for each $G \in \mathcal{K}$ there exists no more than one $F \in \mathcal{H}$, such that $\Lambda F = G$, (uniqueness of the solution)*

- *the solution $F \in \mathcal{H}$ depends continuously on $G \in \mathcal{K}$. (continuity/stability of the inverse Λ^{-1})*

Otherwise Problem 2.1.1 is called ill-posed.

This means that for an ill-posed problem the operator Λ^{-1} does not exist, or is not defined on all of $\mathcal{K}$, or is not continuous.
In practice we are often not confronted with the well-posed problems. First of all a solution of $\Lambda F = G$ exists only if G is in the range of Λ. Errors due to unprecise measurements may cause that $G \notin \mathcal{R}(\Lambda)$. Another difficulty with an ill-posed problem is that even if it is solvable, the solution of $\Lambda F = G$ needs not be close to the solution of $\Lambda F = G^{\varepsilon}$ if G^{ε} is close to G.
In order to define a substitute for the solution of $\Lambda F = G$, if there is none, one introduces a notion of a so-called generalized solution, which roughly speaking is the F for which ΛF is "nearest" (in some sense) to G.
Assume that there exist closed subspaces $M \subset \mathcal{H}$ and $S \subset \mathcal{K}$ such that $\mathcal{H}$ and $\mathcal{K}$ can be represented as a direct sum of $\mathcal{N}(\Lambda)$ and M and respectively of $\overline{\mathcal{R}(\Lambda)}$ and S, i.e. $\mathcal{H} = \mathcal{N}(\Lambda) \dot{+} M$ and $\mathcal{K} = \overline{\mathcal{R}(\Lambda)} \dot{+} S$. Let P be the projector of $\mathcal{H}$ onto $\mathcal{N}(\Lambda)$ along M and Q be the projector of $\mathcal{K}$ onto $\overline{\mathcal{R}(\Lambda)}$ along S. However, it is known that (see e.g. [65]) if a Banach space is represented as a direct sum of two closed subspaces then this direct sum is topological, i.e. the corresponding projectors are continuous. Hence, P and Q are continuous, i.e. $\mathcal{H} = \mathcal{N}(\Lambda) \oplus M$ and $\mathcal{K} = \overline{\mathcal{R}(\Lambda)} \oplus S$. Let Λ_0 be the restriction of Λ to M, $\Lambda_0 := \Lambda|M$. Then $\Lambda_0 : M \to \mathcal{R}(\Lambda)$ is bijective. The *generalized inverse* (see [55]) Λ^+ of Λ is defined as the unique extension of Λ_0^{-1} to $\mathcal{R}(\Lambda) \dot{+} S$ such that $\Lambda^+(S) = 0$. Clearly, Λ^+ is linear. It can also be shown that Λ^+ is characterized by the following equations:

$$
\begin{aligned}
&\Lambda^+ \Lambda \Lambda^+ = \Lambda^+ && \text{on} \quad \mathcal{D}(\Lambda^+) := \mathcal{R}(\Lambda) \dot{+} S \\
&\Lambda \Lambda^+ = Q && \text{on} \quad \mathcal{D}(\Lambda^+) \\
&\Lambda^+ \Lambda = I - P
\end{aligned}
$$

This implies that $\Lambda \Lambda^+ \Lambda = \Lambda$. We also have that $\Lambda^+ = \Lambda_0^{-1} Q$ on $\mathcal{D}(\Lambda^+)$, $\mathcal{R}(\Lambda^+) = M$ and $\mathcal{N}(\Lambda^+) = S$. For $G \in \mathcal{D}(\Lambda^+)$, $F := \Lambda^+ G$ is the unique solution of

$$\Lambda F = QG \tag{2.2}$$

in M. Hence, the set of all solutions of (2.2) is $\Lambda^+ G + \mathcal{N}(\Lambda)$.
Note that if $\mathcal{H}$ and $\mathcal{K}$ are Hilbert spaces then $\mathcal{N}(\Lambda)$ and $\overline{\mathcal{R}(\Lambda)}$ have topological complements. In particular, if we take $M := \mathcal{N}(\Lambda)^\perp$ and $S := \mathcal{R}(\Lambda)^\perp$, then Λ^+ is also called *Moore-Penrose* inverse of Λ (see e.g. [55],[59]). Moreover, in that case, for any $G \in \mathcal{D}(\Lambda^+)$, $\Lambda^+ G$ is the unique least-squares solution of minimal norm of (2.1). For Hilbert spaces one can prove also the following theorem (see e.g. [54]).

Theorem 2.1.3 *Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces and $\Lambda : \mathcal{H} \to \mathcal{K}$ be a linear bounded operator. Then, the generalized (Moore-Penrose) inverse of Λ, Λ^+ is continuous if and only if $\mathcal{R}(\Lambda)$ is closed.*

We mention that motivated from this result in Hilbert spaces one can also give another definition of ill-posedness.

Definition 2.1.4 *Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces and $\Lambda : \mathcal{H} \to \mathcal{K}$ be a linear bounded operator. Problem 2.1.1 is called ill-posed in the sense of Nashed, if the range of $\mathcal{R}(\Lambda)$ is not closed. Otherwise, it is called well-posed in the sense of Nashed.*

In general, Λ^+ is not a continuous operator, this means that "small" changes in the data can cause "big" changes in the solution. In order to have a continuous dependence of the solution on the data one introduces the concept of a regularization of Λ^+ (see e.g. [53], [72]).

Definition 2.1.5 *Let $(\mathcal{H}, \|\cdot\|_{\mathcal{H}})$ and $(\mathcal{K}, \|\cdot\|_{\mathcal{K}})$ be Banach spaces and $\Lambda : \mathcal{H} \to \mathcal{K}$ be a linear bounded operator. Assume that the closure $\overline{\mathcal{R}(\Lambda)}$ has a topological complement in $\mathcal{K}$, say S. The family of operators $\Lambda_J : \mathcal{K} \to \mathcal{H}$, $J \in \mathbb{Z}$, is called a regularization of the generalized inverse Λ^+ if*

(i) for any $J \in \mathbb{Z}$, Λ_J is linear and bounded on $\mathcal{K}$,

(ii) for any $G \in \mathcal{R}(\Lambda) \dot{+} S$,

$$\lim_{J\to\infty} \|\Lambda_J G - \Lambda^+ G\|_{\mathcal{H}} = 0.$$

The function $F_J = \Lambda_J G$ is called J-level regularization of Problem 2.1.1 and the parameter J is called regularization parameter.

Obviously, $\|\Lambda_J\| \to \infty$ as $J \to \infty$ if Λ^+ is not bounded.
With the help of regularization one can solve Problem 2.1.1 approximately in the following sense. Let G^ε be an approximation of G such that $\|G^\varepsilon - G\|_{\mathcal{K}} \leq \varepsilon$. Let also $F^+ = \Lambda^+ G$, and $F_J = \Lambda_J G^\varepsilon$, $J \in \mathbb{Z}$. Then

$$\begin{aligned}\|F_J - F^+\|_{\mathcal{H}} &\leq \|\Lambda_J G^\varepsilon - \Lambda_J G\|_{\mathcal{H}} + \|\Lambda_J G - \Lambda^+ G\|_{\mathcal{H}} \\ &\leq \|\Lambda_J\| \|G^\varepsilon - G\|_{\mathcal{K}} + \|\Lambda_J G - \Lambda^+ G\|_{\mathcal{H}} \\ &\leq \varepsilon \|\Lambda_J\| + \|\Lambda_J G - \Lambda^+ G\|_{\mathcal{H}}\,.\end{aligned}$$

This decomposition shows that the error consists of two parts: the first term reflects the influence of the incorrect data, while the second term is represent the approximation error between Λ_J and Λ^+. Usually the first term increases with the increasing of J because of the ill-posed nature of the problem, whereas the second term will decrease as $J \to \infty$ according the definition of a regularization. Every regularization scheme requires a strategy for choosing the parameter J in dependence on the error level ε in order to achieve an acceptable total error for the regularized solution.
There are several methods for constructing a regularization, e.g. the Truncated Singular Value Decomposition, the Method of Tikhonov-Philips, Iterative Methods (see e.g. [10], [19], [72]), Regularization with Wavelets (see e.g. [23], [46], [47], [58]), etc. In the following chapter we will present a spline approximation method and in particular we will show that it can be considered as a regularization.

2.2 Seismic Traveltime Linearized Tomography

The task of seismic traveltime tomography is to determine the seismic wave velocity function/model out of traveltime data related to the positions of the epicenters and the recording stations. This is an inverse problem, which can be represented as follows:

Problem 2.2.1 *Given traveltimes $T_q; q = 1, ..., N$ of seismic waves between epicenters E_q and receivers R_q on the Earth's surface. Find a (slowness) function S, such that*

$$T_q = \int_{\gamma_q} S(x)\, d\sigma(x), \quad q = 1, ..., N, \tag{2.3}$$

where $\gamma_q; q = 1, ..., N$ are seismic rays between E_q and R_q, and $d\sigma(x)$ is the arc-length element.

Seismic rays $\gamma_q; q = 1, ..., N$ are dependent on the slowness model S, and this brings nonlinearity into Problem 2.2.1. To avoid this nonlinearity we will use the most common approach in seismological literature (see e.g. [12], [42], [57]), the so-called traveltime perturbation method (see Section A.3). That is in Equations (2.3) instead of traveltimes we will use traveltime differences or so called delay times, with respect to traveltimes in a reference slowness model:

$$\delta T_q = T_q - T_q^0 = \int_{\gamma_q} S(x)\, d\sigma(x) - \int_{\gamma_q^0} S_0(x)\, d\sigma(x) \quad q = 1, ..., N, \tag{2.4}$$

where T_q^0 and γ_q^0, $q = 1, ..., N$, are respectively traveltimes and raypaths of seismic waves in a reference slowness model $S_0(x)$. Therefore, assuming that $\delta S = S - S_0$ is not "big", using Equation A.13, we can substitute the unknown raypaths in a slowness model $S(x)$ by raypaths in a reference model $S_0(x)$.
We mention that the assumption that δS is not "big" in seismological literature usually means that S_0 and S differ from one another no more than 10%, i.e. $|\delta S| \leq \min(|S|, |S_0|)/10$.
So, with the accuracy of small quantities of the order of δS^2 (see Section A.3) we can rewrite (2.4) approximately as:

$$\delta T_q = T_q - T_q^0 \approx \int_{\gamma_q^0} \delta S(x)\, d\sigma(x) \quad q = 1, ..., N. \tag{2.5}$$

This (approximate) equation already expresses a linear relationship between the observed delay times and the perturbations $\delta S =: \mathcal{S}$ to the reference slowness model S_0. In the present work we only discuss the linear formulation of seismic traveltime tomography. For investigations on the nonlinear formulation of our problem, see e.g. [2], [8], [14] and references therein.

In seismic body wave tomography the domain of the unknown slowness function S and the raypaths γ_q are lying in the Earth's interior; whereas in seismic surface wave tomography the domain of S and γ_q are lying on the Earth's surface. In this chapter we will consider only the case of body wave tomography, as long as for surface wave tomography the results are analogous.

We shall present a more precise mathematical formulation of Problem 2.2.1. Throughout this work we will use the unit ball B in $\mathbb{R}^3$ as an approximation to the Earth, and the unit sphere $\Omega = \partial B$ therefore will be used as an approximation to the Earth's surface.

Assumption 2.2.2 *Seismic rays are uniquely determined by the given data about the type of the considered seismic waves, reference model S_0 and by the source and receiver coordinates.*

This is not a restriction since if there are several seismic rays between the given source and receiver we will just take any particular one of them (see Section A.1).

Assumption 2.2.3 *The perturbation $\mathcal{S}$ is a continuous function in B, i.e. $\mathcal{S} \in \mathrm{C}(B)$.*

It should be mentioned that usually the slowness perturbation function $\mathcal{S}$ is supposed to possess continuous derivatives of second and sometimes higher order. It will be additionally mentioned if such a requirement arises.

Assumption 2.2.4 *The seismic sources and receivers are located on the Earth's surface.*

Taking this into account we reformulate Problem 2.2.1 as follows:

Problem 2.2.5 *Given real numbers $T_q; q = 1, ..., N$ and pairs of points $(E_q, R_q) \in \Omega \times \Omega$. Find $\mathcal{S} \in \mathrm{C}(B)$ such that*

$$T_q = \int_{\gamma_q} \mathcal{S}(x)\, d\sigma(x), \quad q = 1, ..., N, \tag{2.6}$$

where $\gamma_q; q = 1, ..., N$, are given curves/raypaths (independent from $\mathcal{S}$) between E_q and R_q.

This is the so-called discrete formulation of the seismic traveltime linear inversion problem, since traveltimes are given only for finitely many rays. For further discussions and analysis it is convenient to write Problem 2.2.5 in continuous form as well (see e.g. [41],[61]).

By $\gamma_{S_0}(\nu_1, \nu_2) =: \gamma_{S_0}(u)$, $u = (\nu_1, \nu_2) \in \Omega \times \Omega$ we denote the seismic raypath between ν_1 and ν_2, according to the reference model S_0. If no confusion is likely to arise, we will simply write γ_u instead of $\gamma_{S_0}(u)$.

In this case Problem 2.2.5 in continuous form can be formulated as follows:

Problem 2.2.6 *Given a function $\tau(u) = \tau(\nu_1, \nu_2)$, $u = (\nu_1, \nu_2) \in \Omega \times \Omega$, find a continuous function $\mathcal{S}$ in B such that*

$$\tau(u) := \tau(\nu_1, \nu_2) := \int_{\gamma_{S_0}(u)} \mathcal{S}(x) d\sigma(x). \tag{2.7}$$

This problem in the nonlinear case, i.e. when we have $\gamma_{\mathcal{S}}(u)$ instead of $\gamma_{S_0}(u)$ in Equation (2.7), is also called the inverse kinematic problem of seismology, and was first considered in 1905-1907 by G. Herglotz (see [34]) and E. Wiechert, assuming spherical symmetry of the Earth.
We will show now that $\tau(\nu_1, \nu_2)$ can be assumed to be a continuous function of ν_1 and ν_2. First, let us show that the traveltime in a non-linearized model is a continuous function. That is

Theorem 2.2.7 *Let for any $u = (\nu_1, \nu_2) \in \Omega \times \Omega$,*

$$\tau_S'(u) := \tau_S'(\nu_1, \nu_2) := \int_{\gamma_S(u)} S(x) d\sigma(x).$$

Then for any non-negative measurable and bounded function S in B $\tau_S'(\cdot, \cdot)$ is a continuous function on $\Omega \times \Omega$.

Proof: Take arbitrary points $\nu_1^0, \nu_2^0 \in \Omega$. We show that $\tau_S'(\cdot, \cdot)$ is continuous at (ν_1^0, ν_2^0). For any $\nu_1, \nu_2 \in \Omega$ denote by $\Gamma(\nu_1, \nu_2)$ the set of all smooth curves γ lying in B and joining the points ν_1 and ν_2. Let also

$$\Upsilon_{(\nu_1,\nu_2)}(\gamma) := \int_\gamma S(x) d\sigma(x), \quad \gamma \in \Gamma(\nu_1, \nu_2).$$

In this case according to Fermat's principle (see Section A.1) the seismic ray between ν_1 and ν_2 (according to the slowness model S) is the curve $\gamma \in \Gamma(\nu_1, \nu_2)$ on which the functional $\Upsilon(\gamma)$ achieves its minimum, i.e.

$$\tau_S'(\nu_1, \nu_2) = \Upsilon_{(\nu_1,\nu_2)}(\gamma_S(\nu_1, \nu_2)) = \min_{\gamma \in \Gamma(\nu_1,\nu_2)} \int_\gamma S(x) d\sigma(x).$$

Now take any $\varepsilon > 0$. Clearly, for sufficiently small $\delta > 0$ and for any $\nu_1, \nu_2 \in \Omega$, if $|\nu_1 - \nu_1^0| < \delta$ and $|\nu_2 - \nu_2^0| < \delta$, then ν_1 and ν_2 can be smoothly connected to $\gamma_S(\nu_1^0, \nu_2^0)$ with the curves l_1, l_2 with the lengths smaller than $C_1\delta$, where C_1 is some positive constant (see Figure 2.1). The obtained smooth curve that connects

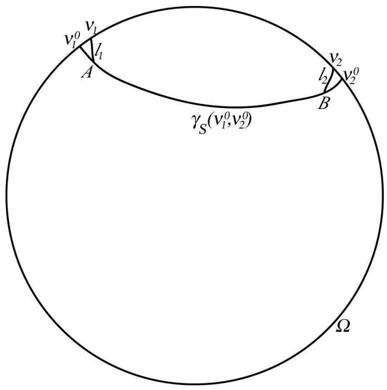


Figure 2.1: Construction of γ_1.

the points ν_1, A, B, ν_2 will be denoted by γ_1.
Let S be bounded by the constant $C_2 > 0$. Since S is non-negative,

$$\begin{aligned} \tau'_S(\nu_1, \nu_2) &= \min_{\gamma \in \Gamma(\nu_1,\nu_2)} \int_\gamma S(x)d\sigma(x) \leq \int_{\gamma_1} S(x)d\sigma(x) \\ &\leq \int_{l_1} S(x)d\sigma(x) + \int_{l_2} S(x)d\sigma(x) + \int_{\gamma_S(\nu_1^0,\nu_2^0)} S(x)d\sigma(x) \\ &\leq 2\delta C_1 C_2 + \tau'_S(\nu_1^0, \nu_2^0). \end{aligned}$$

Hence, taking $\delta = \varepsilon/2C_1C_2$ we obtain

$$\tau'_S(\nu_1, \nu_2) \leq \varepsilon + \tau'_S(\nu_1^0, \nu_2^0).$$

In an analogous way we obtain that

$$\tau'_S(\nu_1^0, \nu_2^0) \leq \varepsilon + \tau'_S(\nu_1, \nu_2).$$

Therefore

$$|\tau'_S(\nu_1, \nu_2) - \tau'_S(\nu_1^0, \nu_2^0)| \leq \varepsilon,$$

as $|\nu_1 - \nu_1^0| < \delta$ and $|\nu_2 - \nu_2^0| < \delta$.
Since $\nu_1^0, \nu_2^0 \in \Omega$ was arbitrary, $\tau'_S(\cdot,\cdot) \in \mathrm{C}(\Omega \times \Omega)$. ■

The approximate Equation (2.5) (in a continuous form) can be written as

$$\tau'_S(\nu_1, \nu_2) - \tau'_{S_0}(\nu_1, \nu_2) \approx \int_{\gamma_{S_0}(u)} (S(x) - S_0(x))d\sigma(x) \quad \text{for any} \quad \nu_1, \nu_2 \in \Omega. \quad (2.8)$$

where S and S_0 represent real and reference slowness model respectively, and therefore are non-negative and bounded. Theorem 2.2.7 implies that $\tau'_S(\cdot, \cdot)$, $\tau'_{S_0}(\cdot, \cdot) \in \mathrm{C}(\Omega \times \Omega)$. Therefore, if we set $\mathcal{S} := S - S_0$ then $\tau(\cdot, \cdot)$ defined by the Equation (2.7) can be written as

$$\tau(\cdot, \cdot) \approx \tau'_S(\nu_1, \nu_2) - \tau'_{S_0}(\nu_1, \nu_2).$$

That is $\tau(\cdot, \cdot)$ can be represented (approximately) as a difference of continuous functions, therefore, in the context of linear tomography it is realistic to make the following assumption.

Assumption 2.2.8 $\tau(\cdot, \cdot)$ *is a continuous function on* $\Omega \times \Omega$.

Next, we will assume the following properties.

Assumption 2.2.9 *There exists an integer* L *such that for any* $u_1, u_2 \in \Omega \times \Omega$, *with* $u_1 \neq u_2$ *the number of intersection points of* γ_{u_1} *and* γ_{u_2} *is smaller than* L.

For example if γ_u, $u \in \Omega \times \Omega$ are straight lines then any number greater than 1 can be taken as L. If γ_u, $u \in \Omega \times \Omega$ can be represented as a part of an ellipse then any number greater than 2 can be taken as L.

Assumption 2.2.10 *There exists* $M^{S_0} \in \mathbb{R}$ *such that for any ball* $B_\alpha \subset B$ *with radius* α,

$$\mathrm{length}\left(\gamma_u^{B_\alpha}\right) < M^{S_0}\alpha, \quad \textit{for all} \quad u \in \Omega \times \Omega,$$

where length$\left(\gamma_u^{B_\alpha}\right)$ *is the length of the part of* γ_u *whose image is in* B_α.

In particular, taking $B_\alpha = B$ we will have that

$$\mathrm{length}(\gamma_u) < M^{S_0} \quad \text{for all} \quad u \in \Omega \times \Omega.$$

For example if γ_u, $u \in \Omega \times \Omega$ are straight lines then any number greater than 2 can be taken as M^{S_0}. If γ_u, $u \in \Omega \times \Omega$ can be represented as a part of an ellipse

then any number greater than 2π can be taken as M^{S_0}.
Denote by T the operator, defined on $\mathrm{C}(B)$, by $T(F) = TF =: \tau_F$, where

$$\tau_F(u) = \int_{\gamma_u} F(x) d\sigma(x), \quad u \in \Omega \times \Omega.$$

Using our notations we can write Problem 2.2.6 in the following form:

Problem 2.2.11 *Given a function τ defined on $\Omega \times \Omega$, find a function $F \in \mathrm{C}(B)$ such that*

$$TF = \tau\,. \tag{2.9}$$

Note that in Problem 2.2.5, as well as in practice, τ is given only in finitely many points of $\Omega \times \Omega$.
According to Assumption 2.2.8 $\tau(\cdot, \cdot)$ is a continuous function on $\Omega \times \Omega$. Hence the range of T is in the space of continuous functions on $\Omega \times \Omega$, i.e. $T : \mathrm{C}(B) \to \mathrm{C}(\Omega \times \Omega)$.
Clearly, T is linear. Using Assumption 2.2.10 we obtain that for any $F \in \mathrm{C}(B)$,

$$\|TF\|_{\mathrm{C}(\Omega\times\Omega)} = \max_{u\in\Omega\times\Omega} \left| \int_{\gamma_u} F(x) d\sigma(x) \right| < M^{S_0} \max_{x \in B} |F(x)| = M^{S_0} \|F\|_{\mathrm{C}(B)}.$$

This means that T is bounded and therefore continuous as well.

We remark also that Problem 2.2.11 can be considered as a special case of the main problem of integral geometry, which in general case can be formulated as follows (see [28]): Let $u(x)$ be a sufficiently smooth function defined in n-dimensional space, i.e. $x = (x_1, ..., x_n)$, and let $\{\mathcal{M}(\lambda)\}$ be a family of smooth manifolds in this space depending on a parameter $\lambda = (\lambda_1, ..., \lambda_k)$ defined on a parameter space Λ. For a given function $v(\lambda)$, it is required to find the function $u(x)$, with

$$\int_{\mathcal{M}(\lambda)} u(x)\, d\sigma = v(\lambda), \quad \lambda \in \Lambda,$$

where $d\sigma$ defines the element of measure on $\mathcal{M}(\lambda)$.
Another special case of Integral Geometry is the so-called Computerized Tomography (see e.g. [56]), which has important applications in medicine. In that case the corresponding transform which maps a function into the set of its line integrals is called Radon transform.

2.2.1 On Uniqueness of the Solution

Clearly, the uniqueness of the solution of the integral geometry problem, and in particular Problem 2.2.11 depends on the family of the curves on which the integral of the target function is given. That is, it depends on the reference slowness function according to which these curves are generated.
The first general results on uniqueness of the integral geometry problem, in linear and nonlinear case, were obtained by R. G. Mukhometov in [48], [49] in the two-dimensional case. The multidimensional generalization of these results have been done by R. G. Mukhometov himself [50], [51], by I. N. Bernstein and M. L. Gerver [7] as well as by some other authors V. G. Romanov [60], Y. E. Anikonov and V. G. Romanov [3].
The question on uniqueness of the integral geometry problem is also discussed in differential geometry and known as *boundary rigidity problem* (see e.g. [66], [69], [78] and the references therein).

Here we present (without proof) the result of I. N. Bernstein and M. L. Gerver obtained in [7].

Definition 2.2.12 *The family Γ of curves is called regular in B if the following holds true.*
a) For any point $x \in B$ and every direction θ, a unique curve $\gamma_{x,\theta} \in \Gamma$ passes through the point x and its tangent has the direction θ at x.
*b) Denote by $y(x, \theta, s)$ the point of the curve $\gamma_{x,\theta}$, which we arrive moving along $\gamma_{x,\theta}$ from x at a direction θ at a distance s. $y(x, \theta, s)$ is a smooth * function of x, θ, s on its domain, say $\mathcal{M}$.*
c) $\mathcal{M}$ is compact. In particular lengths of the curves of Γ are uniformly bounded.
d) One unique curve from Γ passes through any two different points from B, i.e. the equality $y(x, \theta, s) = y$ has a unique solution (θ, s) for any $x, y \in B$, $x \neq y$.
e) That solution (θ, s) depends smoothly on x, y with $x \neq y$.

Theorem 2.2.13 *([7]) If the family of seismic curves Γ is regular, then Problem 2.2.11 for a smooth function F has no more than one solution.*

*For simplicity "smooth" is understood here as infinitely often differentiable.

In case of surface wave tomography and for a special case of Problem 2.2.11, analogous uniqueness problems will be discussed in later chapters.

2.2.2 The Instability of the Solution

To prove the instability of the solution of Problem 2.2.11 we have to show that if T^{-1} exists then it is not continuous. For this we use the following well known theorem from functional analysis (see e.g. [84]).

Theorem 2.2.14 *Let $(X, \|\cdot\|_X)$, $(Y, \|\cdot\|_Y)$ be normed linear spaces. Then a linear operator $\mathcal{T} : X \to Y$ admits a continuous inverse $\mathcal{T}^{-1}$ on the range of T if and only if there exists a constant $c > 0$ such that*

$$c\|x\|_X \leq \|\mathcal{T}x\|_Y, \quad \textit{for all} \quad x \in X.$$

The following theorem, as far as we know, is a new result.

Theorem 2.2.15 *If $T^{-1} : T(\mathrm{C}(B)) \to \mathrm{C}(B)$ exists then it is not continuous.*

Proof: From Theorem 2.2.14 we see that for discontinuity of T^{-1} it is enough to show that for any $c > 0$ there exists $F \in \mathrm{C}(B)$ such that $c\|F\|_{\mathrm{C}(B)} > \|TF\|_{\mathrm{C}(\Omega\times\Omega)}$. Take any $c > 0$, we can construct a continuous non-negative function $F_c \in \mathrm{C}(B)$ such that $\max_{x\in B} |F_c(x)| = F_c(x_0) \neq 0$ for some $x_0 \in B$ and $F_c(x) = 0$ for any $x \notin x_0(c/M^{S_0})$, where $x_0(c/M^{S_0})$ is the c/M^{S_0} neighborhood of x_0.
Hence using Assumption 2.2.10 we obtain that

$$\|TF\|_{\mathrm{C}(\Omega\times\Omega)} = \max_{u\in\Omega\times\Omega} \left| \int_{\gamma_u} F(x) d\sigma(x) \right| < \frac{c}{M^{S_0}} M^{S_0} \|F\|_{\mathrm{C}(B)} = c \, \|F\|_{\mathrm{C}(B)}.$$

This completes our proof. ■

2.2.3 On Existence of the Solution

The question on existence of the solution of the seismic tomography problem (in general case) is not widely discussed and is still open. At present we can only say that if the operator T is injective, i.e. the solution of Problem 2.2.11 is unique, then T is not surjective, i.e. there exists $\tau_0 \in \mathrm{C}(\Omega \times \Omega)$ for which Equation (2.9) has no solution. This fact holds true due to the following theorem.

Theorem 2.2.16 *([36]) An injective continuous linear operator between two Banach spaces has a continuous inverse if it is surjective.*

Hence, if T is injective then it is not surjective, since T^{-1} is not continuous (see Theorem 2.2.15).

Chapter 3

Approximation by Splines

In this chapter we introduce spline functions in a reproducing kernel Sobolev space $\mathcal{W}(\{A_k\}; X)$ to interpolate/approximate prescribed data. Concerning to this the following fields of interest are discussed in more detail, namely smoothing, best approximation, error estimates, convergence results and regularization via splines.

In order to be able to apply the spline approximation concept to surface wave as well as to body wave tomography problems, the spherical spline approximation concept, introduced by W. Freeden in [21] and [22], is extended for the case where the domain of the function to be approximated is an arbitrary compact set in $\mathbb{R}^n$. Results are mostly based on works of W. Freeden et al. (see [21], [22], [23], [24]) for the unit sphere, and on [4], [15] for the theory of reproducing kernels.
Note that there are alternative approaches to construct interpolating or approximating structures by use of the reproducing kernel Hilbert space theory such as in [9], [63], [64].

3.1 Sobolev Spaces

Throughout this chapter, let $X \subset \mathbb{R}^n$, $n \in \mathbb{N}$ be an arbitrary compact set. We will call X the *initial set* for spline approximation. Let also $W^X := \{W_k^X : X \to \mathbb{R}; W_k^X \in \mathrm{C}_\Theta(X); k \in \mathbb{N}_0\}$ be a complete and orthonormal (both in $\mathrm{L}^2(X)$ sense) system on X, where $\mathrm{C}_\Theta(X)$ is defined in Section 1.1. We will call W^X the *initial basis system* on X.

3.1.1 Definition and basic properties

Definition 3.1.1 *Let $\{A_k\}_{k\in\mathbb{N}_0}$ be an arbitrary real sequence. By $\mathcal{E} := \mathcal{E}(\{A_k\}; X)$ we denote the space of all $F \in \mathrm{L}^2(X)$ satisfying*

$$\left(F, W_k^X\right)_{\mathrm{L}^2(X)} = 0 \quad \text{for all} \quad k \in \mathbb{N} \quad \text{with} \quad A_k = 0$$

and

$$\sum_{\substack{k=0\\A_k\neq 0}}^{\infty} A_k^{-2} \left(F, W_k^X\right)^2_{\mathrm{L}^2(X)} < +\infty$$

From the Cauchy-Schwarz inequality it follows that for all $F, G \in \mathcal{E}$

$$\left| \sum_{\substack{k=0\\A_k\neq 0}}^{\infty} A_k^{-2} \left(F, W_k^X\right)_{\mathrm{L}^2(X)} (G, W_k^X)_{\mathrm{L}^2(X)} \right|$$
$$\leq \left(\sum_{\substack{k=0\\A_k\neq 0}}^{\infty} A_k^{-2} \left(F, W_k^X\right)^2_{\mathrm{L}^2(X)} \right)^{1/2} \left(\sum_{\substack{k=0\\A_k\neq 0}}^{\infty} A_k^{-2} (G, W_k^X)^2_{\mathrm{L}^2(X)} \right)^{1/2} < \infty$$

Therefore, $\mathcal{E}$ is a pre-Hilbert space if it is equipped with the inner product

$$(F,G)_{\mathcal{W}(\{A_k\};X)} := \sum_{\substack{k=0\\A_k\neq 0}}^{\infty} A_k^{-2} \left(F, W_k^X\right)_{\mathrm{L}^2(X)} (G, W_k^X)_{\mathrm{L}^2(X)} \quad F, G \in \mathcal{E}.$$

The associated norm $\|\cdot\|_{\mathcal{W}(\{A_k\};X)}$ is given by $\|F\|_{\mathcal{W}(\{A_k\};X)} := \sqrt{(F,F)_{\mathcal{W}(\{A_k\};X)}}$.

Definition 3.1.2 *The Sobolev space $\mathcal{W}(\{A_k\}; X)$ is defined as the completion of $\mathcal{E}(\{A_k\}; X)$ with respect to the inner product $(\cdot,\cdot)_{\mathcal{W}(\{A_k\};X)}$.*

If no confusion is likely to arise, we will simply write $\mathcal{W}$ instead of $\mathcal{W}(\{A_k\}; X)$. It is clear that $\mathcal{W}$ equipped with the inner product $(\cdot,\cdot)_{\mathcal{W}}$ is a Hilbert space.

Elements of Sobolev spaces may be interpreted as formal orthogonal expansions in terms of functions of W^X. However, Lemma 3.1.5 (see bellow), which is an analog of the Sobolev lemma, says that under certain circumstances the formal orthogonal expansion actually converges uniformly to a function in ordinary sense.

Definition 3.1.3 *A real sequence $\{A_k\}_{k\in\mathbb{N}_0}$ is called summable if the sum*

$$\sum_{k=0}^{\infty} A_k^2 \left\|W_k^X\right\|_\infty^2$$

is convergent.

Assumption 3.1.4 *We always assume that the used sequences $\{A_k\}_{k\in\mathbb{N}_0}$ are summable.*

The summability of the sequence $\{A_k\}_{k\in\mathbb{N}_0}$ automatically guarantees that every element of the Hilbert space $\mathcal{W}(\{A_k\};X)$ can be related to a piecewise continuous function such that $\mathcal{W}(\{A_k\};X) \subset \mathrm{C}_\Theta(X)$.

Lemma 3.1.5 *$\mathcal{W}(\{A_k\};X) \subset \mathrm{C}_\Theta(X)$ and for every $F \in \mathcal{W}(\{A_k\};X)$ the Fourier series*

$$F(x) = \sum_{k=0}^{\infty} \left(F, W_k^X\right)_{\mathrm{L}^2(X)} W_k^X(x) \tag{3.1}$$

is uniformly convergent on X.

Proof: Application of the Cauchy-Schwarz inequality yields for $F \in \mathcal{W}(\{A_k\},X)$ the estimate

$$\begin{aligned}
\left|\sum_{k=K}^{\infty} \left(F, W_k^X\right)_{\mathrm{L}^2(X)} W_k^X(x)\right| &= \left|\sum_{\substack{k=K\\A_k\neq 0}}^{\infty} \left(F, W_k^X\right)_{\mathrm{L}^2(X)} A_k^{-1} A_k W_k^X(x)\right| \\
&\leq \left(\sum_{\substack{k=K\\A_k\neq 0}}^{\infty} \left(F, W_k^X\right)_{\mathrm{L}^2(X)}^2 A_k^{-2}\right)^{1/2} \left(\sum_{\substack{k=K\\A_k\neq 0}}^{\infty} A_k^2 (W_k^X(x))^2\right)^{1/2} \\
&\leq \|F\|_{\mathcal{W}(\{A_k\},X)} \left(\sum_{\substack{k=K\\A_k\neq 0}}^{\infty} A_k^2 \left\|W_k^X\right\|_\infty^2\right)^{1/2} \underset{K\to\infty}{\longrightarrow} 0,
\end{aligned}$$

where the right hand side converges as $K \to \infty$ uniformly with respect to $x \in X$ due to the summability condition. Finally, from $W_k^X \in \mathrm{C}_\Theta(X)$, $k \in \mathbb{N}_0$, and from the uniform convergence of the series in (3.1) follows that $F \in \mathrm{C}_\Theta(X)$. ■

Corollary 3.1.6 *From the proof of Lemma 3.1.5 we see that*

$$\|F\|_\infty \leq \|F\|_{\mathcal{W}} \left(\sum_{k=0}^{\infty} A_k^2 \left\| W_k^X \right\|_\infty^2 \right)^{1/2} \tag{3.2}$$

In the following examples we will see how the summability of the sequence $\{A_k\}_{k\in\mathbb{N}_0}$ can be understood for certain types of X and W^X.

3.1.2 Examples

a) unit sphere
In case of $X = \Omega$, where $\Omega = \{x \in \mathbb{R}^3 \mid |x| = 1\}$ is the unit sphere in $\mathbb{R}^3$, the system $\{Y_{k,j}\}_{k\in\mathbb{N}_0; j=-k,\dots,k}$ of spherical harmonics can be taken as initial basis system on Ω (see Section 1.4). Since the spherical harmonics are continuous on Ω, $\Theta = \emptyset$, i.e. $\mathrm{C}_\Theta(\Omega) = \mathrm{C}(\Omega)$.

Moreover, we have the addition theorem for spherical harmonics (see Theorem 1.4.9)

$$\sum_{j=-k}^{k} Y_{k,j}(\xi) Y_{k,j}(\eta) = \frac{2k+1}{4\pi} P_k(\xi \cdot \eta); \quad \xi, \eta \in \Omega, \tag{3.3}$$

where P_k is the Legendre polynomial of degree k.
In order to use the addition theorem, we take $A_{k,j} = A_k$, $k \in \mathbb{N}_0, j = -k, \dots, k$. Hence, for any $\xi \in \Omega$

$$\sum_{k=0}^{\infty} \sum_{j=-k}^{k} A_k^2 \left(Y_{k,j}(\xi)\right)^2 = \sum_{k=0}^{\infty} A_k^2 \frac{2k+1}{4\pi} P_n(1) = \sum_{k=0}^{\infty} A_k^2 \frac{2k+1}{4\pi},$$

and therefore, the sequence $\{A_k\}_{k\in\mathbb{N}_0}$ is summable if and only if

$$\sum_{k=0}^{\infty} \frac{2k+1}{4\pi} A_k^2 < \infty. \tag{3.4}$$

We also bring several examples of such a summable sequence $\{A_k\}_{k\in\mathbb{N}_0}$.
a1) The Shannon sequence. For a non-negative integer m

$$A_k = \begin{cases} 1, & \text{if} \quad k \in [0, m+1), \\ 0, & \text{if} \quad k \in [m+1, \infty). \end{cases} \tag{3.5}$$

a2) The Abel–Poisson sequence. For a real $h \in (0,1)$

$$A_k = h^{k/2}, \quad k \in \mathbb{N}_0. \tag{3.6}$$

a3) The Gauß–Weierstraß sequence. For a real $h \in (0,1)$

$$A_k = h^{k(k+1)/2}, \quad k \in \mathbb{N}_0. \tag{3.7}$$

b) unit ball
In case of $X = B$, where $B = \{x \in \mathbb{R}^3 \,|\, |x| \leq 1\}$ is the unit ball in $\mathbb{R}^3$, the system $\left\{W^B_{k,n,j}\right\}_{k,n\in\mathbb{N}_0; j=-n,\ldots,n}$ defined by (1.11) can be taken as W^B, an initial basis system on B. In this case the system W^B is complete and orthonormal in $\mathrm{L}^2(B)$ and $W^B \subset \mathrm{C}_\Theta(B)$, where $\Theta = \{0\}$ (see Section 1.5).
Hence, for any $x \in B \setminus \{0\}$

$$\begin{aligned}\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{j=-n}^{n} A^2_{k,n}\left(W^B_{k,n,j}(x)\right)^2 &= \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{j=-n}^{n} A^2_{k,n}\left(g_k(r_x)\right)^2\left(Y_{n,j}(\xi_x)\right)^2 \\ &= \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} A^2_{k,n}\left(\sqrt{2k+3}P^{(0,2)}_k(2r_x-1)\right)^2 \frac{2n+1}{4\pi}.\end{aligned}$$

However, from Theorem 1.3.3, we see that

$$\max_{-1\leq 2r_x-1\leq 1}\left|P^{(0,2)}_k(2r_x-1)\right| = \mathcal{O}(k^2) \quad \text{as} \quad k \to \infty.$$

Therefore, the sequence $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ is summable if

$$\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} A^2_{k,n} k^5 n < \infty. \tag{3.8}$$

In applications it is convenient to write $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ in the form of a product of two sequences, i.e. $A_{k,n} = B_k C_n$, $k,n \in \mathbb{N}_0$. Clearly, in this case the sequence $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ will be summable if we take any of the sequences defined in (3.5). (3.6) and (3.7) as B_k and C_n. For example $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ is summable if

$$A_{k,n} = B_k C_n, \quad \text{with} \quad B_k = h_1^{k(k+1)/2}, C_n = h_2^{n/2}, \quad k,n \in \mathbb{N}_0, \tag{3.9}$$

where $h_1, h_2 \in (0,1)$ are some reals.

3.2 Reproducing Kernels

Essential for the construction of the splines here is the existence of a reproducing kernel. This is also guaranteed by the summability of the sequence $\{A_k\}_{k\in\mathbb{N}_0}$ (see also [4], [15]).

3.2.1 Definition and basic properties

Definition 3.2.1 *A function $K_{\mathcal{W}} : X \times X \to \mathbb{R}$ is called a reproducing kernel of $\mathcal{W}$ if*
(i) $K_{\mathcal{W}}(x, \cdot) \in \mathcal{W}$ for all $x \in X$.
(ii) $(F(\cdot), K_{\mathcal{W}}(x, \cdot))_{\mathcal{W}} = F(x)$ for all $F \in \mathcal{W}$ and for all $x \in X$ (reproducing property).

Theorem 3.2.2 *$\mathcal{W}$ has a unique reproducing kernel $K_{\mathcal{W}} : X \times X \to \mathbb{R}$ given by*

$$K_{\mathcal{W}}(x, y) = \sum_{k=0}^{\infty} A_k^2 W_k^X(x) W_k^X(y) \tag{3.10}$$

Proof: A necessary and sufficient condition that $\mathcal{W}$ has a reproducing kernel is that, for each fixed $x \in X$, the evaluation functional $\mathcal{L}_x : \mathcal{W} \to \mathbb{R}$ given by $\mathcal{L}_x F = F(x), x \in X$ is bounded for all $F \in \mathcal{W}$ (see [4]). Suppose first that $K_{\mathcal{W}}$ is a reproducing kernel, then

$$\begin{aligned} |\mathcal{L}_x F| = |F(x)| &= |(F, K_{\mathcal{W}}(\cdot, x))_{\mathcal{W}}| \leq \|F\|_{\mathcal{W}} \left(K_{\mathcal{W}}(\cdot, x), K_{\mathcal{W}}(\cdot, x)\right)^{1/2} \\ &= \|F\|_{\mathcal{W}} (K_{\mathcal{W}}(x, x))^{1/2} < \infty. \end{aligned}$$

And conversely if $\mathcal{L}_x F$ is bounded (and therefore, continuous), then by Theorem 1.1.11 there exists a function $G_x \in \mathcal{W}$ such that $\mathcal{L}_x F = F(x) = (F, G_x)_{\mathcal{W}}$. Thus, we can take $K_{\mathcal{W}}(x, \cdot) = G_x$, which clearly fulfils properties (i) and (ii) of Definition 3.2.1, and therefore, is a reproducing kernel.
In $\mathcal{W}$ the boundedness of the evaluation functional is guaranteed by Corollary 3.1.6, since for any $F \in \mathcal{W}$,

$$|F(x)| \leq \|F\|_\infty \leq \|F\|_{\mathcal{W}} \left(\sum_{k=0}^{\infty} A_k^2 \left\| W_k^X \right\|_\infty^2 \right)^{1/2}, \quad x \in X.$$

If there exists another reproducing kernel $K'_{\mathcal{W}}$, then for each fixed $x \in X$

$$\begin{aligned}\|K_{\mathcal{W}}(x,\cdot) - K'_{\mathcal{W}}(x,\cdot)\|^2 &= \left((K_{\mathcal{W}} - K'_{\mathcal{W}})(x,\cdot), (K_{\mathcal{W}} - K'_{\mathcal{W}})(x,\cdot)\right) \\ &= \left((K_{\mathcal{W}} - K'_{\mathcal{W}})(x,\cdot), K_{\mathcal{W}}(x,\cdot)\right) \\ &\quad - \left((K_{\mathcal{W}} - K'_{\mathcal{W}})(x,\cdot), K'_{\mathcal{W}}(x,\cdot)\right) = 0\end{aligned}$$

because of the reproducing property of $K_{\mathcal{W}}$ and $K'_{\mathcal{W}}$.
Now, it is easy to check that the reproducing kernel $K_{\mathcal{W}}$ is given by (3.10). Because of the reproducing property, for each $n \in \mathbb{N}_0$ with $A_n \neq 0$ and $x \in X$

$$\begin{aligned}W_n^X(x) &= (K_{\mathcal{W}}(x,\cdot), W_n^X(\cdot))_{\mathcal{W}} = \sum_{\substack{k=0 \\ A_k \neq 0}}^{\infty} A_k^{-2} (K_{\mathcal{W}}(x,\cdot), W_k^X(\cdot))_{\mathrm{L}^2(X)} (W_k^X, W_n^X)_{\mathrm{L}^2(X)} \\ &= A_n^{-2} (K_{\mathcal{W}}(x,\cdot), W_n^X(\cdot))_{\mathrm{L}^2(X)}.\end{aligned}$$

Therefore for each $n \in \mathbb{N}_0$ (see also Definition 3.1.1 and property *(i)* of $K_{\mathcal{W}}$) and $x \in X$

$$(K_{\mathcal{W}}(x,\cdot))^\wedge(n) = (K_{\mathcal{W}}(x,\cdot), W_n^X(\cdot))_{\mathrm{L}^2(X)} = A_n^2 W_n^X(x).$$

Hence, $K_{\mathcal{W}}$ is given by (3.10). ■

Corollary 3.2.3 *Clearly from (3.10) follows that* $K_{\mathcal{W}}(x,y) = K_{\mathcal{W}}(y,x)$ *for all* $x, y \in X$

Theorem 3.2.4 *Let* $\mathcal{F}$ *be a bounded linear functional on* $\mathcal{W}$*. Then the function* $y \mapsto \mathcal{F}_x K_{\mathcal{W}}(x,y)$ *is in* $\mathcal{W}$ *and*

$$\mathcal{F}(F) = (F, \mathcal{F}_x K_{\mathcal{W}}(x,\cdot))_{\mathcal{W}}$$

for all $F \in \mathcal{W}$*.*

(Here, $\mathcal{F}_x K_{\mathcal{W}}(x,\cdot)$ means that $\mathcal{F}$ is applied to the function $x \mapsto K_{\mathcal{W}}(x,y)$ where y is arbitrary but fixed.)
Proof: Let $R_{\mathcal{F}}$ be the representer of $\mathcal{F}_x$, i.e. $\mathcal{F}_x F = (F, R_{\mathcal{F}})_{\mathcal{W}}$ for all $F \in \mathcal{W}$. Then,

$$\mathcal{F}_x K_{\mathcal{W}}(x,y) = (K_{\mathcal{W}}(\cdot,y), R_{\mathcal{F}})_{\mathcal{W}} = R_{\mathcal{F}}(y).$$

Hence, for all $F \in \mathcal{W}$

$$\mathcal{F}_x F = (F, R_{\mathcal{F}})_{\mathcal{W}} = (F, \mathcal{F}_x K_{\mathcal{W}}(x,\cdot))_{\mathcal{W}}. \quad ■$$

This theorem implies that we can define an inner product in the dual space $\mathcal{W}^*$ of $\mathcal{W}$ as

$$(\mathcal{F},\mathcal{G})_{\mathcal{W}^*} := (R_{\mathcal{F}}, R_{\mathcal{G}})_{\mathcal{W}} = \mathcal{F}\mathcal{G}K_{\mathcal{W}}(\cdot,\cdot),$$

where $R_{\mathcal{F}}$ and $R_{\mathcal{G}}$ are representers corresponding to $\mathcal{F}$ and $\mathcal{G}$. $\mathcal{W}^*$ is a Hilbert space with respect to $(\cdot,\cdot)_{\mathcal{W}^*}$. The spaces $\mathcal{W}$ and $\mathcal{W}^*$ are known to be isomorphic and isometric (see e.g. [15]).

Reproducing kernel representations may be used to act as a basis system in reproducing Sobolev spaces.

Theorem 3.2.5 *Assume that $D \supset \Theta$ is a countable and dense set of points in X. Then*

$$\overline{\operatorname{span}_{x\in D}\{K_{\mathcal{W}}(x,\cdot)\}}^{\|\cdot\|_{\mathcal{W}}} = \mathcal{W}.$$

Proof: According to Theorem 1.1.3 it is enough to show that the properties $F \in \mathcal{W}$ and $(F, K_{\mathcal{W}}(x,\cdot))_{\mathcal{W}} = 0$ for all $x \in D$ imply that $F = 0$, i.e. the system $\{K_{\mathcal{W}}(x,\cdot)\}_{x\in D}$ is complete and therefore closed in X. By definition of $K_{\mathcal{W}}$, the condition $(K_{\mathcal{W}}(x,\cdot), F)_{\mathcal{W}} = 0$ is equivalent to $F(x) = 0$ for all $x \in D$. However according to our construction, F is continuous on $X \setminus \Theta$ (see Lemma 3.1.5). Hence, if $F(x) \neq 0$ for some $x \in X \setminus \Theta$ then F would be different from zero for some neighborhood of x. But this is a contradiction to the fact that D is dense in X. ■

The following theorem shows that in $\mathcal{W}(\{A_k\}; X)$ complete sets of functions can be generated from complete sets of functionals.

Theorem 3.2.6 *The sequence $\{\mathcal{F}_n\}_{n\in\mathbb{N}}$ of bounded linear functionals is complete in $\mathcal{W}^*$, i.e. $f \in \mathcal{W}, \mathcal{F}_n(f) = 0, n = 1,2,...,$ implies $f \equiv 0$, if and only if the functions*

$$g_n(y) := (\mathcal{F}_n)_x K_{\mathcal{W}}(x,y), \quad y \in X, n = 1,2,...$$

form a complete set for $\mathcal{W}$.

Proof: By Theorem 3.2.4, $\mathcal{F}_n(f) = (f(\cdot), g_n(\cdot))$. Hence, we see that the completeness of the sequence of functions $\{g_n\}$ in $\mathcal{W}$ is equivalent to the completeness of the sequence of functionals $\{\mathcal{F}_n\}_{n\in\mathbb{N}}$ in $\mathcal{W}^*$. ■

Since in Hilbert spaces closure and completeness are equivalent concepts, we get the following result.

Corollary 3.2.7 *The system of bounded linear functionals $\{\mathcal{F}_n\}_{n\in\mathbb{N}}$ is complete in $\mathcal{W}^*$ if and only if*

$$\overline{\text{span}_{n\in\mathbb{N}}\{(\mathcal{F}_n)_x K_{\mathcal{W}}(x,y)\}}^{\|\cdot\|_{\mathcal{W}}} = \mathcal{W}. \tag{3.11}$$

3.2.2 Examples

Here we bring some examples of reproducing kernels and demonstrate their localization character in case of the unit sphere and the unit ball.
a) unit sphere
As we have already seen in case of $X = \Omega$ the system $\{Y_{k,j}\}_{k\in\mathbb{N}_0;j=-k,\ldots,k}$ of spherical harmonics can be taken as an initial basis system on Ω. Hence, using (3.3) we obtain that

$$K_{\mathcal{W}}(\xi,\eta) = \sum_{k=0}^{\infty} A_k^2 \frac{2k+1}{4\pi} P_k(\xi\cdot\eta); \quad \xi,\eta\in\Omega, \tag{3.12}$$

where P_k is the Legendre polynomial of degree k.
In Figure 3.1, Figure 3.2 and Figure 3.3 the reproducing kernel $K_{\mathcal{W}}(\xi,\eta)$ with the corresponding sequences (symbols) defined in Section 3.1.2 is plotted. $K_{\mathcal{W}}(\xi,\eta)$ is plotted in dependence of $\xi\cdot\eta = \cos(\vartheta)$, $\vartheta\in[-\pi,\pi]$.
It should be mentioned that for the case of the Abel–Poisson sequence we obtain a closed representation of the reproducing kernel $K_{\mathcal{W}}$. According to [24], p. 45 we find, that for all $t\in[-1,1]$, and $h\in(-1,1)$

$$\sum_{n=0}^{\infty}(2n+1)h^n P_n(t) = \frac{1-h^2}{(1+h^2-2ht)^{(3/2)}}.$$

Hence, the Abel–Poisson kernel has the well–known form

$$K_{\mathcal{W}}(\xi,\eta) = \frac{1}{4\pi}\frac{1-h^2}{(1+h^2-2h(\xi\cdot\eta))^{(3/2)}} \tag{3.13}$$

where $h = A_1^2$.
b) unit ball
In case of $X = B$, the system $\left\{W_{k,n,j}^B\right\}_{k,n\in\mathbb{N}_0;j=-n,\ldots,n}$ defined in Section 1.5 can

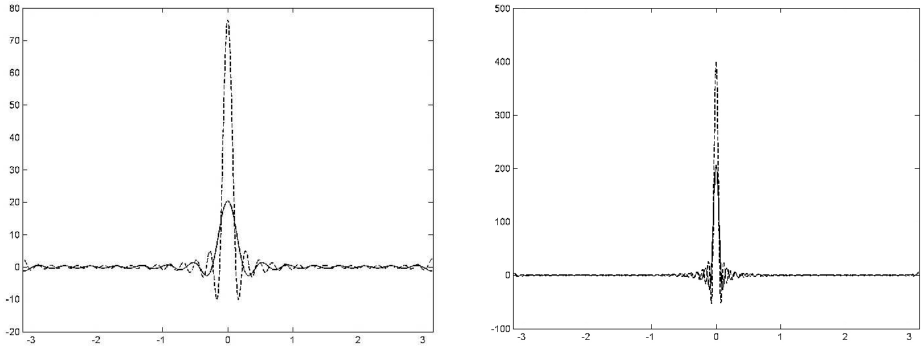


Figure 3.1: Shannon kernel for $m = 15$ (solid line, left), $m = 30$ (dashed line, left), $m = 50$ (solid line, right), and $m = 70$ (dashed line, right)

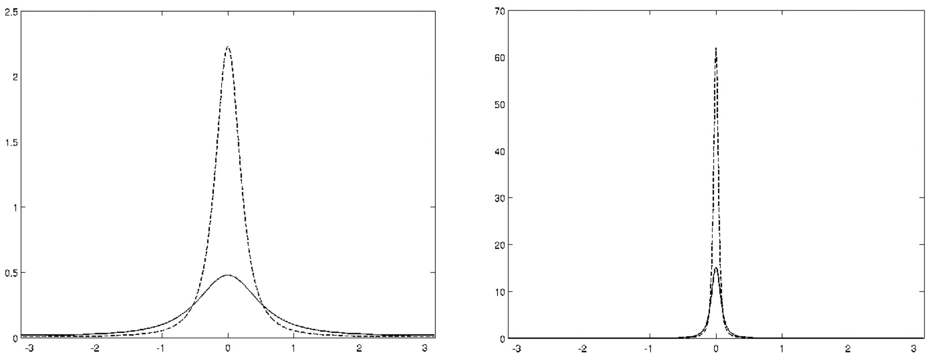


Figure 3.2: Abel–Poisson kernel for $h = 0.5$ (solid line, left), $h = 0.75$ (dashed line, left), $h = 0.9$ (solid line, right), and $h = 0.95$ (dashed line, right)

be taken as an initial basis system on B (see also Section 3.1.2). Hence, again using (3.3) we obtain that for all $x, y \in B \setminus \{0\}$

$$K_{\mathcal{W}}(x,y) = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty} A_{k,n}^2 (2k+3) P_k^{(0,2)}(2|x|-1) P_k^{(0,2)}(2|y|-1)\, \frac{2n+1}{4\pi} P_n\left(\frac{x}{|x|}\cdot\frac{y}{|y|}\right).$$

where $P_k^{(0,2)}$ is the corresponding Jacobi polynomial of degree k, and P_n is the Legendre polynomial of degree n (for similar kernels see [76]).

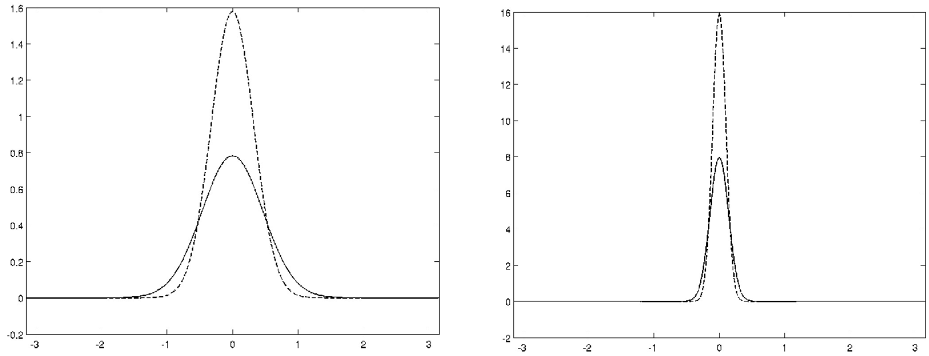


Figure 3.3: Gauß–Weierstraß kernel for $h = 0.9$ (solid line, left), $h = 0.95$ (dashed line, left), $h = 0.99$ (solid line, right), and $h = 0.995$ (dashed line, right)

In Figure 3.4 and Figure 3.5 the localization character of $K_{\mathcal{W}}(x,y)$, with $A_{k,n} = B_k C_n$, $k,n \in \mathbb{N}_0$ for some B_k and C_n is demonstrated. In both figures we have $x = (0, x_2, x_3)$, $y = (0, y_2, y_3)$, and the reproducing kernel $K_{\mathcal{W}}(x,y)$ is plotted in dependence of y_2 and y_3, with $y_2^2 + y_3^2 \leq 1$ and the value of $K_{\mathcal{W}}(0,0)$ is ignored.

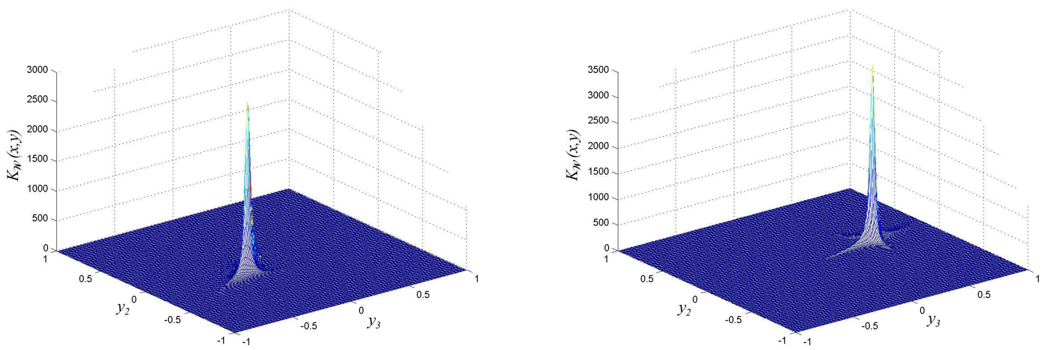


Figure 3.4: The reproducing kernel $K_{\mathcal{W}}(x,y)$ with $B_k = e^{-0.1k}$, $C_n = e^{-0.1n}$, $x_2 = -0.1$, $x_3 = -0.2$ (left), $B_k = e^{-0.05k}$, $C_n = e^{-0.05n}$, $x_2 = 0.1$, $x_3 = 0.5$ (right)

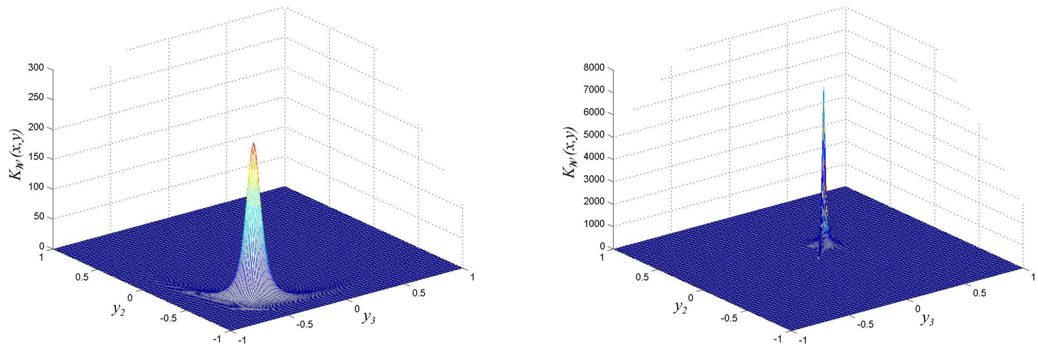


Figure 3.5: The reproducing kernel $K_{\mathcal{W}}(x, y)$ with $B_k = e^{-0.05k(k+1)}$, $C_n = e^{-0.1n}$, $x_2 = -0.6$, $x_3 = -0.5$ (left), $B_k = e^{-0.05k(k+1)}$, $C_n = e^{-0.05n}$, $x_2 = 0.2$, $x_3 = 0.2$ (right)

3.3 Spline Interpolation

Let $\mathcal{F}^N := \{\mathcal{F}_n\}_{n=1,...,N}$ be a linearly independent system of linear continuous functionals on $\mathcal{W}(\{A_k\}; X)$.

Definition 3.3.1 *A function $S \in \mathcal{W}$ of the form*

$$S(x) = \sum_{k=1}^{N} a_k \mathcal{F}_k K_{\mathcal{W}}(\cdot, x), \quad x \in X,$$

$a = (a_1, ..., a_N)^{\mathrm{T}} \in \mathbb{R}^N$ is called spline in $\mathcal{W}(\{A_k\}; X)$ relative to $\mathcal{F}^N$. The scalars $a_1, ..., a_N$ are called the coefficients of the spline $S(x)$. Such splines are collected in the space $\mathrm{Spline}(\{A_k\}; \mathcal{F}^N)$ *or simply* $\mathrm{Spl}_{\mathcal{F}^N}$.

A spline interpolation problem can be formulated as follows.

Problem 3.3.2 *For a given linearly independent system $\mathcal{F}^N = \{\mathcal{F}_1, ..., \mathcal{F}_N\}$ of linear continuous functionals and a vector $y = (y_1, ..., y_N)^{\mathrm{T}} \in \mathbb{R}^N$ determine $S \in \mathrm{Spline}(\{A_k\}; \mathcal{F}^N)$ such that*

$$\mathcal{F}_i S = y_i \quad \textit{for all} \quad i = 1, ..., N$$

Or, equivalently, determine $a \in \mathbb{R}^N$ such that

$$\sum_{j=1}^{N} a_j \mathcal{F}_i \mathcal{F}_j K_{\mathcal{W}}(\cdot,\cdot) = y_i \quad \text{for all} \quad i = 1, ..., N \tag{3.14}$$

This yields a linear equation system with the matrix

$$\mathbf{k}_N = (\mathcal{F}_i \mathcal{F}_j K_{\mathcal{W}}(\cdot,\cdot))_{i,j=1,...,N} \tag{3.15}$$

which is positive definite according to the following theorem.

Theorem 3.3.3 *Let $\mathcal{F}^N := \{\mathcal{F}_1, ..., \mathcal{F}_N\}$ be a system of bounded linear functionals on $\mathcal{W}$. This system is linearly independent if and only if the matrix $\mathbf{k}_N$ is positive definite.*

Proof: Due to Theorem 3.2.4 we see that $\mathbf{k}_N$ is a Gram matrix since

$$(\mathcal{F}_i)_x (\mathcal{F}_j)_y K_{\mathcal{W}}(x,y) = ((\mathcal{F}_j)_y K_{\mathcal{W}}(\cdot,y), (\mathcal{F}_i)_x K_{\mathcal{W}}(x,\cdot))_{\mathcal{W}}. \tag{3.16}$$

Moreover, according to this theorem the linear independence of the system $\{(\mathcal{F}_i)_x K_{\mathcal{W}}(x,\cdot))\}_{i=1,...,N}$, meaning that

$$G(y) := \sum_{i=1}^{N} a_i (\mathcal{F}_i)_x K_{\mathcal{W}}(x,y) = 0 \quad \text{for all} \quad y \in X \Leftrightarrow a_i = 0 \quad \text{for all} \quad i = 1, ..., N,$$

is equivalent to the statement that

$$(F,G)_{\mathcal{W}} = \sum_{i=1}^{N} a_i \mathcal{F}_i F = 0 \quad \text{for all} \quad F \in \mathcal{W} \Leftrightarrow a_i = 0 \quad \text{for all} \quad i = 1, ..., N$$

which is true if and only if $\mathcal{F}^N$ is linearly independent. Since a Gram matrix is positive definite if and only if the corresponding system of vectors is linearly independent, the statement of the theorem is valid. ■

Therefore, we obtain the following theorem.

Theorem 3.3.4 *The formulated (spline interpolation) Problem 3.3.2 is always uniquely solvable.*

Remark 3.3.5 *Theorem 3.3.3 implies that the system* $\{\mathcal{F}_1 K_{\mathcal{W}}(x,\cdot), ..., \mathcal{F}_N K_{\mathcal{W}}(x,\cdot)\}$ *is linearly independent, and therefore,* $\text{Spline}(\{A_k\};\mathcal{F}^N)$ *is an* N*-dimensional subspace of* $\mathcal{W}$*.*

Next, we will prove the $\mathcal{W}$ - *spline formula* and the Shannon Sampling Theorem.

Lemma 3.3.6 ***($\mathcal{W}$-spline formula)*** *Let* $S \in \text{Spl}_{\mathcal{F}^N}$ *with*

$$S(x) = \sum_{l=1}^{N} a_l \mathcal{F}_l K_{\mathcal{W}}(.,x), \quad x \in X.$$

Then, for arbitrary $F \in \mathcal{W}$

$$(F,S)_{\mathcal{W}} = \sum_{l=1}^{N} a_l \mathcal{F}_l F. \tag{3.17}$$

Proof: From Theorem 3.2.4 it follows directly that

$$(F,S)_{\mathcal{W}} = \sum_{l=1}^{N} a_l \left(F, (\mathcal{F}_l)_y K_{\mathcal{W}}(y,.)\right)_{\mathcal{W}} = \sum_{l=1}^{N} a_l \mathcal{F}_l F.$$

■

Theorem 3.3.7 ***(Shannon Sampling Theorem)*** *Any spline function* $S \in \text{Spline}(\{A_n\};\mathcal{F}^N)$ *is representable by its "samples"* $\mathcal{F}_i S$ *as*

$$S(x) = \sum_{k=1}^{N} (\mathcal{F}_k S) L_k(x), \quad x \in X, \tag{3.18}$$

where

$$L_k(x) = \sum_{j=1}^{N} a_j^{(k)} \mathcal{F}_j K_{\mathcal{W}}(x,\cdot), \quad x \in X, \tag{3.19}$$

with $a_j^{(k)}$ *given as solution of the linear equation systems*

$$\sum_{j=1}^{N} a_j^{(k)} \mathcal{F}_i \mathcal{F}_j K_{\mathcal{W}}(\cdot,\cdot) = \delta_{i,k} \quad \text{for all} \quad i,k = 1,...,N. \tag{3.20}$$

Proof: The set of equation systems in (3.20) guarantees that

$$\mathcal{F}_i L_k = \delta_{i,k},$$

such that

$$\mathcal{F}_i \left(\sum_{k=1}^{N} (\mathcal{F}_k S) L_k \right) = \sum_{k=1}^{N} \mathcal{F}_k S \mathcal{F}_i L_k = \mathcal{F}_i S$$

for all $i = 1, ..., N$. Thus, the uniqueness of the interpolating spline implies (3.18). ■

Next, we derive the following minimum properties.

Theorem 3.3.8 ***(1st Minimum Property)*** *Let $y \in \mathbb{R}^N$ be given and $\mathcal{F}^N := \{\mathcal{F}_1, ..., \mathcal{F}_N\} \subset \mathcal{W}^*$ be linearly independent. If $S^* = \sum_{i=1}^{N} a_i (\mathcal{F}_i)_x K_{\mathcal{W}}(\cdot, x)$ is the unique spline satisfying $\mathcal{F}_i S^* = y_i$ for all $i = 1, ..., N$ then S^* is the unique minimizer of*

$$\|S^*\|_{\mathcal{W}} = \min\{\|F\|_{\mathcal{W}} | F \in \mathcal{W}, \mathcal{F}_i F = y_i \ \ \forall i = 1, ..., N\}.$$

Proof: For any $F \in \mathcal{W}$ we have

$$\begin{aligned} \|S^* - F\|_{\mathcal{W}}^2 &= (S^* - F, S^* - F)_{\mathcal{W}} \\ &= (S^*, S^*)_{\mathcal{W}} - 2(S^*, F)_{\mathcal{W}} + (F, F)_{\mathcal{W}} \\ &= (S^*, S^* - 2F)_{\mathcal{W}} + \|F\|_{\mathcal{W}}^2. \end{aligned}$$

Now, if $\mathcal{F}_i F = y_i \quad \forall i = 1, ..., N$, then using Lemma 3.3.6 we get

$$\begin{aligned} (S^*, S^* - 2F)_{\mathcal{W}} &= \sum_{i=1}^{N} a_i \mathcal{F}_i (S^* - 2F) = \sum_{i=1}^{N} a_i (-y_i) \\ &= -\sum_{i=1}^{N} a_i \mathcal{F}_i S^* = -(S^*, S^*)_{\mathcal{W}}. \end{aligned}$$

Altogether

$$\begin{aligned} \|F\|_{\mathcal{W}}^2 &= -(S^*, S^* - 2F)_{\mathcal{W}} + \|S^* - F\|_{\mathcal{W}}^2 \\ &= \|S^*\|_{\mathcal{W}}^2 + \|S^* - F\|_{\mathcal{W}}^2. \end{aligned}$$

Therefore, for any $F \in \mathcal{W}$, with $\mathcal{F}_i F = y_i \ \forall i = 1, ..., N$,

$$\|F\|_{\mathcal{W}} \geq \|S^*\|_{\mathcal{W}} \text{ and } \|F\|_{\mathcal{W}} = \|S^*\|_{\mathcal{W}} \text{ if and only if } F = S^*.$$

■

The obtained result shows that the formulated spline interpolation problem 3.3.2 is equivalent to the *minimum norm interpolation* problem:

Problem 3.3.9 *Let* $\mathcal{F}^N = \{\mathcal{F}_1, ..., \mathcal{F}_N\} \subset \mathcal{W}^*$ *be a linearly independent system and* $y = (y_1, ..., y_N)^{\mathrm{T}} \in \mathbb{R}^N$*. Let also* $F \in \mathcal{W}$*, with* $\mathcal{F}_i F = y_i$ *for* $i = 1, ..., N$*. Determine* $S^F_{\mathcal{F}^N} \in \mathcal{W}$ *such that*

$$\left\|S^F_{\mathcal{F}^N}\right\|_{\mathcal{W}} = \inf_{G \in \mathcal{I}_N(y)} \|G\|_{\mathcal{W}}, \tag{3.21}$$

where

$$\mathcal{I}_N(y) = \{G \in \mathcal{W} | \mathcal{F}_i G = \mathcal{F}_i F = y_i, i = 1, ..., N\} \tag{3.22}$$

In general, the name 'spline' refers to a function with a property of minimizing a certain measure among all interpolants. In the classical Euclidean case the natural cubic spline s minimizes the linearized deformation energy $\|s''\|_{\mathrm{L}^2}$.

Theorem 3.3.10 ***(2nd Minimum Property)*** *Let* $F \in \mathcal{W}$ *be given and* $\mathcal{F}^N := \{\mathcal{F}_1, ..., \mathcal{F}_N\} \subset \mathcal{W}^*$ *be linearly independent. If* $S^* \in \mathrm{Spline}(\{A_k\}; \mathcal{F}^N)$ *is the unique spline satisfying* $\mathcal{F}_i S^* = \mathcal{F}_i F$ *for all* $i = 1, ..., N$*, then* S^* *is the unique minimizer of*

$$\|F - S^*\|_{\mathcal{W}} = \min\{\|F - S\|_{\mathcal{W}} | S \in \mathrm{Spline}(\{A_k\}; \mathcal{F}^N)\}.$$

Proof: For any $S \in \mathrm{Spline}(\{A_k\}; \mathcal{F}^N)$ we have

$$\begin{aligned} \|S - F\|^2_{\mathcal{W}} &= \|S - S^* + S^* - F\|^2_{\mathcal{W}} \\ &= (S - S^* + S^* - F, S - S^* + S^* - F)_{\mathcal{W}} \\ &= \|S - S^*\|^2_{\mathcal{W}} + 2(S - S^*, S^* - F)_{\mathcal{W}} + \|S^* - F\|^2_{\mathcal{W}}. \end{aligned}$$

For the splines we will use the notations

$$S = \sum_{i=1}^{N} a_i^S \mathcal{F}_i K_{\mathcal{W}}(x, \cdot)$$

and

$$S^* = \sum_{i=1}^{N} a_i^{S^*} \mathcal{F}_i K_{\mathcal{W}}(x, \cdot).$$

Applying Lemma 3.3.6 we see that

$$\begin{aligned}(S - S^*, S^* - F)_{\mathcal{W}} &= (S, S^* - F)_{\mathcal{W}} - (S^*, S^* - F)_{\mathcal{W}} \\ &= \sum_{i=1}^{N} a_i^S \mathfrak{F}_i(S^* - F) - \sum_{i=1}^{N} a_i^{S^*} \mathfrak{F}_i(S^* - F) \\ &= 0.\end{aligned}$$

Hence, we have

$$\|F - S\|_{\mathcal{W}}^2 = \|S - S^*\|_{\mathcal{W}}^2 + \|F - S^*\|_{\mathcal{W}}^2.$$

Therefore, for any $S \in \text{Spline}(\{A_k\}; \mathfrak{F}^N)$,

$$\|F - S\|_{\mathcal{W}} \geq \|F - S^*\|_{\mathcal{W}}$$

and

$$\|F - S\|_{\mathcal{W}} = \|F - S^*\|_{\mathcal{W}} \quad \text{if and only if} \quad S = S^*. \quad \blacksquare$$

Thus, if F represents an unknown function in $\mathcal{W}$, the interpolating spline S^* represents the best possible approximation to F among all splines, measured with respect to the metric induced by the Sobolev norm $\|\cdot\|_{\mathcal{W}}$. Moreover, among all functions in $\mathcal{W}$ that fit to the known data y_i the spline S^* is the 'smoothest' (in $\|\cdot\|_{\mathcal{W}}$-sense).

Summarizing our results we obtain the following theorem.

Theorem 3.3.11 *Problem 3.3.9 is well-posed, in the sense that its solution exists, is unique, and depends continuously on the data $y_1, ..., y_N$. The uniquely determined solution is given by*

$$S_{\mathfrak{F}^N}^F(x) = \sum_{i=1}^{N} a_i \mathfrak{F}_i K_{\mathcal{W}}(\cdot, x) \quad x \in X,$$

where the coefficients $a_1, ..., a_N$ satisfy the linear equation system (3.14).

3.4 Smoothing

In practice, the observations are affected by errors and irregularities and we have to deal with 'noisy data'. In this case strict interpolation is inappropriate and a *combined interpolation-smoothing method* should be used (for more see e.g. [22], [26] [27], [79]). More precisely, the quantities $y_1, ..., y_N$, corresponding to a set of linear bounded functionals $\mathcal{F}_1, ..., \mathcal{F}_N$, are affected with uncertainties and it is more reasonable to look for a 'smoothing' function rather than for an interpolating function, i.e. we have to determine a function $F \in \mathcal{W}$ such that

$$\mathcal{F}_i F \approx y_i \quad i = 1, ..., N, \tag{3.23}$$

and which minimizes some quantity $\mu(F)$.
As $\mu(F)$ we will take

$$\mu(F) = \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - y_i}{\beta_i} \right]^2 + \rho(F, F)_{\mathcal{W}}. \tag{3.24}$$

In this case the method is called Least Squares Adjustment.
Here $\beta_1^2, ..., \beta_N^2$ and ρ are some positive constants, which should be adapted to the data situation (see e.g. [19], [21], [79]).

Theorem 3.4.1 ***(spline smoothing)*** *Given $y = (y_1, ..., y_N)^{\mathrm{T}} \in \mathbb{R}^N$ corresponding to a set of N linearly independent bounded linear functionals $\mathcal{F}^N = \{\mathcal{F}_1, ..., \mathcal{F}_N\}$ on $\mathcal{W}$. Then there exists a unique element $S \in \mathrm{Spl}_{\mathcal{F}^N}$ satisfying*

$$\mu(S) \leq \mu(F) \quad \textit{whenever} \quad F \in \mathcal{W}. \tag{3.25}$$

Equality holds if and only if $S = F$. Moreover, the coefficients $a = (a_1, ..., a_N)^{\mathrm{T}} \in \mathbb{R}^N$ of the spline $S = \sum_{i=1}^{N} a_i (\mathcal{F}_i)_x K_{\mathcal{W}}(\cdot, x)$ are uniquely determined by the linear equation system

$$\mathcal{F}_i S + \rho \beta_i^2 a_i = y_i \quad i = 1, ..., N. \tag{3.26}$$

Proof: First of all, if we set

$$D = \begin{pmatrix} \beta_1^2 & & 0 \\ & \ddots & \\ 0 & & \beta_N^2 \end{pmatrix},$$

then (3.26) can be written in vectorial form as

$$(\mathbf{k}_N + \rho D) a = y, \tag{3.27}$$

where $\mathbf{k}_N$ is defined in (3.15). Now, since $\mathbf{k}_N$ and D are positive definite, hence, $\mathbf{k}_N + \rho D$ is positive definite, too, therefore (3.27) is uniquely solvable.
Next, for any $F \in \mathcal{W}(\{A_k\}; X)$ and any $S \in \mathrm{Spl}_{\mathcal{F}^N}$ satisfying (3.26), it is easy to see that

$$\sum_{i=1}^{N} \mathcal{F}_i F \left[\frac{y_i - \mathcal{F}_i S}{\beta_i^2}\right] = \rho \sum_{i=1}^{N} a_i \mathcal{F}_i F \tag{3.28}$$

Hence, according to Lemma 3.3.6

$$\sum_{i=1}^{N} \mathcal{F}_i F \left[\frac{y_i - \mathcal{F}_i S}{\beta_i^2}\right] = \rho(S, F)_{\mathcal{W}}. \tag{3.29}$$

Now, from the definition of $\mu(F)$ and from (3.29) we obtain that

$$\begin{aligned}
\mu(F) - \mu(S) &= \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - y_i}{\beta_i}\right]^2 + \rho(F,F)_{\mathcal{W}} - \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i S - y_i}{\beta_i}\right]^2 - \rho(S,S)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \frac{(\mathcal{F}_i F)^2 - 2y_i \mathcal{F}_i F + y_i^2 - (\mathcal{F}_i S)^2 + 2y_i \mathcal{F}_i S - y_i^2}{\beta_i^2} + \rho(F,F)_{\mathcal{W}} - \rho(S,S)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \frac{(\mathcal{F}_i F)^2 - 2y_i \mathcal{F}_i F + y_i \mathcal{F}_i S}{\beta_i^2} + \sum_{i=1}^{N} \mathcal{F}_i S \left[\frac{y_i - \mathcal{F}_i S}{\beta_i^2}\right] + \rho(F,F)_{\mathcal{W}} - \rho(S,S)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \frac{(\mathcal{F}_i F)^2 - 2y_i \mathcal{F}_i F + y_i \mathcal{F}_i S}{\beta_i^2} + \rho(F,F)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \frac{(\mathcal{F}_i F)^2 - 2\mathcal{F}_i F \mathcal{F}_i S + (\mathcal{F}_i S)^2 + 2\mathcal{F}_i F \mathcal{F}_i S - (\mathcal{F}_i S)^2 - 2y_i \mathcal{F}_i F + y_i \mathcal{F}_i S}{\beta_i^2} + \rho(F,F)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - \mathcal{F}_i S}{\beta_i}\right]^2 - 2\sum_{i=1}^{N} \mathcal{F}_i F \left[\frac{y_i - \mathcal{F}_i S}{\beta_i^2}\right] + \sum_{i=1}^{N} \mathcal{F}_i S \left[\frac{y_i - \mathcal{F}_i S}{\beta_i^2}\right] + \rho(F,F)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - \mathcal{F}_i S}{\beta_i}\right]^2 + \rho(F,F)_{\mathcal{W}} - 2\rho(S,F)_{\mathcal{W}} + \rho(S,S)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - \mathcal{F}_i S}{\beta_i}\right]^2 + \rho(F-S, F-S)_{\mathcal{W}} \\
&= \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - \mathcal{F}_i S}{\beta_i}\right]^2 + \rho\|F-S\|_{\mathcal{W}}^2.
\end{aligned}$$

Hence,

$$\mu(F) = \mu(S) + \sum_{i=1}^{N} \left[\frac{\mathcal{F}_i F - \mathcal{F}_i S}{\beta_i} \right]^2 + \rho \|F - S\|_{\mathcal{W}}^2.$$

This proves the theorem. ■

Clearly, the condition of $\mathbf{k}_N + \rho D$ is better than the condition of $\mathbf{k}_N$, and the larger ρ the better gets the condition of $\mathbf{k}_N + \rho D$. Since the system of linear equations obtained by the spline interpolation problem can be very ill-conditioned, this is one way to stabilize the matrix and make such systems numerically solvable.
The constant ρ is some kind of quantifier between smoothing and closeness to the measurements. A small value of ρ emphasizes precision of the observed data and less smoothness for F, while a large value does the opposite. The problem of choosing the "optimal" smoothing parameter is widely discussed in the literature. There exist numerous strategies for such an "optimal" parameter choice (see e.g. the L-curve criterion [5], [19], [32], [33], the generalized cross-validation [79] and the quasi-optimality criterion [43], [32]), however there is no general method that works in every situation. The L-curve is a plot of the norm of the regularized solution (y-axis) versus the norm of the corresponding residual (x-axis). In our case the L-curve can be constructed by plotting $\|S^\rho\|_{\mathcal{W}}$ versus $\|\mathbf{k}_N a^\rho - y\|$, where for each ρ, a^ρ is the solution of Equation (3.27) and S^ρ is the corresponding spline, i.e. the spline with coefficients a^ρ. Here, this ρ which corresponds to the "corner" point of L-curve (see [32], [33]) should be taken as an "optimal" smoothing parameter. Using (3.15) and (3.16), $\|S^\rho\|_{\mathcal{W}}$ can be written as follows.

$$\begin{aligned} \|S^\rho\|_{\mathcal{W}}^2 &= (S^\rho, S^\rho)_{\mathcal{W}} = \left(\sum_{i=1}^{N} a_i^\rho \mathcal{F}_i K_{\mathcal{W}}(x, \cdot), \sum_{j=1}^{N} a_j^\rho \mathcal{F}_j K_{\mathcal{W}}(\cdot, y) \right)_{\mathcal{W}} \\ &= \sum_{i=1}^{N} \sum_{j=1}^{N} a_i^\rho a_j^\rho (\mathbf{k}_N)_{i,j} = (a^\rho)^{\mathrm{T}} \mathbf{k}_N (a^\rho). \end{aligned}$$

3.5 Best Approximation of Functionals

Let $\mathcal{F}$ be a bounded linear functional on $\mathcal{W}$. Consider an approximation of $\mathcal{F}$ by a linear combination $\mathcal{J}_N$ of the form

$$\mathcal{J}_N = \sum_{i=1}^{N} a_i \mathcal{F}_i, \tag{3.30}$$

where $a_i \in \mathbb{R}, i = 1, ..., N$ and $\mathcal{F}^N = \{\mathcal{F}_1, ..., \mathcal{F}_N\}$ form a linearly independent system of bounded linear functionals on $\mathcal{W}$. The *error* or *reminder*, when $\mathcal{J}_N$ is used to approximate $\mathcal{F}$ is defined by $\mathcal{R}_N = \mathcal{F} - \mathcal{J}_N$.

Definition 3.5.1 *The best approximation to $\mathcal{F} \in \mathcal{W}^*$ by the system $\mathcal{F}^N \subset \mathcal{W}^*$ is the functional $\mathcal{J}'_N \in \mathcal{W}^*$, with*

$$\mathcal{J}'_N = \sum_{i=1}^{N} a'_i \mathcal{F}_i, \quad a'_i \in \mathbb{R}, i = 1, ..., N,$$

for which, for every $\mathcal{J}_N$ in a form of (3.30) and $\mathcal{R}_N = \mathcal{F} - \mathcal{J}_N$, we have

$$\|\mathcal{R}'_N\|_{\mathcal{W}^*} \leq \|\mathcal{R}_N\|_{\mathcal{W}^*}, \tag{3.31}$$

where $\mathcal{R}'_N = \mathcal{F} - \mathcal{J}'_N$.

It is clear that for all $F \in \mathcal{W}$ (see Theorem 3.2.4)

$$\mathcal{R}_N F = (\mathcal{R}_N K_{\mathcal{W}}(\cdot,\cdot), F)_{\mathcal{W}} = (R_N, F)_{\mathcal{W}}, \tag{3.32}$$

where $R_N = \mathcal{R}_N K_{\mathcal{W}}(\cdot,\cdot)$ is the representer of $\mathcal{R}_N$, and hence, $\|\mathcal{R}_N\|_{\mathcal{W}^*} = \|R_N\|_{\mathcal{W}}$. So, we see that the problem of finding the best approximation to $\mathcal{F} \in \mathcal{W}^*$ by the system $\mathcal{F}^N \subset \mathcal{W}^*$ is equivalent to finding $a'_i \in \mathbb{R}, i = 1, ..., N$ for which $\|R_N\|_{\mathcal{W}}$ is minimal.

We have that

$$\begin{aligned} R_N &= \mathcal{R}_N K_{\mathcal{W}}(\cdot,\cdot) = (\mathcal{F} - \mathcal{J}_N) K_{\mathcal{W}}(\cdot,\cdot) = \left(\mathcal{F} - \sum_{i=1}^{N} a_i \mathcal{F}_i\right) K_{\mathcal{W}}(\cdot,\cdot) \\ &= \mathcal{F} K_{\mathcal{W}}(\cdot,\cdot) - \sum_{i=1}^{N} a_i \mathcal{F}_i K_{\mathcal{W}}(\cdot,\cdot) =: F - S, \end{aligned}$$

where $F := \mathcal{F}K_{\mathcal{W}}(\cdot,\cdot) \in \mathcal{W}$ and $S := \sum_{i=1}^{N} a_i \mathcal{F}_i K_{\mathcal{W}}(\cdot,\cdot) \in \mathrm{Spl}_{\mathcal{F}^N}$. Therefore, for minimizing $\|R_N\|_{\mathcal{W}}$ we need to find a spline $S \in \mathrm{Spl}_{\mathcal{F}^N}$ that minimizes $\|F-S\|_{\mathcal{W}}$. But from Theorem 3.3.10 we see that for every $F \in \mathcal{W}$ the spline that minimizes $\|F-S\|_{\mathcal{W}}$ is unique and is uniquely determined by the equations

$$\mathcal{F}_i F = \mathcal{F}_i S, \quad i = 1, ..., N,$$

that is

$$\mathcal{F}_i \mathcal{F} K_{\mathcal{W}}(\cdot,\cdot) = \sum_{k=1}^{N} a_k \mathcal{F}_i \mathcal{F}_k K_{\mathcal{W}}(\cdot,\cdot), \quad i = 1, ..., N. \tag{3.33}$$

By applying the Cauchy-Schwarz inequality to (3.32) we get also that for any $F \in \mathcal{W}$

$$|\mathcal{R}_N F| \leq \|R_N\|_{\mathcal{W}} \|F\|_{\mathcal{W}}.$$

Thus, we arrive at the following theorem.

Theorem 3.5.2 *Let $\mathcal{F} \in \mathcal{W}^*$ and $\mathcal{F}^N = \{\mathcal{F}_1, ..., \mathcal{F}_N\} \subset \mathcal{W}^*$ be a linearly independent system. Let also $a_1^N, ..., a_N^N$ be the solution of the (uniquely solvable) linear equation system (3.33). Then, the linear functional $\mathcal{J}'_N$ given by*

$$\mathcal{J}'_N = \sum_{i=1}^{N} a_i^N \mathcal{F}_i$$

represents the unique best approximation to $\mathcal{F}$ by the system $\mathcal{F}^N$. The approximation formula

$$\mathcal{F}F \approx \mathcal{J}'_N F, \quad F \in \mathcal{W},$$

admits the a posteriori estimate

$$|\mathcal{F}F - \mathcal{J}'_N F| \leq \|\mathcal{F}K_{\mathcal{W}}(\cdot,\cdot) - \mathcal{J}'_N K_{\mathcal{W}}(\cdot,\cdot)\|_{\mathcal{W}} \|F\|_{\mathcal{W}}.$$

3.6 Error Estimates

Here we obtain some new results, namely error estimates, for our spline interpolation problem. For spherical splines error estimates can be found in [24].

Theorem 3.6.1 *Let F be a function in $\mathcal{W}$, $y = (y_1, ..., y_N)^{\mathrm{T}} \in \mathbb{R}^N$ and let $\mathcal{F}^N = \{\mathcal{F}_1, ..., \mathcal{F}_N\} \subset \mathcal{W}^*$ be a linearly independent system. Denote by $S^F_{\mathcal{F}^N} \in \mathcal{W}$ the uniquely determined solution of the Problem 3.3.9. Then*

$$\sup_{\substack{\mathcal{L}\in\mathcal{W}^* \\ \|\mathcal{L}\|_{\mathcal{W}^*}=1}} |\mathcal{L}F - \mathcal{L}S^F_{\mathcal{F}^N}| \le 2\Lambda_{\mathcal{F}^N}\|F\|_{\mathcal{W}}, \tag{3.34}$$

where the $\mathcal{F}^N -$ width $\Lambda_{\mathcal{F}^N}$ is defined by

$$\Lambda_{\mathcal{F}^N} := \sup_{\substack{\mathcal{L}\in\mathcal{W}^* \\ \|\mathcal{L}\|_{\mathcal{W}^*}=1}} \left(\min_{\mathcal{J}\in\mathrm{span}(\mathcal{F}^N)} \|\mathcal{L} - \mathcal{J}\|_{\mathcal{W}^*} \right). \tag{3.35}$$

Remark 3.6.2 *Note that in the definition of $\Lambda_{\mathcal{F}^N}$ the* "min" *exists due to Theorem 3.5.2. Moreover, for any $\mathcal{L} \in \mathcal{W}^*$ with $\|\mathcal{L}\|_{\mathcal{W}^*} = 1$*

$$\min_{\mathcal{J}\in\mathrm{span}(\mathcal{F}^N)} \|\mathcal{L} - \mathcal{J}\|_{\mathcal{W}^*} \le \|\mathcal{L}\|_{\mathcal{W}^*} = 1. \tag{3.36}$$

Thus, for arbitrary $\mathcal{F}^N \subset \mathcal{W}^*$

$$0 \le \Lambda_{\mathcal{F}^N} \le 1.$$

Hence, we see that (3.34) is a more precise version of the fact that for all $\mathcal{L} \in \mathcal{W}^*$, with $\|\mathcal{L}\|_{\mathcal{W}^*} = 1$ and for all $F \in \mathcal{W}$

$$|\mathcal{L}F - \mathcal{L}S^F_{\mathcal{F}^N}| \le \|\mathcal{L}\|_{\mathcal{W}^*}\|F - S^F_{\mathcal{F}^N}\|_{\mathcal{W}} \le \|F\|_{\mathcal{W}} + \|S^F_{\mathcal{F}^N}\|_{\mathcal{W}} \le 2\|F\|_{\mathcal{W}}.$$

Proof of Theorem 3.6.1: For any $\mathcal{L} \in \mathcal{W}^*$ with $\|\mathcal{L}\|_{\mathcal{W}^*} = 1$ there exists $\mathcal{J}_\mathcal{L} \in \mathrm{span}(\mathcal{F}^N)$ such that $\|\mathcal{L} - \mathcal{J}_\mathcal{L}\|_{\mathcal{W}^*} \le \Lambda_{\mathcal{F}^N}$. Since $\mathcal{F}_k F = \mathcal{F}_k S^F_{\mathcal{F}^N}$ for all $k = 1, .., N$, hence $\mathcal{J}_\mathcal{L} F = \mathcal{J}_\mathcal{L} S^F_{\mathcal{F}^N}$, and therefore

$$\mathcal{L}F - \mathcal{L}S^F_{\mathcal{F}^N} = \mathcal{L}F - \mathcal{J}_\mathcal{L}F + \mathcal{J}_\mathcal{L}S^F_{\mathcal{F}^N} - \mathcal{L}S^F_{\mathcal{F}^N} = (\mathcal{L} - \mathcal{J}_\mathcal{L})F - (\mathcal{L} - \mathcal{J}_\mathcal{L})S^F_{\mathcal{F}^N}.$$

From Theorem 3.2.4 we see that

$$\begin{aligned} (\mathcal{L} - \mathcal{J}_\mathcal{L})F &= (F, (\mathcal{L} - \mathcal{J}_\mathcal{L})_x K_\mathcal{W}(x, \cdot))_\mathcal{W} \\ (\mathcal{L} - \mathcal{J}_\mathcal{L})S^F_{\mathcal{F}^N} &= (S^F_{\mathcal{F}^N}, (\mathcal{L} - \mathcal{J}_\mathcal{L})_x K_\mathcal{W}(x, \cdot))_\mathcal{W} \end{aligned}$$

Next, using the Cauchy-Schwarz inequality we get

$$\begin{aligned} |(F, (\mathcal{L} - \mathcal{J}_\mathcal{L})_x K_\mathcal{W}(x, \cdot))_\mathcal{W}| &\le \|F\|_\mathcal{W} (\kappa_\mathcal{W}(\mathcal{L}, \mathcal{J}_\mathcal{L}))^{1/2} \\ \left|(S^F_{\mathcal{F}^N}, (\mathcal{L} - \mathcal{J}_\mathcal{L})_x K_\mathcal{W}(x, \cdot))_\mathcal{W}\right| &\le \left\|S^F_{\mathcal{F}^N}\right\|_\mathcal{W} (\kappa_\mathcal{W}(\mathcal{L}, \mathcal{J}_\mathcal{L}))^{1/2} \end{aligned}$$

where

$$\kappa_{\mathcal{W}}(\mathfrak{L}, \mathfrak{J}_{\mathfrak{L}}) = ((\mathfrak{L} - \mathfrak{J}_{\mathfrak{L}})_x K_{\mathcal{W}}(x, \cdot), (\mathfrak{L} - \mathfrak{J}_{\mathfrak{L}})_x K_{\mathcal{W}}(x, \cdot))_{\mathcal{W}}.$$

Therefore, again using Theorem 3.2.4 we get

$$(\kappa_{\mathcal{W}}(\mathfrak{L}, \mathfrak{J}_{\mathfrak{L}}))^{1/2} = ((\mathfrak{L} - \mathfrak{J}_{\mathfrak{L}})(\mathfrak{L} - \mathfrak{J}_{\mathfrak{L}}) K_{\mathcal{W}}(\cdot, \cdot))^{1/2} = \|\mathfrak{L} - \mathfrak{J}_{\mathfrak{L}}\|_{\mathcal{W}^*} \leq \Lambda_{\mathfrak{F}^N}.$$

Now, since $S^F_{\mathfrak{F}^N}$ is the 'smoothest' interpolant (see Theorem 3.3.8), thus

$$\left\| S^F_{\mathfrak{F}^N} \right\|_{\mathcal{W}} \leq \|F\|_{\mathcal{W}}.$$

Therefore, summarizing our results we obtain

$$|\mathfrak{L}F - \mathfrak{L}S^F_{\mathfrak{F}^N}| \leq 2\Lambda_{\mathfrak{F}^N} \|F\|_{\mathcal{W}}$$

which proves the theorem, since $\mathfrak{L} \in \mathcal{W}^*$ with $\|\mathfrak{L}\|_{\mathcal{W}^*} = 1$ was arbitrary. ■

Theorem 3.6.3 *Let F be a function in $\mathcal{W}$, $y = (y_1, ..., y_N)^{\mathrm{T}} \in \mathbb{R}^N$ and let $\mathfrak{F}^N = \{\mathfrak{F}_1, ..., \mathfrak{F}_N\} \subset \mathcal{W}^*$ be a linearly independent system. Then*

$$\left\| F - S^F_{\mathfrak{F}^N} \right\|_{\mathcal{W}} \leq 2\Lambda^{1/2}_{\mathfrak{F}^N} \|F\|_{\mathcal{W}}, \tag{3.37}$$

where $S^F_{\mathfrak{F}^N}$ and $\Lambda_{\mathfrak{F}^N}$ are defined in Theorem 3.6.1.

Proof: Due to Theorem 1.1.11 for every $F \in \mathcal{W}$ and for the corresponding $S^F_{\mathfrak{F}^N}$ there exists $\mathfrak{L} \in \mathcal{W}^*$ such that $F - S^F_{\mathfrak{F}^N}$ is the representer of $\mathfrak{L}$, i.e. for any $G \in \mathcal{W}$ we have $\mathfrak{L}G = (G, F - S^F_{\mathfrak{F}^N})_{\mathcal{W}}$. By taking $G = K_{\mathcal{W}}(x, \cdot)$, we will have

$$\mathfrak{L}K_{\mathcal{W}}(x, \cdot) = (K_{\mathcal{W}}(x, \cdot), F - S^F_{\mathfrak{F}^N})_{\mathcal{W}} = \left(F - S^F_{\mathfrak{F}^N}\right)(x).$$

Note that since $\mathfrak{L}$ is the representer of $F - S^F_{\mathfrak{F}^N}$ and due to Theorem 3.3.8

$$\|\mathfrak{L}\|_{\mathcal{W}^*} = \|F - S^F_{\mathfrak{F}^N}\|_{\mathcal{W}} \leq \|F\|_{\mathcal{W}} + \|S^F_{\mathfrak{F}^N}\|_{\mathcal{W}} \leq 2\|F\|_{\mathcal{W}}.$$

Let $\|F - S^F_{\mathfrak{F}^N}\|_{\mathcal{W}} \neq 0$ (otherwise there is nothing to prove, since the right hand side of (3.37) is non-negative). We set $\mathfrak{L}_0 := \mathfrak{L}/\|\mathfrak{L}\|_{\mathcal{W}^*}$, so $\mathfrak{L}_0 \in \mathcal{W}^*$ and $\|\mathfrak{L}_0\|_{\mathcal{W}^*} = 1$. Hence, we obtain

$$\begin{aligned}
\|F - S^F_{\mathfrak{F}^N}\|_{\mathcal{W}} &= (F - S^F_{\mathfrak{F}^N}, F - S^F_{\mathfrak{F}^N})^{1/2}_{\mathcal{W}} = (F - S^F_{\mathfrak{F}^N}, \mathfrak{L}K_{\mathcal{W}}(x, \cdot))^{1/2}_{\mathcal{W}} \\
&= (\mathfrak{L}(F - S^F_{\mathfrak{F}^N}))^{1/2} = \|\mathfrak{L}\|^{1/2}_{\mathcal{W}^*} (\mathfrak{L}_0(F - S^F_{\mathfrak{F}^N}))^{1/2} \\
&= \|\mathfrak{L}\|^{1/2}_{\mathcal{W}^*} (\mathfrak{L}_0 F - \mathfrak{L}_0 S^F_{\mathfrak{F}^N})^{1/2} \leq \|\mathfrak{L}\|^{1/2}_{\mathcal{W}^*} (2\Lambda_{\mathfrak{F}^N} \|F\|_{\mathcal{W}})^{1/2} \\
&\leq 2\Lambda^{1/2}_{\mathfrak{F}^N} \|F\|_{\mathcal{W}},
\end{aligned}$$

where we used Theorem 3.2.4 and Theorem 3.6.1. ■

3.7 Convergence Results

One of the important questions of every interpolation problem is whether (and under which circumstances) the interpolating function converges to the initial function. Here we obtain a necessary and sufficient condition, under which the sequence of interpolating splines converges to the initial function, in the sense of a strong as well as a weak convergence.

Let $F \in \mathcal{W}$ be arbitrary and $\mathcal{F} := \{\mathcal{F}_1, \mathcal{F}_2, ...\}$ be a sequence of linearly independent bounded linear functionals on $\mathcal{W}$. For any $N \in \mathbb{N}$ define $\mathcal{F}^N := \{\mathcal{F}_1, ..., \mathcal{F}_N\}$ and consider the sequence $\left\{S^F_{\mathcal{F}^N}\right\}_{N\in\mathbb{N}}$ of the (uniquely determined) solutions of the spline interpolation problems

$$\left\|S^F_{\mathcal{F}^N}\right\|_{\mathcal{W}} = \min_{\substack{G\in\mathcal{W} \\ \mathcal{F}_i G = \mathcal{F}_i F, i=1,...,N}} \|G\|_{\mathcal{W}}, \quad N \in \mathbb{N}. \tag{3.38}$$

Then the following theorem holds true.

Theorem 3.7.1 *The following statements are equivalent*

(*i*) $\lim_{N\to\infty} \|F - S^F_{\mathcal{F}^N}\|_{\mathcal{W}} = 0$ *for any* $F \in \mathcal{W}$,

(*ii*) *the system* $\{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, ...\}$ *is closed in* $\mathcal{W}^*$ *(in the sense of the approximation theory),*

where for any $N \in \mathbb{N}$, $S^F_{\mathcal{F}^N} \in \mathcal{W}$ *is the unique solution of the interpolation problem (3.38).*

Remark 3.7.2 *In [23] another proof of the fact* $(ii) \Rightarrow (i)$ *(for the spherical case) is given. The result* $(ii) \Rightarrow (i)$ *in the current general formulation and the result* $(i) \Rightarrow (ii)$ *(to the knowledge of the author) are new.*

Proof of Theorem 3.7.1:

Due to Theorem 1.1.3 the closeness of $\{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, ...\}$ is equivalent to its completeness. Thus, using Corollary 3.2.7 we get that (ii) is equivalent to

$$\overline{\mathrm{span}_{N\in\mathbb{N}}\{(\mathcal{F}_N)_y K(\cdot, y)\}}^{\|\cdot\|_{\mathcal{W}}} = \mathcal{W}.$$

Next, it is clear that if (i) holds, then

$$\overline{\bigcup_{N=1}^{\infty} \mathrm{Spl}_{\mathcal{F}^N}}^{\|\cdot\|_{\mathcal{W}}} = \mathcal{W}, \tag{3.39}$$

However, (3.39) means that for any $F \in \mathcal{W}$ and for any $\varepsilon > 0$ there exists $N_0 \in \mathbb{N}$ and $S_{N_0} \in \mathrm{Spl}_{\mathcal{F}^{N_0}}$ such that $\|F - S_{N_0}\|_{\mathcal{W}} \leq \varepsilon$. Therefore, using Theorem 3.3.10 we obtain that

$$\|F - S^F_{\mathcal{F}^N}\|_{\mathcal{W}} \leq \|F - S^F_{\mathcal{F}^{N_0}}\|_{\mathcal{W}} \leq \|F - S_{N_0}\|_{\mathcal{W}} \leq \varepsilon \quad \text{for all} \quad N > N_0.$$

Hence, (i) is equivalent to (3.39). Finally, observing the fact that

$$\overline{\bigcup_{N=1}^{\infty} \mathrm{Spl}_{\mathcal{F}^N}}^{\|\cdot\|_{\mathcal{W}}} = \overline{\mathrm{span}_{N\in\mathbb{N}}\{(\mathcal{F}_N)_y K(\cdot, y)\}}^{\|\cdot\|_{\mathcal{W}}},$$

we get the desired result. ■

Remark 3.7.3 *In functional analytic language, the statement (i) in Theorem 3.7.1 means that $S^F_{\mathcal{F}^N} \to F$ as $N \to \infty$ in the sense of strong convergence, and during the proof we have seen that it is true if the system $\{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, ...\}$ is complete in $\mathcal{W}^*$, i.e. it uniquely determines a function $F \in \mathcal{W}$.*

The following (as far as we know - new) theorem shows that the completeness of $\{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, ...\}$ in $\mathcal{W}^*$ is a necessary and sufficient condition for a weak convergence of a sequence of interpolating splines to the initial function as well.

Theorem 3.7.4 *The following statements are equivalent*

(i) $\lim_{N\to\infty} |\mathcal{L}F - \mathcal{L}S^F_{\mathcal{F}^N}| = 0$ *for any* $F \in \mathcal{W}$, *and for any* $\mathcal{L} \in \mathcal{W}^*$,

(ii) *the system* $\{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, ...\}$ *is complete in* $\mathcal{W}^*$.

where for any $N \in \mathbb{N}$, $S^F_{\mathcal{F}^N} \in \mathcal{W}$ is the unique solution of the interpolation problem (3.38).

Proof: Taking into account the fact that from the strong convergence of a sequence follows the weak convergence of one, and using Theorem 3.7.1 we obtain that $(ii) \Rightarrow (i)$ (i.e. (ii) implies (i)). So, to prove the theorem, it is enough to show that $(i) \Rightarrow (ii)$, or equivalently $\mathsf{Not}\,(ii) \Rightarrow \mathsf{Not}\,(i)$.
Assume now that (ii) is not true, i.e. there exists $G \in \mathcal{W}$ such that $\mathcal{F}_i G = 0$,

$i \in \mathbb{N}$, but $G \neq 0$. Denote by $\mathcal{L}_G$ the functional, whose representer is G. In this case using Lemma 3.3.6 we get

$$\mathcal{L}_G S^G_{\mathcal{F}^N} = (S^G_{\mathcal{F}^N}, G)_{\mathcal{W}} = \sum_{i=1}^{N} a_i^N \mathcal{F}_i G = 0, \quad \text{for any} \quad N \in \mathbb{N},$$

where for any $N \in \mathbb{N}$, $a_1^N, ..., a_N^N$ are the coefficients of the spline $S^G_{\mathcal{F}^N}$. Hence,

$$\lim_{N\to\infty} |\mathcal{L}_G G - \mathcal{L}_G S^G_{\mathcal{F}^N}| = |\mathcal{L}_G G| = |(G, G)_{\mathcal{W}}| = \|G\|^2_{\mathcal{W}} \neq 0.$$

That is, Not $(ii) \Rightarrow$ Not (i). ∎

Combining Theorem 3.7.1 and Theorem 3.7.4, and taking into account Theorem 1.1.3 we obtain

Theorem 3.7.5 *The following statements are equivalent*

(i) $\lim_{N\to\infty} |\mathcal{L}F - \mathcal{L}S^F_{\mathcal{F}^N}| = 0$ *for any* $F \in \mathcal{W}$, *and for any* $\mathcal{L} \in \mathcal{W}^*$,

(ii) $\lim_{N\to\infty} \|F - S^F_{\mathcal{F}^N}\|_{\mathcal{W}} = 0$ *for any* $F \in \mathcal{W}$,

(iii) *the system* $\{\mathcal{F}_1, \mathcal{F}_2, \mathcal{F}_3, ...\}$ *is complete in* $\mathcal{W}^*$.

where for any $N \in \mathbb{N}$, $S^F_{\mathcal{F}^N} \in \mathcal{W}$ *is the unique solution of the interpolation problem (3.38).*

We have shown that, roughly speaking, any function in $\mathcal{W}$ can be arbitrarily well (in $\mathcal{W}$-norm) approximated by a certain spline function (of course under the assumption of completeness of the given system of functionals). A question arises here, whether it is possible for an $\mathrm{L}^2(X)$ function to get an arbitrarily good approximation with corresponding spline functions too. In this context we are able to prove the following theorem.
The set of all linear bounded functionals on $\mathrm{L}^2(X)$ will be denoted by $\mathrm{L}^2(X)^*$. Let $F \in \mathrm{L}^2(X)$ be arbitrary and $\mathcal{F} := \{\mathcal{F}_1, \mathcal{F}_2, ...\}$ be a system of linearly independent linear bounded functionals on $\mathrm{L}^2(X)$. For any $N \in \mathbb{N}$ denote $\mathcal{F}^N := \{\mathcal{F}_1, ..., \mathcal{F}_N\}$.

Theorem 3.7.6 *Let the system* $\mathcal{F} = \{\mathcal{F}_1, \mathcal{F}_2, ...\}$ *be complete in* $\mathcal{W}^*$, *and let* $F \in \mathrm{L}^2(X)$ *be arbitrary. Then for any real* $\varepsilon > 0$ *and for any* $T \in \mathbb{N}$ *there exist* $N \in \mathbb{N}$ *and a spline* $S_N \in \mathrm{Spl}_{\mathcal{F}^N}$ *such that*

$$\mathcal{F}_i S_N = \mathcal{F}_i F, \quad i = 1, ..., T \tag{3.40}$$

and

$$\|F - S_N\|_{\mathrm{L}^2(X)} \leq \varepsilon. \tag{3.41}$$

Proof: First of all, note that $\mathcal{W} \subset \mathrm{L}^2(X)$. Moreover, from Lemma 1.1.1 and Corollary 3.1.6 follows that for any $\mathcal{L} \in \mathrm{L}^2(X)^*$ and $F \in \mathcal{W}$

$$|\mathcal{L}F| \leq \|\mathcal{L}\|\|F\|_{\mathrm{L}^2(X)} \leq C_1\|F\|_\infty \leq C_2\|F\|_{\mathcal{W}},$$

where

$$\begin{aligned} C_1 &= \|\mathcal{L}\| \sqrt{\text{measure}(X)} = \text{const}, \\ C_2 &= \|\mathcal{L}\| \sqrt{\text{measure}(X)} \left(\sum_{k=0}^{\infty} A_k^2 \left\| W_k^X(x) \right\|_\infty^2 \right)^{1/2} = \text{const}. \end{aligned}$$

Therefore, $\mathcal{F}$ can be considered as a system of linear bounded functionals on $\mathcal{W}$, too.
By definition W^X is complete and therefore closed in $\mathrm{L}^2(X)$. Thus,

$$\overline{\mathcal{W}(\{A_k\}; X)}^{\|\cdot\|_{\mathrm{L}^2(X)}} = \mathrm{L}^2(X). \tag{3.42}$$

Let now $F \in \mathrm{L}^2(X)$, $\varepsilon > 0$ and $T \in \mathbb{N}$ be arbitrary. From (3.42) and from Theorem 1.1.12 (note that $\mathcal{W}$ is a linear space, and therefore is convex) follows that there exists a function $G \in \mathcal{W}$ such that

$$\|F - G\|_{\mathrm{L}^2(X)} \leq \frac{\varepsilon}{2}, \tag{3.43}$$

and

$$\mathcal{F}_i F = \mathcal{F}_i G, \quad i = 1, ..., T. \tag{3.44}$$

Moreover, since $G \in \mathcal{W}$, due to Theorem 3.7.5 there exists $N_0 = N_0(\varepsilon)$ such that for any $N > N_0$ there exists $S^G_{\mathcal{F}^N} \in \mathrm{Spl}_{\mathcal{F}^N}$ such that

$$\|G - S^G_{\mathcal{F}^N}\|_{\mathcal{W}} \leq \frac{\varepsilon}{2C_3}, \tag{3.45}$$

with

$$\mathcal{F}_i G = \mathcal{F}_i S^G_{\mathcal{F}^N}, \quad i = 1, ..., N, \tag{3.46}$$

where

$$C_3 = \sqrt{\text{measure}(X)} \left(\sum_{k=0}^{\infty} A_k^2 \left\| W_k^X(x) \right\|_\infty^2 \right)^{1/2} = \text{const}.$$

Thus, again using Lemma 1.1.1 and Corollary 3.1.6 we obtain that

$$\|G - S^G_{\mathcal{F}^N}\|_{\mathrm{L}^2(X)} \leq \frac{\varepsilon}{2}. \tag{3.47}$$

Hence, taking $N > \max(N_0, T)$ and combining (3.43), (3.44), (3.46) and (3.47) we obtain that there exists $S_N := S^G_{\mathcal{F}^N} \in \mathrm{Spl}_{\mathcal{F}^N}$ which satisfies (3.40) and (3.41).
■

3.8 Regularization with Splines

Let $Y \subset \mathbb{R}^n$, $n \in \mathbb{N}$ be an arbitrary compact set and let $\mathrm{B}(Y)$ be the Banach space of all bounded functions on Y.
Let also $\Lambda : \mathcal{W}(\{A_k\}; X) \to \mathrm{B}(Y)$ be a linear bounded operator. We discuss the following inverse problem.

Problem 3.8.1 *Given $G \in \mathrm{B}(Y)$, find $F \in \mathcal{W}$ such that $\Lambda F = G$.*

Suppose that the solution of this problem is unstable. Hence, in order to get a stable approximate solution of the Problem 3.8.1, we need to use a regularization (see Section 2.1).
Let the closure of $\mathcal{R}(\Lambda)$ have a topological complement in $\mathrm{B}(Y)$, say S. Let also $\mathcal{P}$ be the projector of $\mathrm{B}(Y)$ onto $\overline{\mathcal{R}(\Lambda)}$ along S. Denote by Λ^+ the generalized inverse of Λ. For any $y \in Y$ denote by $\mathcal{F}_y$ the functional defined on $\mathcal{W}$ with

$$\mathcal{F}_y F := \Lambda F(y), \quad \text{where} \quad F \in \mathcal{W}.$$

From the linearity of Λ follows that for any $y \in Y$, $\mathcal{F}_y$ is linear, too. Moreover, since for any $y \in Y$

$$|\mathcal{F}_y F| = |\Lambda F(y)| \leq \max_{z \in Y} |\Lambda F(z)| = \|\Lambda F\|_\infty \leq \|\Lambda\| \|F\|_{\mathcal{W}}$$

and Λ is bounded, $\mathcal{F}_y$ is bounded as well. Now, let $\{y_1, y_2, ...\}$ be a sequence of points in Y such that the corresponding system of linear bounded functionals $\{\mathcal{F}_{y_1}, \mathcal{F}_{y_2}, ...\}$ is linearly independent and is complete in $\mathcal{W}(\{A_k\}; X)^*$. Denote $\mathcal{F}_i := \mathcal{F}_{y_i}$, $i \in \mathbb{N}$ and $\mathcal{F}^N := \{\mathcal{F}_1, ..., \mathcal{F}_N\}$, $N \in \mathbb{N}$.
Consider the sequence of operators $\Lambda_N : \mathcal{R}(\Lambda) \dot{+} S \to \mathcal{W}$ defined by

$$\Lambda_N G = S^F_{\mathcal{F}^N} \quad \text{for any} \quad G \in \mathcal{R}(\Lambda) \dot{+} S, \;\; N \in \mathbb{N}, \tag{3.48}$$

where $F := \Lambda^+ G$, and for any $N \in \mathbb{N}$, $S^F_{\mathcal{F}^N}$ is the (uniquely determined) solution of the spline interpolation problem

$$\left\| S^F_{\mathcal{F}^N} \right\|_{\mathcal{W}} = \min_{\substack{H \in \mathcal{W} \\ \mathcal{F}_i H = \mathcal{F}_i F, i=1,\dots,N}} \|H\|_{\mathcal{W}}. \tag{3.49}$$

It is not hard to check that using the linearity of Λ^+ and $\mathcal{F}_i$, $i \in \mathbb{N}$, and applying Theorem 3.3.11, one obtains that for any $N \in \mathbb{N}$, Λ_N is linear as well.
Now take an arbitrary $G \in \mathcal{R}(\Lambda) \dot{+} S$ and denote $G_1 := \mathcal{P}G$. Note that from the definition of Λ^+ follows that $\Lambda^+ G = \Lambda^+ G_1$. Thus, for an arbitrary $N \in \mathbb{N}$

$$\Lambda_N G = S^{(\Lambda^+ G)}_{\mathcal{F}^N} = S^{(\Lambda^+ G_1)}_{\mathcal{F}^N} = \Lambda_N G_1.$$

Therefore, for every fixed $N \in \mathbb{N}$ using Lemma 1.1.1, Theorem 3.3.7 and the continuity of $\mathcal{P}$ we obtain that

$$\begin{aligned} \|\Lambda_N G\|_{\mathrm{L}^2(X)} &= \|\Lambda_N G_1\|_{\mathrm{L}^2(X)} = \left\| S^F_{\mathcal{F}^N} \right\|_{\mathrm{L}^2(X)} \\ &\le \sqrt{\text{measure}(X)} \, \left\| S^F_{\mathcal{F}^N} \right\|_{\mathrm{C}(X)} \le C_1 \sup_{x \in X} \left| \sum_{k=1}^N (\mathcal{F}_k F) L_k(x) \right| \\ &\le C_1 \max_{k=1,\dots,N} |\mathcal{F}_k F| \sup_{x \in X} \left| \sum_{k=1}^N L_k(x) \right| \le C_1 \sup_{y \in Y} |\Lambda F(y)| \, C_2 \\ &= \|G_1\|_\infty C_1 \, C_2 \le \|\mathcal{P}\| \|G\|_\infty C_1 \, C_2 \\ &\le C \, \|G\|_\infty, \end{aligned} \tag{3.50}$$

where $F := \Lambda^+ G_1$, $L_k(x)$ is defined by (3.19), $C = C_1 \, C_2$, $C_1 = \sqrt{\text{measure}(X)}$ and

$$C_2 = \sup_{x \in X} \left| \sum_{k=1}^N L_k(x) \right| = \text{const}$$

is bounded since $\sum_{k=1}^N L_k$ is in $\mathcal{W}$ and thus, bounded. So, for any $N \in \mathbb{N}$, Λ_N is a linear bounded and therefore continuous operator on $\mathcal{R}(\Lambda) \dot{+} S$. However since $\mathrm{B}(Y) = \overline{\mathcal{R}(\Lambda) \dot{+} S}$, Λ_N admits a uniquely determined extension Λ'_N to $\mathrm{B}(Y)$, for any $N \in \mathbb{N}$ (see e.g. [39]) with $\|\Lambda'_N\| = \|\Lambda_N\|$, $N \in \mathbb{N}$.
Hence, we obtain a family of linear bounded operators $\Lambda'_N : \mathrm{B}(Y) \to \mathcal{W}$, $N \in \mathbb{N}$ such that for any $G \in \mathcal{R}(\Lambda) \dot{+} S$ (see Theorem 3.7.5)

$$\lim_{N \to \infty} \|\Lambda'_N G - \Lambda^+ G\|_{\mathcal{W}} = \lim_{N \to \infty} \|S^F_{\mathcal{F}^N} - F\|_{\mathcal{W}} = 0.$$

That is, the family of operators Λ'_N, $N \in \mathbb{N}$ defined via splines can be considered as a regularization of the generalized inverse Λ^+ (see Definition 2.1.5).

It should also be mentioned that the described method of the construction of a regularization can work only if in the range space of the operator Λ from the closeness (nearness) in norm follows pointwise closeness, as e.g. in $\mathrm{B}(Y)$ or $\mathrm{C}(Y)$ with the supremum norm. Otherwise, the operators Λ_N can be non-continuous.

Chapter 4

Application to Seismic Surface Wave Tomography

In this chapter we present an application of a spline approximation method, described in Chapter 3, to seismic surface wave traveltime tomography.
As we have already mentioned, the task of seismic (traveltime) tomography is to determine the seismic wave velocity function/model out of traveltime data related to the positions of the epicenters and the recording stations. The problem of seismic surface wave traveltime tomography can be formulated as follows:
Given traveltimes $T_q; q = 1, ..., N$ of seismic surface waves between epicenters E_q and receivers R_q on the Earth's surface. Find a (slowness) function $\tilde{S}$, such that

$$\int_{\gamma_q} \tilde{S}(x) d\sigma(x) = T_q, \quad q = 1, ..., N, \tag{4.1}$$

where integrals are path integrals over $\gamma_q; q = 1, ..., N$, which, in general, are raypaths of seismic surface waves between E_q and R_q. Following the considerations in Chapter 2 we will discuss the linearized inverse problem, by taking PREM (see [16]) as a reference model. However, since in PREM the surface wave velocity is constant, the minimal spherical distances, i.e. the geodesic minimal arcs, between E_q and R_q should be taken as $\gamma_q; q = 1, ..., N$. As we have already mentioned we will use the unit ball as an approximation for the earth. Therefore, the given data, i.e. E_q, R_q and T_q; $q = 1, ..., N$, also must be normalized accordingly.
So, we can reformulate the discussed inverse problem as follows:

Problem 4.0.2 *Given real numbers T_q; $q = 1, ..., N$ and points E_q,R_q; $q = 1, ..., N$ on the unit sphere Ω. Find a function $\tilde{S} \in \mathrm{C}(\Omega)$ such that*

$$\int_{\gamma_q} \tilde{S}(x) d\sigma(x) = T_q, \quad q = 1, ..., N,$$

where $\gamma_q; q = 1, ..., N$ are the geodesic minimal arcs between E_q and R_q.

Note that here as T_q; $q = 1, ..., N$ the delay times with respect to PREM should be taken and $\tilde{S}$ already will approximate the perturbations of the slowness to PREM. This is allowed due to the linearity of the problem.

Assumption 4.0.3 *We will assume that $\gamma_i \neq \gamma_j$, if $i \neq j$, $i, j = 1, ..., N$.*

4.1 Initial Constructions

Since here the function $\tilde{S}$, which needs to be approximated, is defined on the unit sphere, we will take as an initial set (see Section 3.1) the unit sphere $X = \Omega = \{x \in \mathbb{R}^3 \,|\, |x| = 1\}$. As an initial basis system on Ω we take the system $\{Y_{n,j}\}_{n \in \mathbb{N}_0; j=-n,...,n}$ of spherical harmonics defined by (1.4) (see also Section 3.1.2 and Section 3.2.2). As we have already seen, in this case $\Theta = \emptyset$, i.e. $\mathrm{C}_\Theta(\Omega) = \mathrm{C}(\Omega)$.
The results of the Section 3.1 and Section 3.2 will be summarized briefly here for a special case of initial set and initial basis system.
If $\{A_n\}_{n \in \mathbb{N}_0}$ is an arbitrary real sequence, where $A_n \neq 0$ for all $n \in \mathbb{N}_0$, then $\mathcal{E} := \mathcal{E}(\{A_k\}; X)$ denotes the space of all functions $F \in \mathrm{L}^2(\Omega)$ satisfying

$$\sum_{n=0}^{\infty} \sum_{j=-n}^{n} A_n^{-2} \left((F, Y_{n,j})_{\mathrm{L}^2(\Omega)} \right)^2 < +\infty.$$

This space is a pre-Hilbert space if it is equipped with the inner product

$$(F, G)_{\mathcal{H}(\{A_k\};\Omega)} := \sum_{n=0}^{\infty} \sum_{j=-n}^{n} A_n^{-2} \, (F, Y_{n,j})_{\mathrm{L}^2(\Omega)} \, (G, Y_{n,j})_{\mathrm{L}^2(\Omega)} \, ; \quad F, G \in \mathcal{E}(\{A_k\}; \Omega);$$

which is always finite due to the Cauchy–Schwarz inequality. The Hilbert space $\mathcal{H} := \mathcal{H}(\{A_k\}; \Omega)$ is defined as the completion of $\mathcal{E}(\{A_k\}; \Omega)$ with respect to

$(.,.)_{\mathcal{H}}$. The induced norm is denoted by $\|F\|_{\mathcal{H}} := \sqrt{(F,F)_{\mathcal{H}}}$.
As we have already seen in Section 3.1.2, here $\{A_n\}_n$ will be summable if

$$\sum_{n=0}^{\infty} \frac{2n+1}{4\pi} A_n^2 < +\infty.$$

And if $\{A_n\}_n$ is summable, then this Sobolev space $\mathcal{H}$ possesses a unique reproducing kernel $K_{\mathcal{H}} : \Omega \times \Omega \to \mathbb{R}$ given by

$$K_{\mathcal{H}}(\xi,\eta) = \sum_{n=0}^{\infty} \sum_{j=-n}^{n} A_n^2 Y_{n,j}(\xi) Y_{n,j}(\eta) = \sum_{n=0}^{\infty} A_n^2 \frac{2n+1}{4\pi} P_n(\xi \cdot \eta); \quad \xi, \eta \in \Omega;$$

and is, consequently, a radial basis function.
Moreover, the summability also implies that $\mathcal{H}(\{A_k\};\Omega) \subset \mathrm{C}(\Omega)$, i.e. every function in $\mathcal{H}$ is continuous on Ω (see Lemma 3.1.5), and

$$\|F\|_{\mathrm{C}(\Omega)} \leq \|F\|_{\mathcal{H}} \left(\sum_{n=0}^{\infty} A_n^2 \frac{2n+1}{4\pi} \right)^{1/2}$$

for all $F \in \mathcal{H}$.
Moreover, using Theorem 1.4.10 and the fact $\{Y_{n,j}\}_{n \in \mathbb{N}_0, j=-n,\ldots,n} \subset \mathcal{H} \subset \mathrm{C}(\Omega)$ we obtain the following result.

Theorem 4.1.1

$$\overline{\mathcal{H}}^{\|\cdot\|_{\mathrm{C}(\Omega)}} = \mathrm{C}(\Omega).$$

4.2 Application

We define functionals $\mathcal{F}_q : \mathcal{H} \to \mathbb{R}$, $q = 1, ..., N$ as path integrals of a function in $\mathcal{H}$ over γ_q, i.e. for any $F \in \mathcal{H}$

$$\mathcal{F}_q F := \int_{\gamma_q} F(\xi)\, \mathrm{d}\sigma(\xi), \quad q = 1, ..., N. \tag{4.2}$$

The discussed functionals $\mathcal{F}_q$ are obviously linear, due to the linearity of the integral, and continuous on $\mathcal{H} \subset \mathrm{C}(\Omega)$ since

$$|\mathcal{F}_q F| \leq \|F\|_{\mathrm{C}(\Omega)} \,\mathrm{length}\,(\gamma_q) \leq \|F\|_{\mathcal{H}} \left(\sum_{n=0}^{\infty} A_n^2 \frac{2n+1}{4\pi} \right)^{1/2} \pi$$

for all $F \in \mathcal{H}$.

Theorem 4.2.1 *From Assumption 4.0.3 follows that the system of functionals* $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$ *is linearly independent.*

Proof: Let Assumption 4.0.3 hold, i.e. $\gamma_i \neq \gamma_j$, if $i \neq j$, $i, j = 1, ..., N$, but $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$ is linearly dependent. That is there exist coefficients $a_1, ..., a_N$ where at least one of them is not 0, such that $\sum_{k=1}^N a_k \mathcal{F}_k = 0$. However, this means that for any $F \in \mathcal{H}$

$$\sum_{k=1}^{N} a_k \mathcal{F}_k F = 0. \tag{4.3}$$

Let $a_{i_0} \neq 0$. Assume without loss of generality that $a_{i_0} > 0$. We will construct a function in $\mathcal{H}$ for which (4.3) does not hold. Clearly from Assumption 4.0.3 follows that there exists $x_0 \in \gamma_{i_0}$ and $\varepsilon > 0$ such that $x_0(\varepsilon) \cap \gamma_i = \emptyset$ if $i \neq i_0$, where $x_0(\varepsilon)$ is the ε-neighborhood of x_0. Now, clearly for an arbitrary real $M_0 > 0$ we can construct $F_1 \in \mathrm{C}(\Omega)$ such that $F_1(x) \geq 0$, $x \in \Omega$ and

$$F_1(x) = \begin{cases} M_0, & \text{if} \quad x \in x_0(\varepsilon/2) \\ 0, & \text{if} \quad x \in \Omega \backslash x_0(\varepsilon). \end{cases} \tag{4.4}$$

Hence,

$$\lambda_1 := \sum_{k=1}^{N} a_k \int_{\gamma_k} F_1(\xi) \mathrm{d}\sigma(\xi) = a_{i_0} \int_{\gamma_{i_0}} F_1(\xi) \mathrm{d}\sigma(\xi) > a_{i_0} M_0 \varepsilon / 4 =: M_1 > 0. \tag{4.5}$$

Now since length(γ_i), $i = 1, ..., N$ is bounded

$$M_2 := \sum_{k=1}^{N} |a_k| \, \mathrm{length}(\gamma_k) < \infty.$$

However, due to Theorem 4.1.1 we can arbitrarily well (in $\|\cdot\|_{\mathrm{C}(\Omega)}$ norm) approximate F_1 by a function in $\mathcal{H}$. It follows that for $\delta := M_1 M_2 / 2$ there exists $F_2 \in \mathcal{H}$ such that $\|F_1 - F_2\|_{\mathrm{C}(\Omega)} \leq \delta$. Hence, if we denote

$$\lambda_2 := \sum_{k=1}^{N} a_k \mathcal{F}_k F_2 = \sum_{k=1}^{N} a_k \int_{\gamma_k} F_2(\xi) \mathrm{d}\sigma(\xi),$$

then

$$\begin{aligned} |\lambda_1 - \lambda_2| &= \left| \sum_{k=1}^{N} a_k \int_{\gamma_k} (F_1 - F_2)(\xi) \mathrm{d}\sigma(\xi) \right| \leq \|F_1 - F_2\|_{\mathrm{C}(\Omega)} \sum_{k=1}^{N} |a_k| \, \mathrm{length}(\gamma_k) \\ &\leq \delta M_2 = \frac{M_1}{2}. \end{aligned}$$

That is

$$\lambda_1 - M_1/2 \leq \lambda_2 \leq \lambda_1 + M_1/2,$$

such that using (4.5) we obtain that

$$\sum_{k=1}^{N} a_k \mathcal{F}_k F_2 = \lambda_2 > M_1 - \frac{M_1}{2} = \frac{M_1}{2} > 0.$$

However, this is a contradiction to (4.3), hence, $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$ is linearly independent. ■

The idea that we follow here is to approximate $\tilde{S}$ by a harmonic spline $S \in \mathcal{H}$ based on a system $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$, i.e. by a spline of the form

$$S(\xi) = \sum_{k=1}^{N} a_k \mathcal{F}_k K_{\mathcal{H}}(., \xi), \quad \xi \in \Omega. \tag{4.6}$$

Note that in this case the spline S will be harmonic function since the sum of a uniformly convergent series of harmonic functions (in our case - spherical harmonics) is harmonic (see e.g. [6]).

As we can see from (4.6), the evaluation of the linear functionals $\mathcal{F}_q F$, $F \in \mathcal{W}$, $q = 1, ..., N$, or in our case (see (4.2)) the evaluation of the line integrals over the geodesic minimal arc γ_q between E_q and R_q is essential for the evaluation of the spline function S. Here we present two methods for the evaluation of such functionals.

4.2.1 First Method

It is known that the geodesic minimal arc between two points on a sphere is the arc of the great-circle which contains these points.

Now, let $P = (x_P, y_P, z_P)$, $Q = (x_Q, y_Q, z_Q)$ be points on the unit sphere Ω, $w = Q - (P \cdot Q)P$ and $Q_P = \frac{w}{|w|}$. Then, the parametric equation of the great-circle which is given by the points P and Q can be written as (see e.g. [40])

$$r(t) = \cos(t)P + \sin(t)Q_P\,. \tag{4.7}$$

Moreover $r(0) = P$, $r(d) = Q$, where $d = \arccos(P \cdot Q)$, and the minimal spherical distance between P and Q is equal to d. Note also that $|r'(t)| = 1$, for all $t \in [0, d]$.

It is also known that if L is a curve parameterized by a $\mathrm{C}^{(1)}([a,b],\mathbb{R}^3)$–function l, and F is a continuous scalar field, then

$$\int_L F(\xi)\,\mathrm{d}\sigma(\xi) = \int_a^b F(l(t))\,|l'(t)|\,\mathrm{d}t\,.$$

Let now the curves γ_q; $q = 1, ..., N$; on the unit sphere Ω be parameterized by

$$r_q(x) = \cos(x)E_q + \sin(x)Q_{E_q}, \quad 0 \leq x \leq d_q,$$

where $Q_{E_q} = \dfrac{R_q - (E_q \cdot R_q)E_q}{|R_q - (E_q \cdot R_q)E_q|}$ and $d_q = \arccos(E_q \cdot R_q)$.
Thus, the functionals $\mathcal{F}_q F$, $F \in \mathcal{W}$, $q = 1, ..., N$ can be calculated by the formula

$$\mathcal{F}_q F := \int_{\gamma_q} F(\xi)\,\mathrm{d}\sigma(\xi) = \int_0^{d_q} F(r_q(t))\mathrm{d}t, \quad q = 1, ..., N. \tag{4.8}$$

Therefore, the matrix corresponding to such a spline interpolation problem has the following components:

$$\begin{aligned}
(\mathcal{F}_l)_\xi(\mathcal{F}_k)_\eta K_{\mathcal{H}}(\eta,\xi) &= \int_{\gamma_l}\int_{\gamma_k} K_{\mathcal{H}}(\eta,\xi)\,\mathrm{d}\sigma(\eta)\,\mathrm{d}\sigma(\xi) \\
&= \sum_{n=0}^{\infty} A_n^2 \frac{2n+1}{4\pi} \int_{\gamma_l}\int_{\gamma_k} P_n(\xi\cdot\eta)\mathrm{d}\sigma(\eta)\,\mathrm{d}\sigma(\xi) \\
&= \sum_{n=0}^{\infty} A_n^2 \frac{2n+1}{4\pi} \int_0^{d_l}\int_0^{d_k} P_n\left(r_k(x)\cdot r_l(y)\right)\,\mathrm{d}x\,\mathrm{d}y\,.
\end{aligned}$$

Note that here we can change the order of integration and summation, since the discussed functionals $\mathcal{F}_q$ are linear and continuous. Thus, by solving the linear equation system

$$\sum_{k=1}^{N} a_k (\mathcal{F}_l)_\xi(\mathcal{F}_k)_\eta K_{\mathcal{H}}(\eta,\xi) = T_q \quad \text{for all} \quad q = 1, ..., N;$$

we obtain the coefficients $(a_k)_{k=1,...,N}$ of the spline

$$S(\xi) = \sum_{k=1}^{N} a_k (\mathcal{F}_k)_\eta K_{\mathcal{H}}(\eta,\xi) = \sum_{k=1}^{N} a_k \sum_{n=0}^{\infty} A_n^2 \frac{2n+1}{4\pi} \int_0^{d_k} P_n\left(r_k(x)\cdot\xi\right)\,\mathrm{d}x$$

approximating the function $\tilde{S}$. Note that the obtained integrals can easily be calculated approximately by appropriate quadrature methods such as the trapezoidal rule.

For the case of the Abel–Poisson kernel we obtain a closed representation of the reproducing kernel. As we have seen in Section 3.2.2, the Abel–Poisson kernel is given by

$$K_{\mathcal{H}}(\xi,\eta) = \frac{1}{4\pi}\frac{1-h^2}{(1+h^2-2h(\xi\cdot\eta))^{(3/2)}} \tag{4.9}$$

where $h = A_1^2$.
Therefore, the matrix corresponding to such a spline interpolation problem has the following components:

$$\begin{aligned}(\mathcal{F}_l)_\xi(\mathcal{F}_k)_\eta K_{\mathcal{H}}(\eta,\xi) &= \int_{\gamma_l}\int_{\gamma_k} K_{\mathcal{H}}(\eta,\xi)\,\mathrm{d}\sigma(\eta)\,\mathrm{d}\sigma(\xi)\\ &= \frac{1-h^2}{4\pi}\int_{\gamma_l}\int_{\gamma_k}\left(1+h^2-2h(\eta\cdot\xi)\right)^{(-3/2)}\,\mathrm{d}\sigma(\eta)\,\mathrm{d}\sigma(\xi)\\ &= \frac{1-h^2}{4\pi}\int_0^{d_l}\int_0^{d_k}\frac{1}{(1+h^2-2h(r_k(x)\cdot r_l(y)))^{3/2}}\,\mathrm{d}x\,\mathrm{d}y\quad .\end{aligned}$$

Thus, by solving the linear equation system

$$\sum_{k=1}^{N} a_k(\mathcal{F}_l)_\xi(\mathcal{F}_k)_\eta K_{\mathcal{H}}(\eta,\xi) = T_l \quad \text{for all} \quad l=1,...,N;$$

we obtain the coefficients $(a_k)_{k=1,\dots,N}$ of the spline

$$S(\xi) = \sum_{k=1}^{N} a_k(\mathcal{F}_k)_\eta K_{\mathcal{H}}(\eta,\xi) = \sum_{k=1}^{N} a_k\,\frac{1-h^2}{4\pi}\int_0^{d_k}\frac{1}{(1+h^2-2h(r_k(x)\cdot\xi))^{3/2}}\,\mathrm{d}x$$

approximating the function $\tilde{S}$.

4.2.2 Second Method

For the evaluation of the spline S one can also use an alternative algorithm, which will be described next.
According to [14] (p. 930) we find that for all $n \in \mathbb{N}_0$ and $j = -n, ..., n$

$$\int_{\gamma_q} \mathcal{Y}_{n,j}(\xi)\,\mathrm{d}\sigma(\xi) = \sum_{m=-n}^{n}\frac{i}{m}X_{n,m}\left(\frac{\pi}{2}\right)\left(1-e^{im\vartheta_q}\right)\mathcal{D}^{(n)}_{m,j}(\alpha_q,\beta_q,\eta_q), \tag{4.10}$$

where $\mathcal{Y}_{n,j}$ are the complex spherical harmonics defined by (1.6), $X_{n,m}$ is defined by (1.5) and

$$\begin{aligned}\mathcal{D}^{(n)}_{m,j}(\alpha,\beta,\eta) &= e^{im\eta}P^m_{n,j}(\cos\beta)e^{ij\alpha},\\ P^m_{n,j}(t) &= \frac{1}{2^n}\left(\frac{1}{(n+m)!(n-m)!}\right)^{1/2}\left(\frac{(n+j)!}{(n-j)!}\right)^{1/2}(1-t)^{-\frac{1}{2}(j-m)}\\ &\quad (1+t)^{-\frac{1}{2}(j+m)}\cdot\left(\frac{\mathrm{d}}{\mathrm{d}t}\right)^{n-j}\left((t-1)^{n-m}(t+1)^{n+m}\right).\end{aligned}$$

Here $P^m_{n,j}$ is called generalized Legendre function of degree n, order $j\in\{-n,...,n\}$, and upper index $m\in\{-n,...,n\}$ and can be calculated recursively (see [14], p. 899f). Moreover, the Euler angles $(\alpha_q,\beta_q,\eta_q)$ are given by

$$\begin{aligned}\tan\alpha_q &= \frac{\sin\theta^{\mathrm{R}}_q\cos\theta^{\mathrm{E}}_q\cos\varphi^{\mathrm{R}}_q-\cos\theta^{\mathrm{R}}_q\sin\theta^{\mathrm{E}}_q\cos\varphi^{\mathrm{E}}_q}{\cos\theta^{\mathrm{R}}_q\sin\theta^{\mathrm{E}}_q\sin\varphi^{\mathrm{E}}_q-\sin\theta^{\mathrm{R}}_q\cos\theta^{\mathrm{E}}_q\sin\varphi^{\mathrm{R}}_q},\\ \cos\beta_q &= \frac{\sin\theta^{\mathrm{R}}_q\sin\theta^{\mathrm{E}}_q\sin\left(\varphi^{\mathrm{R}}_q-\varphi^{\mathrm{E}}_q\right)}{\sin\vartheta_q},\\ \tan\eta_q &= \frac{\cos\theta^{\mathrm{E}}_q\cos\vartheta_q-\cos\theta^{\mathrm{R}}_q}{\cos\theta^{\mathrm{E}}_q\sin\vartheta_q}\end{aligned}$$

and the geodesic angular distance ϑ_q between epicenter and receiver is defined via

$$\cos\vartheta_q=\cos\theta^{\mathrm{R}}_q\cos\theta^{\mathrm{E}}_q+\sin\theta^{\mathrm{R}}_q\sin\theta^{\mathrm{E}}_q\cos\left(\varphi^{\mathrm{R}}_q-\varphi^{\mathrm{E}}_q\right).$$

Here $\theta^{\mathrm{E}}_q,\varphi^{\mathrm{E}}_q$ and $\theta^{\mathrm{R}}_q,\varphi^{\mathrm{R}}_q$ are colatitude and longitude of E_q and R_q respectively. From Equation (4.10) we have that

$$\begin{aligned}\int_{\gamma_q}\mathcal{Y}_{n,j}(\xi)\,\mathrm{d}\sigma(\xi) &= \sum_{m=-n}^{n}\frac{i}{m}X_{n,m}\left(\frac{\pi}{2}\right)\left(1-e^{im\vartheta_q}\right)\mathcal{D}^{(n)}_{m,j}(\alpha_q,\beta_q,\eta_q)\\ &= \sum_{m=-n}^{n}\left[\frac{i}{m}\left(1-e^{im\vartheta_q}\right)e^{im\eta_q}e^{ij\alpha_q}\right]X_{n,m}\left(\frac{\pi}{2}\right)P^m_{n,j}(\cos\beta_q)\\ &= \sum_{m=-n}^{n}\left[\frac{1}{m}\left(ie^{im\eta_q+ij\alpha_q}-ie^{im\vartheta_q+im\eta_q+ij\alpha_q}\right)\right]X_{n,m}\left(\frac{\pi}{2}\right)P^m_{n,j}(\cos\beta_q)\\ &= \sum_{m=-n}^{n}\frac{1}{m}\Big[i(\cos(m\eta_q+j\alpha_q)-\cos(m\vartheta_q+m\eta_q+j\alpha_q))\\ &\quad +(\sin(m\vartheta_q+m\eta_q+j\alpha_q)-\sin(m\eta_q+j\alpha_q))\Big]X_{n,m}\left(\frac{\pi}{2}\right)P^m_{n,j}(\cos\beta_q)\end{aligned}$$

Therefore, using Equation (1.7) we obtain that for all $n \in \mathbb{N}_0$ the following holds true:
if $-n \leq j < 0$, then

$$\int_{\gamma_q} Y_{n,j}(\xi)\,\mathrm{d}\sigma(\xi) = \int_{\gamma_q} \sqrt{2}\,\mathrm{Re}\,\mathcal{Y}_{n,|j|}(\xi)\,\mathrm{d}\sigma(\xi) = \sqrt{2}\mathrm{Re}\int_{\gamma_q} \mathcal{Y}_{n,|j|}(\xi)\,\mathrm{d}\sigma(\xi)$$
$$= \sqrt{2}\sum_{m=-n}^{n} \frac{1}{m}\Big[\sin(m\vartheta_q + m\eta_q - j\alpha_q) - \sin(m\eta_q - j\alpha_q)\Big] X_{n,m}\left(\frac{\pi}{2}\right) P_{n,-j}^{m}(\cos\beta_q),$$

if $j = 0$, then

$$\int_{\gamma_q} Y_{n,0}(\xi)\,\mathrm{d}\sigma(\xi) = \int_{\gamma_q} \mathcal{Y}_{n,0}(\xi)\,\mathrm{d}\sigma(\xi) = \sum_{m=-n}^{n} \frac{i}{m} X_{n,m}\left(\frac{\pi}{2}\right)\left(1 - e^{im\vartheta_q}\right)\mathcal{D}_{m,0}^{(n)}(\alpha_q, \beta_q, \eta_q)$$

and if $0 < j \leq n$, then

$$\int_{\gamma_q} Y_{n,j}(\xi)\,\mathrm{d}\sigma(\xi) = \int_{\gamma_q} \sqrt{2}\,\mathrm{Im}\,\mathcal{Y}_{n,j}(\xi)\,\mathrm{d}\sigma(\xi) = \sqrt{2}\mathrm{Im}\int_{\gamma_q} \mathcal{Y}_{n,j}(\xi)\,\mathrm{d}\sigma(\xi)$$
$$= \sqrt{2}\sum_{m=-n}^{n} \frac{1}{m}\Big[\cos(m\eta_q + j\alpha_q) - \cos(m\vartheta_q + m\eta_q + j\alpha_q)\Big] X_{n,m}\left(\frac{\pi}{2}\right) P_{n,j}^{m}(\cos\beta_q).$$

Hence, the matrix corresponding to such a spline interpolation problem has the following components:

$$(\mathcal{F}_l)_\xi\,(\mathcal{F}_k)_\eta\,K_{\mathcal{H}}(\eta,\xi) = \sum_{n=0}^{\infty} A_n^2 \sum_{j=-n}^{n} \int_{\eta_k} Y_{n,j}(\eta)\,\mathrm{d}\sigma(\eta) \int_{\eta_l} Y_{n,j}(\xi)\,\mathrm{d}\sigma(\xi),$$

where the path integrals can be calculated by the obtained formulae.
Thus, by solving the linear equation system

$$\sum_{k=1}^{N} a_k\,(\mathcal{F}_l)_\xi\,(\mathcal{F}_k)_\eta\,K_{\mathcal{H}}(\eta,\xi) = T_l \text{ for all } l = 1, ..., N$$

we obtain the coefficients $(a_k)_{k=1,\dots,N}$ of the spline

$$S(\xi) \;=\; \sum_{k=1}^{N} a_k\,(\mathcal{F}_k)_\eta\,K_{\mathcal{H}}(\eta,\xi) = \sum_{k=1}^{N} a_k \sum_{n=0}^{\infty} A_n^2 \sum_{j=-n}^{n} \int_{\gamma_k} Y_{n,j}(\eta)\,\mathrm{d}\sigma(\eta)\,Y_{n,j}(\xi)$$

approximating the function $\tilde{S}$.

4.3 Numerical Tests

For testing the described spline approximation method we used phase data which were kindly provided by Jeannot Trampert (University of Utrecht) [73], [74]. Using that method we obtain phase velocity maps at 40, 50, 60, 80, 100, 130 and 150 seconds for Rayleigh and Love waves. We calculated the deviation "$\frac{dc}{c}$" from the PREM phase velocity. In all cases the Abel–Poisson kernel with the symbol $A_n^2 = e^{-0.2n} = h^n$ has been used. The parameter $h \in (0, 1)$ determines the "hat-width" of the kernel $K_{\mathcal{H}}$ (see Section 3.2.2), the closer h is to 1 the narrow the hat will be. It should be mentioned that the choice of an "optimal" h depends on the given data "density" and the a priori information about the smoothness of the approximated function. Currently there is no general method to determine an "optimal" symbol for each particular problem.

The integral terms representing the matrix components and the spline basis have been calculated approximately with the trapezoidal rule as described in Section 4.2.1. Moreover, a smoothing (regularization) of the linear equation system has been done (see Section 3.4), where in each case the smoothing parameter ρ has been determined using the L-curve method (see Section 3.4) and the identity matrix has been taken as a matrix D. We choose the smoothing parameters for the construction of L-curves such that every next parameter value is the double of the previous one. As we can see in Figures 4.9, 4.10 and 4.11 in our case L-curves have no sharp "corner", however they suggest an approximate region for the choice of the smoothing parameter. Due to this in each case (unless mentioned otherwise) of the global spline approximation we choose the same smoothing parameter $\rho = 0.123$. In each velocity map N indicates the number of used ray paths.

For comparison purposes we have constructed the spherical harmonic approximation for some phases as well (see Figures 4.13 to 4.18), using the same data as for the corresponding phase in spline approximation. Spherical harmonic approximations are constructed using the real spherical harmonics (up to degree $L = 39$) defined by (1.4) and applying a standard least-squares algorithm (see e.g. [71], [73]). In order to reduce the so-called ringing effect (see e.g. [73]) an $(L+1)^2 \times (L+1)^2$ diagonal matrix C_m given by $(C_m^{-1})_{j,j} = \lambda[l(l+1)]^2$ has been taken as an a priori model covariance matrix, where j is the index numbering the

$(L+1)^2$ coefficients, l is the degree of the corresponding spherical harmonic and λ is a smoothing parameter. In this case also the smoothing parameter λ has been determined using the L-curve method (see Figure 4.12).
The obtained phase velocity maps (see Figures 4.2 to 4.8) in comparison with the corresponding maps obtained via the spherical harmonic approximation method (see Figures 4.13 to 4.18 and also [17], [73], [74]) have similar structure, however, as further tests (with the synthetic data sets) show splines allow more "accurate" reconstruction. The advantages of our spline method are particularly visible in the tests with local/localized models (see Figures 4.32 and 4.25).
It should be mentioned that we do not claim that the chosen smoothing parameter ρ is the "optimal" one. For example the phase velocity maps in [17], [73], [74] are visually more "smooth" than our ones. However, if an a priori information about the smoothness of a model is known the desired smoothness degree can be obtained by manipulating the parameter ρ (see e.g. Figure 4.1 vs Figure 4.5(a)).

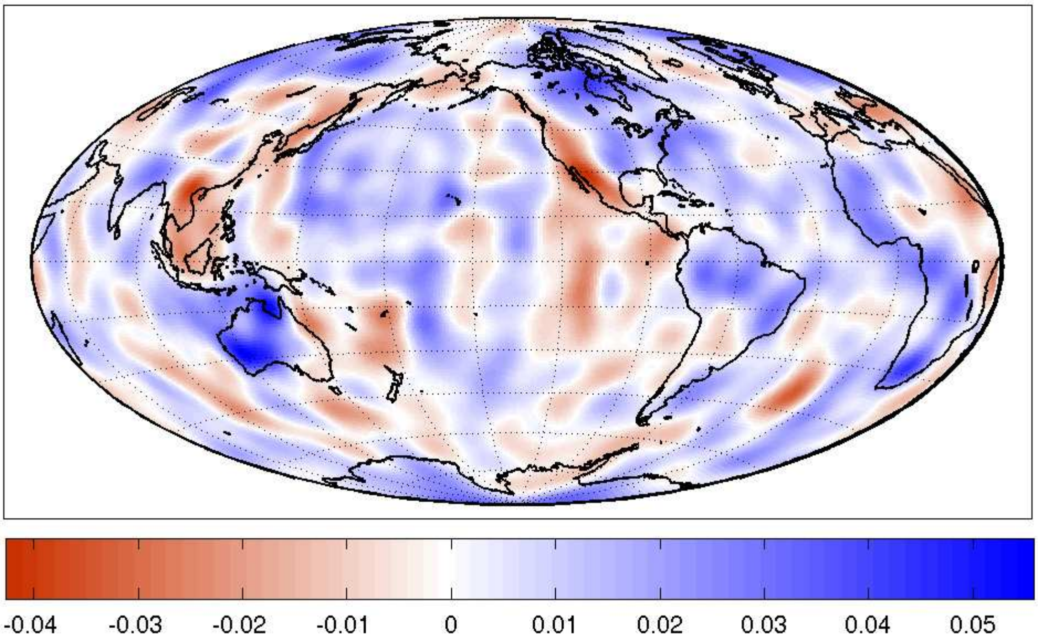
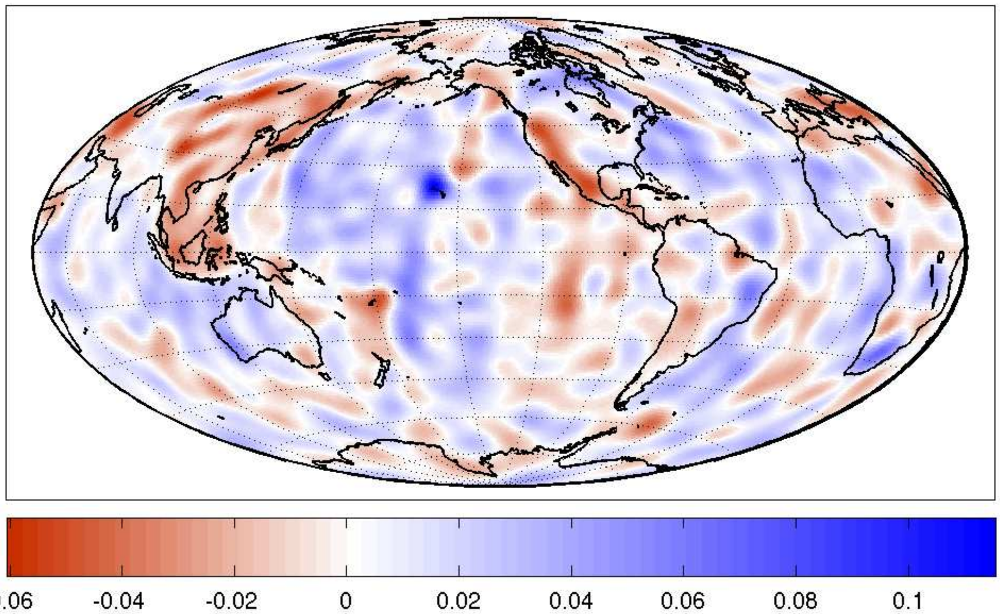
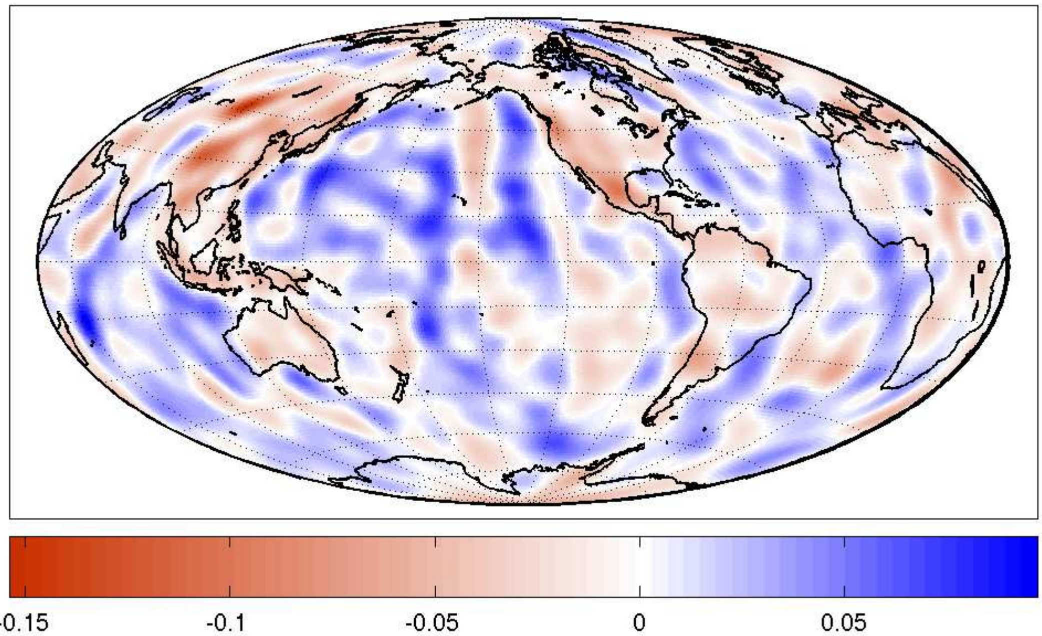


Figure 4.1: Rayleigh wave phase velocity maps at 80 seconds, with $N = 8490$, $\rho = 0.491$ obtained using the spline approximation method

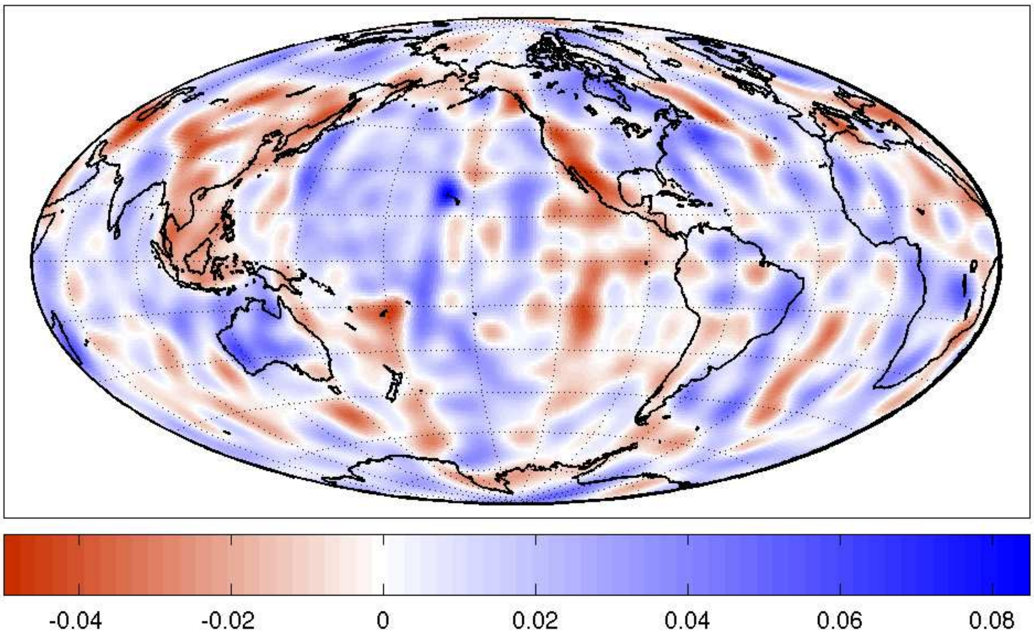


(a) Rayleigh wave phase velocity map at 40 seconds, with $N = 8433$, $\rho = 0.123$

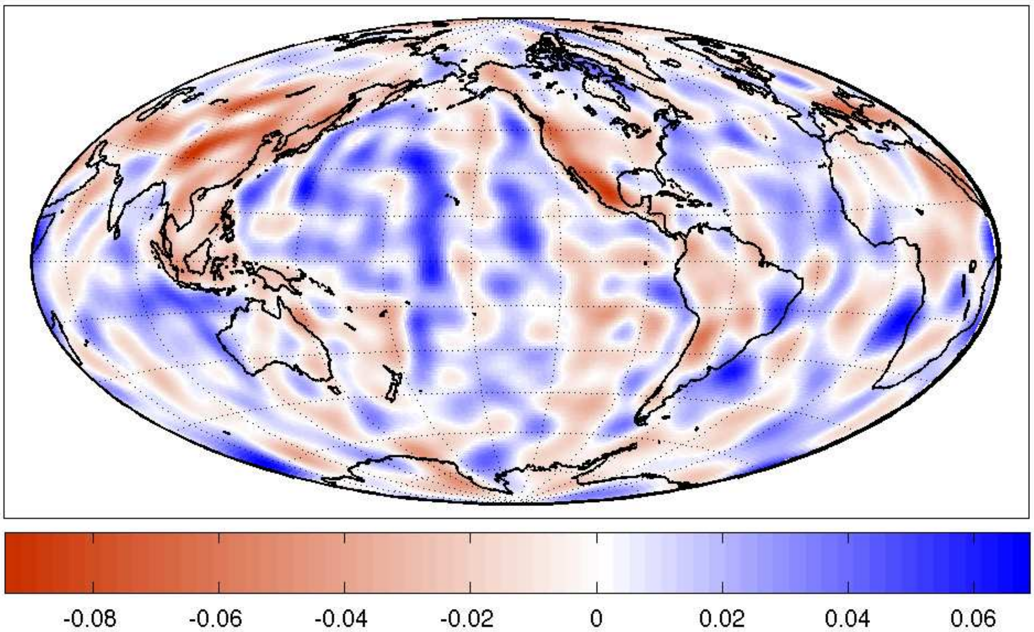


(b) Love wave phase velocity map at 40 seconds, with $N = 8022$, $\rho = 0.123$

Figure 4.2: Rayleigh and Love wave phase velocity maps at 40 seconds obtained using the spline approximation method

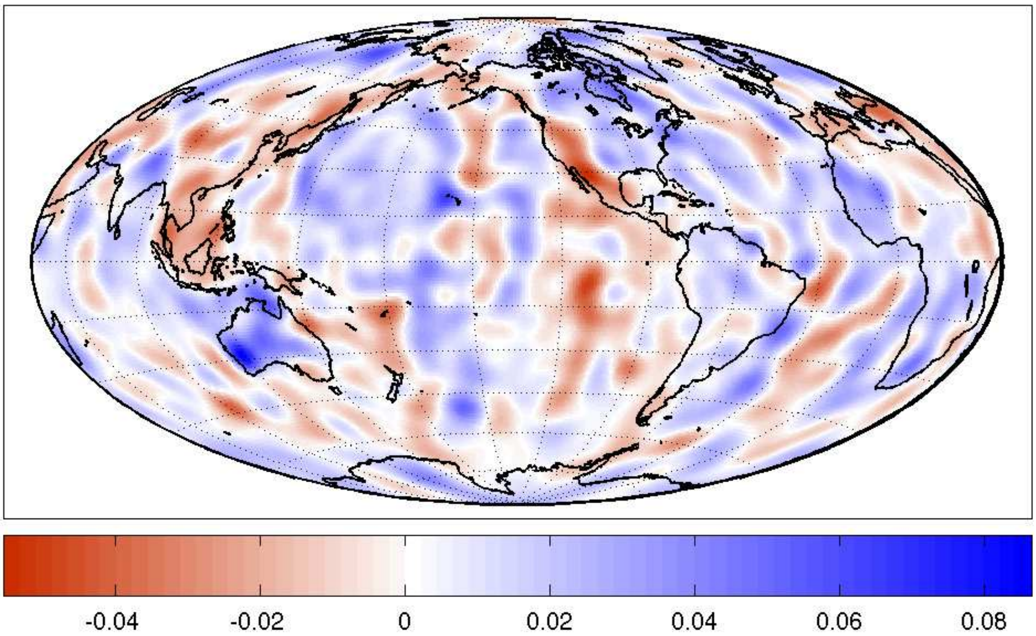


(a) Rayleigh wave phase velocity map at 50 seconds, with $N = 8459$, $\rho = 0.123$

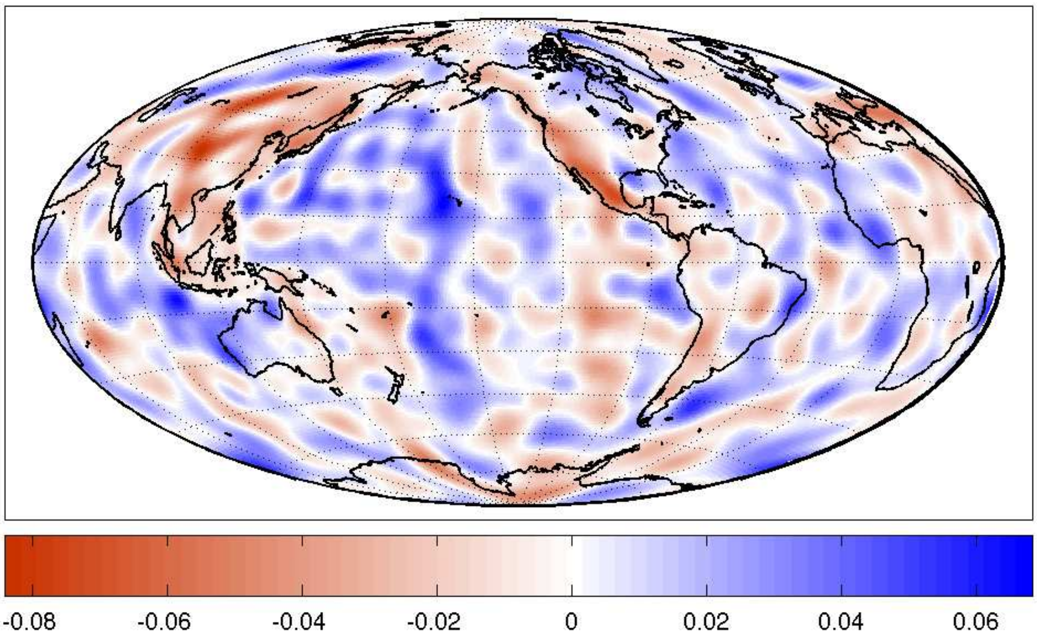


(b) Love wave phase velocity map at 50 seconds, with $N = 7995$, $\rho = 0.123$

Figure 4.3: Rayleigh and Love wave phase velocity maps at 50 seconds obtained using the spline approximation method

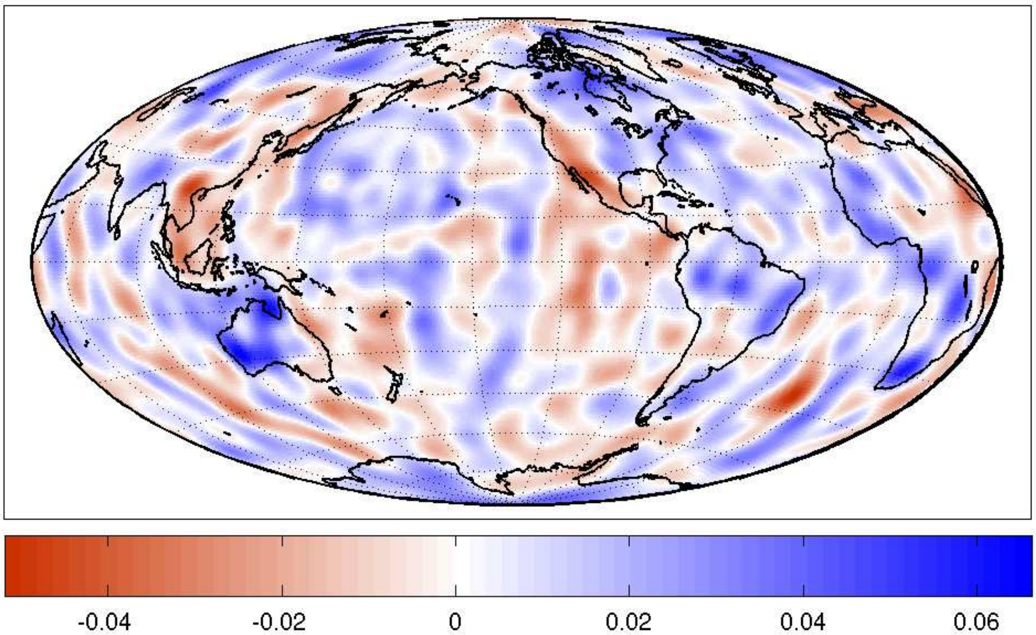


(a) Rayleigh wave phase velocity map at 60 seconds, with $N = 8521$, $\rho = 0.123$

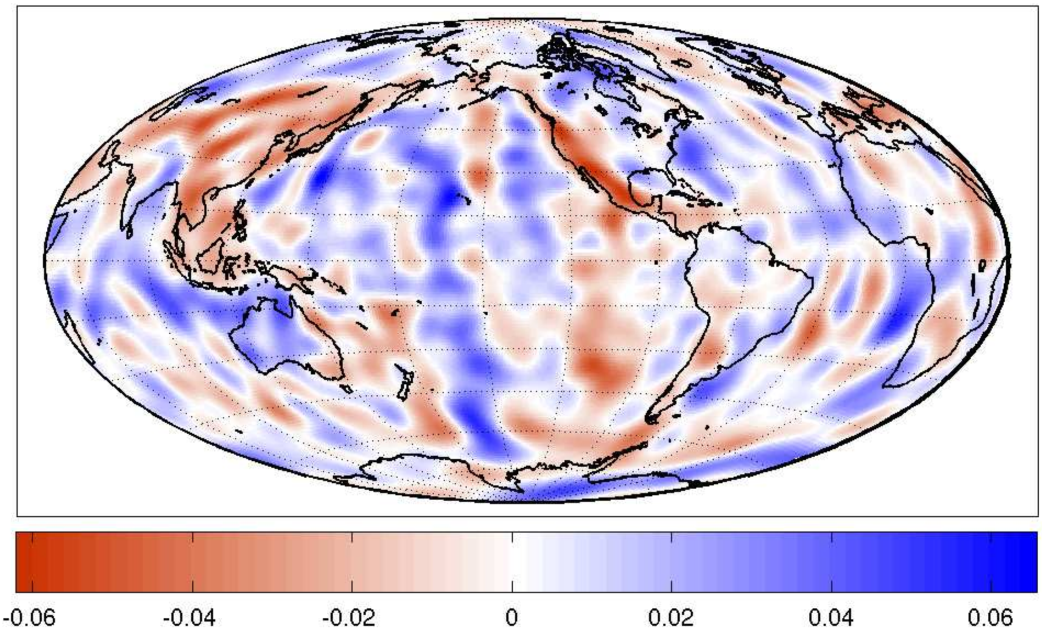


(b) Love wave phase velocity map at 60 seconds, with $N = 8062$, $\rho = 0.123$

Figure 4.4: Rayleigh and Love wave phase velocity maps at 60 seconds obtained using the spline approximation method

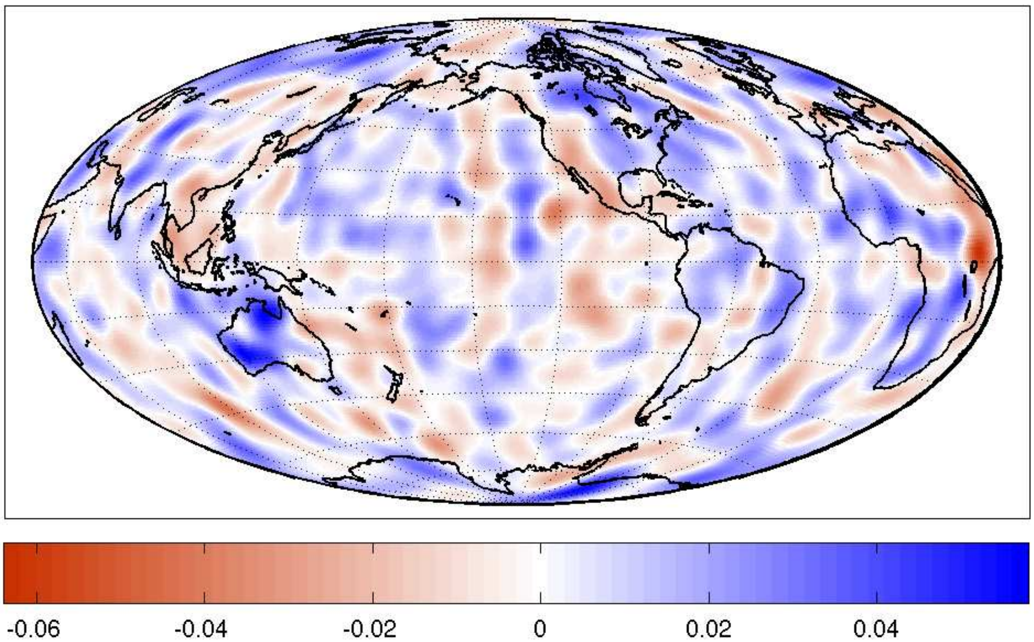


(a) Rayleigh wave phase velocity map at 80 seconds, with $N = 8490$, $\rho = 0.123$

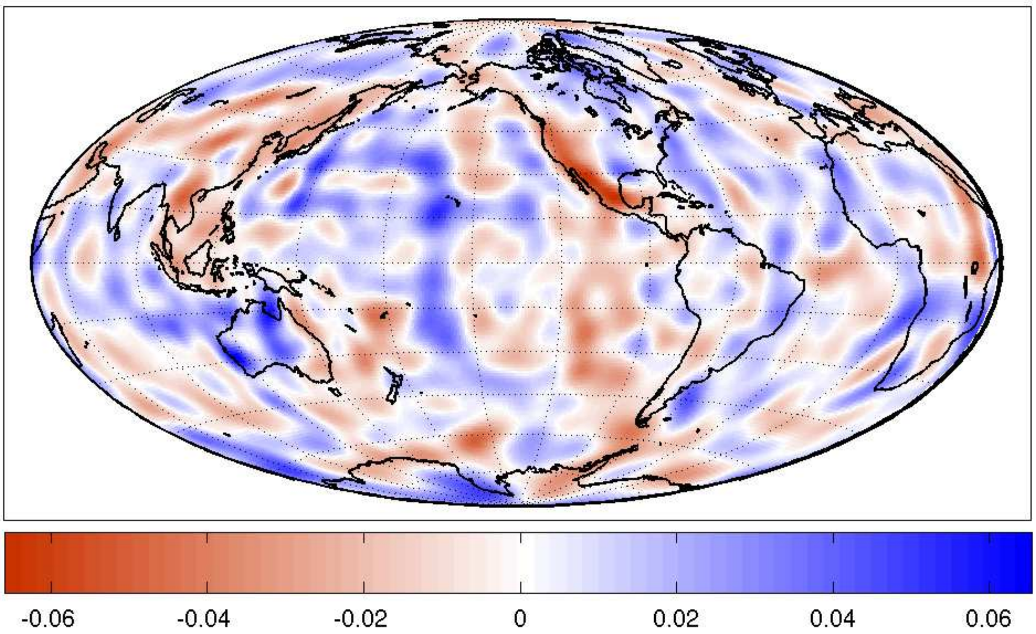


(b) Love wave phase velocity map at 80 seconds, with $N = 8089$, $\rho = 0.123$

Figure 4.5: Rayleigh and Love wave phase velocity maps at 80 seconds obtained using the spline approximation method

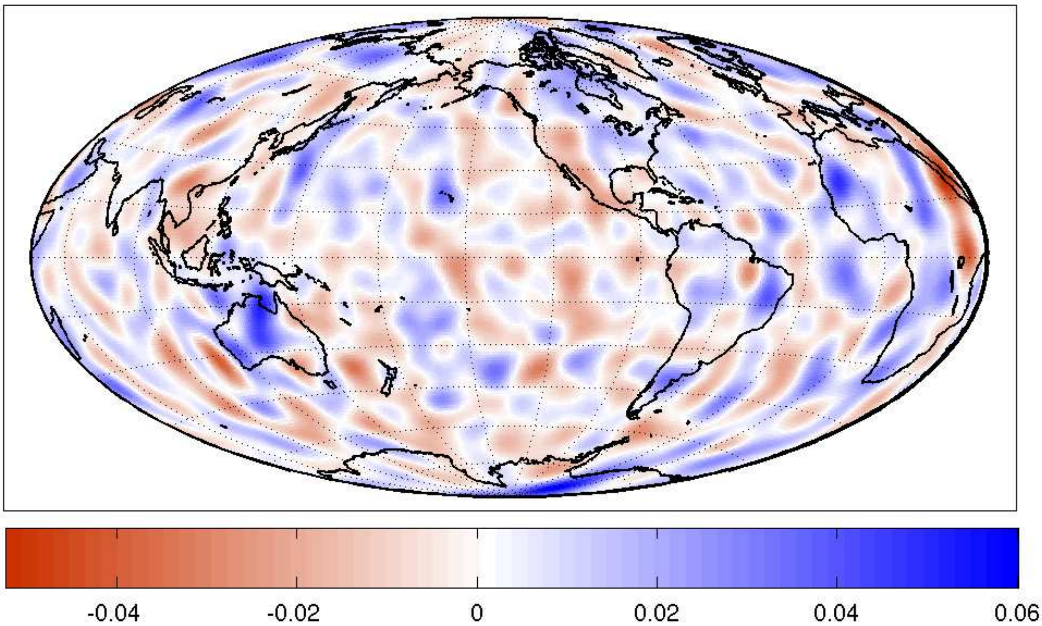


(a) Rayleigh wave phase velocity map at 100 seconds, with $N = 8490$, $\rho = 0.123$

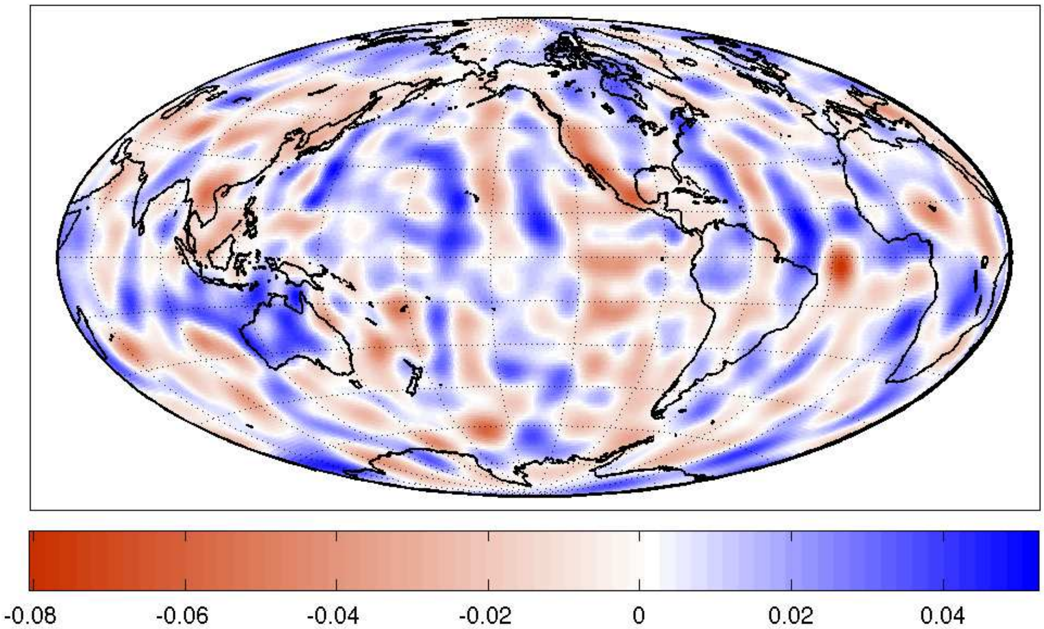


(b) Love wave phase velocity map at 100 seconds, with $N = 8600$, $\rho = 0.123$

Figure 4.6: Rayleigh and Love wave phase velocity maps at 100 seconds obtained using the spline approximation method

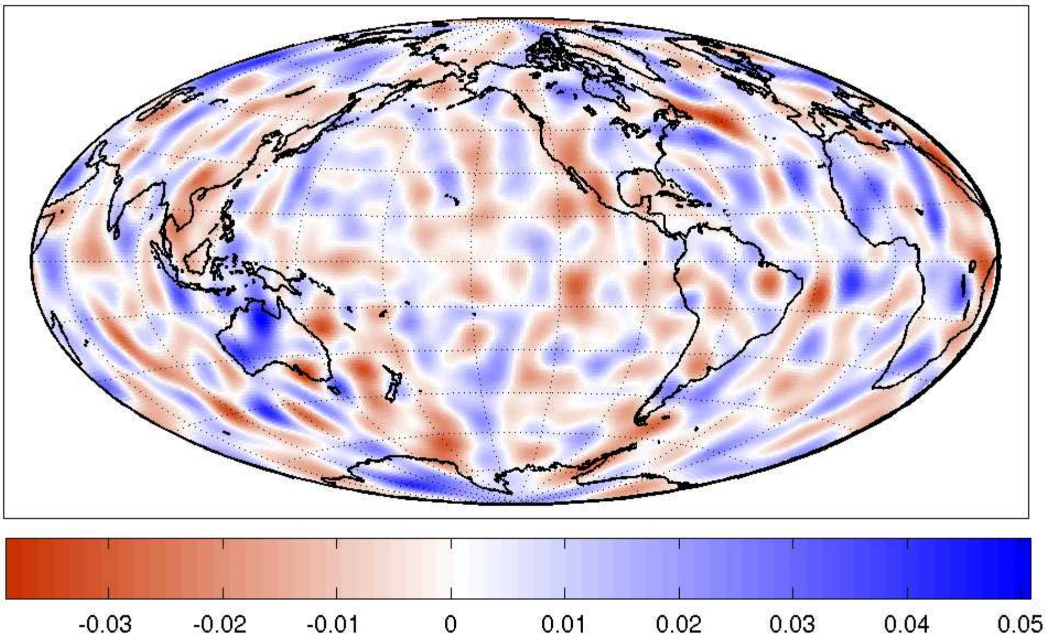


(a) Rayleigh wave phase velocity map at 130 seconds. with $N = 8545$, $\rho = 0.123$

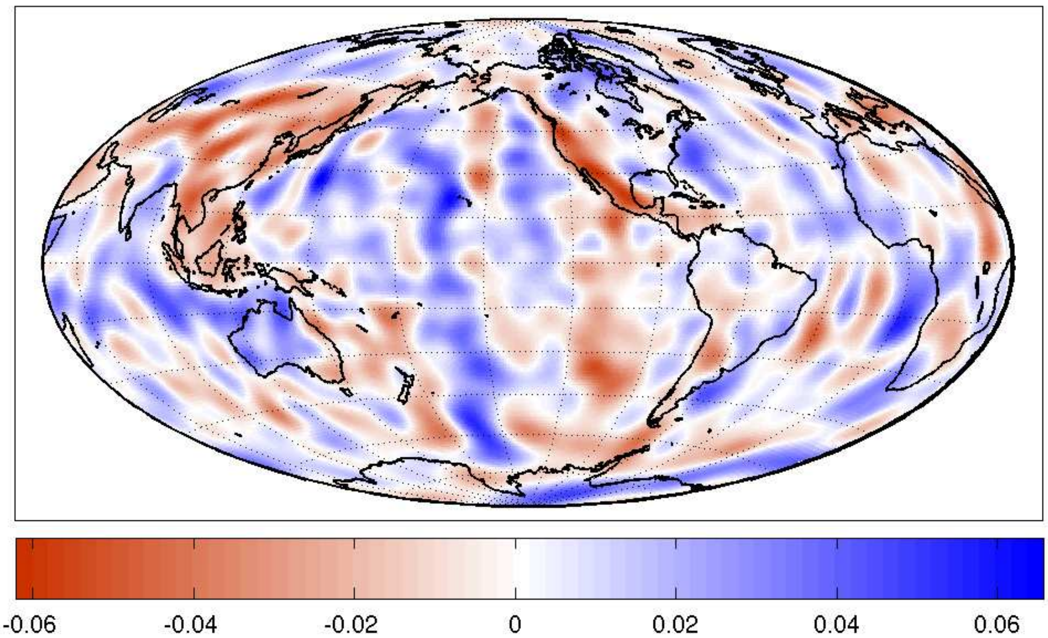


(b) Love wave phase velocity map at 130 seconds, with $N = 7941$, $\rho = 0.123$

Figure 4.7: Rayleigh and Love wave phase velocity maps at 130 seconds obtained using the spline approximation method

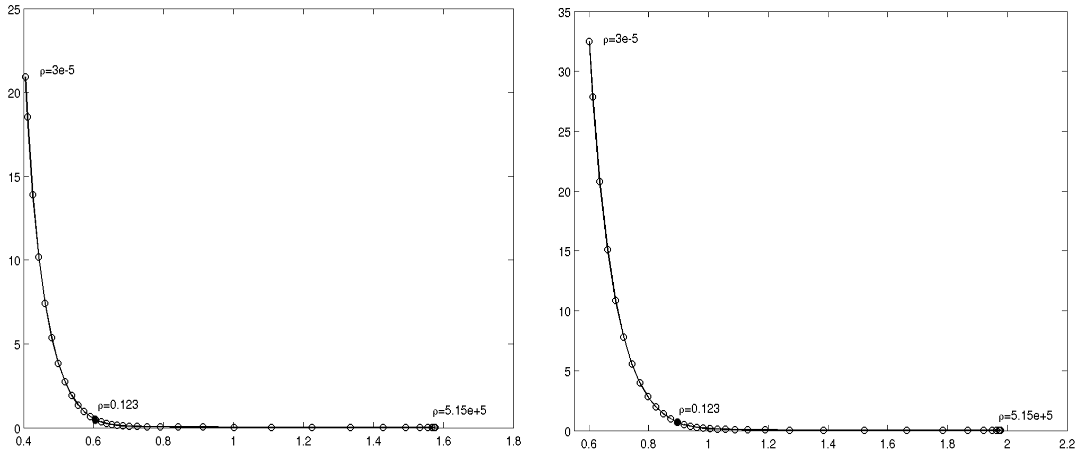


(a) Rayleigh wave phase velocity map at 150 seconds, with $N = 8424$, $\rho = 0.123$



(b) Love wave phase velocity map at 150 seconds, with $N = 8100$, $\rho = 0.123$

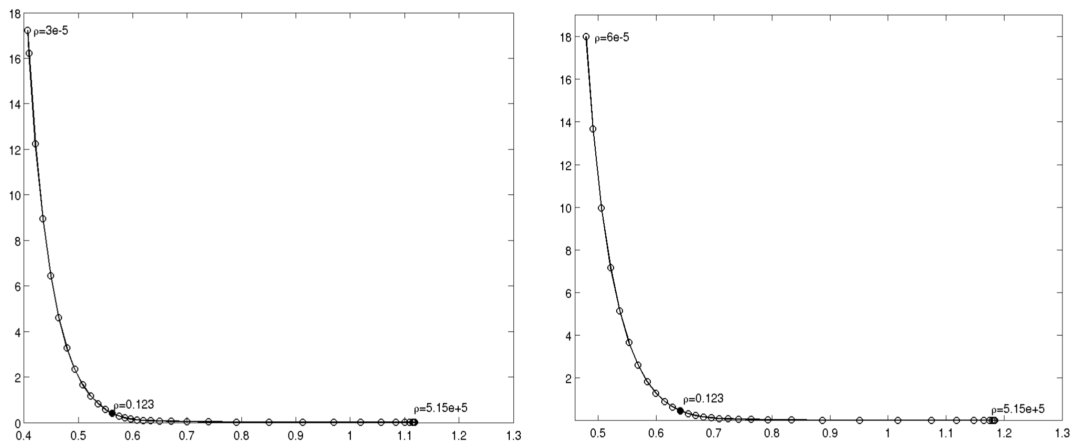
Figure 4.8: Rayleigh and Love wave phase velocity maps at 150 seconds obtained using the spline approximation method



(a) L-curve for Rayleigh waves at 40 s

(b) L-curve for Love waves at 40 s

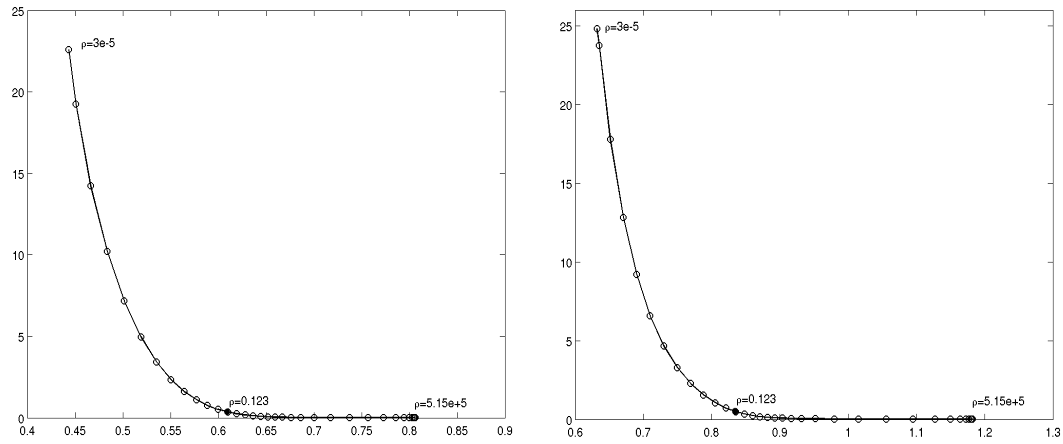
Figure 4.9: L-curve corresponding to the spline approximation of Rayleigh (left) and Love (right) wave phase velocity at 40 seconds



(a) L-curve for Rayleigh waves at 80 s

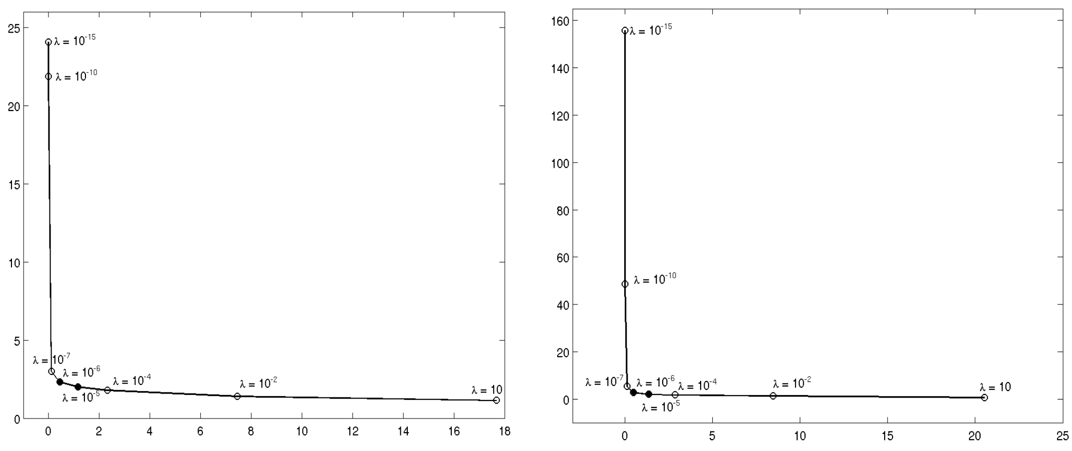
(b) L-curve for Love waves at 80 s

Figure 4.10: L-curve corresponding to the spline approximation of Rayleigh (left) and Love (right) wave phase velocity at 80 seconds



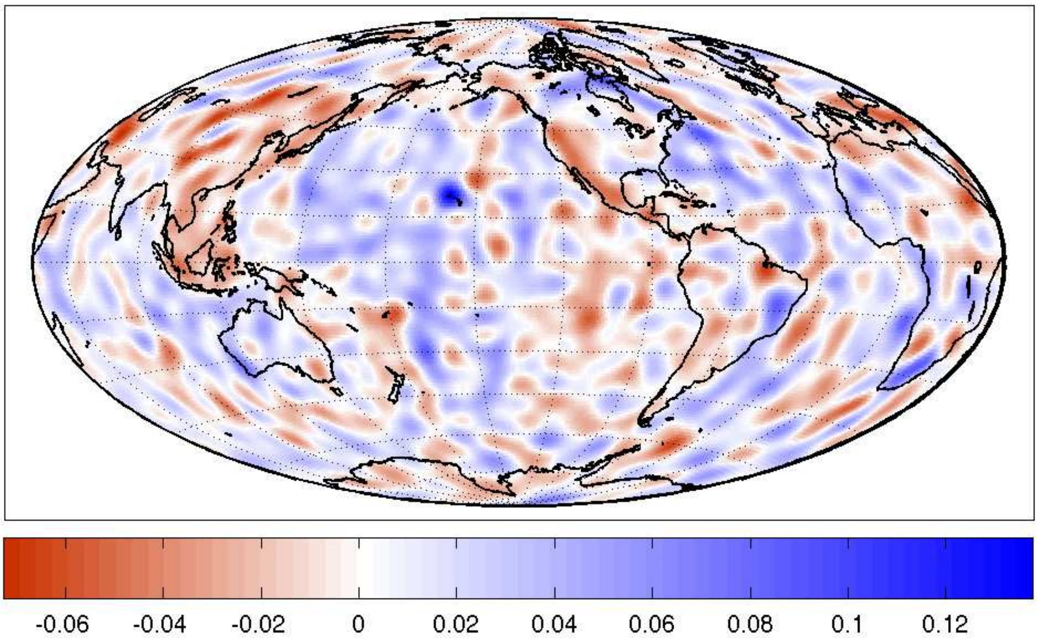
(a) L-curve for Rayleigh waves at 150 s (b) L-curve for Love waves at 150 s

Figure 4.11: L-curve corresponding to the spline approximation of Rayleigh (left) and Love (right) wave phase velocity at 150 seconds

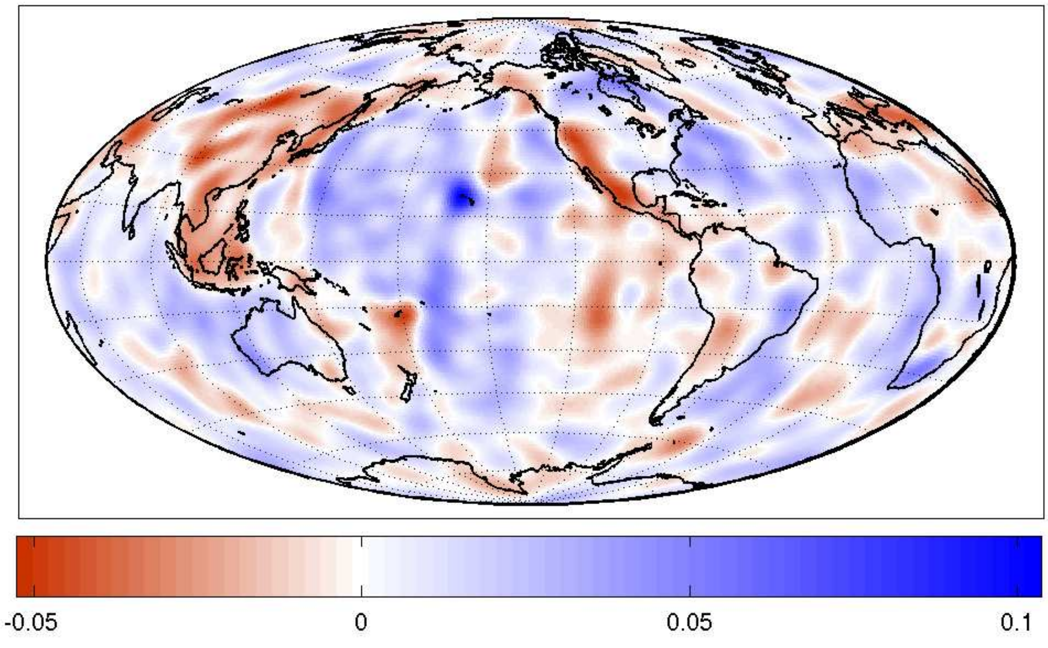


(a) L-curve for Rayleigh waves at 80 s (b) L-curve for Love waves at 80 s

Figure 4.12: L-curve corresponding to the spherical harmonic approximation of Rayleigh (left) and Love (right) wave phase velocity at 80 seconds

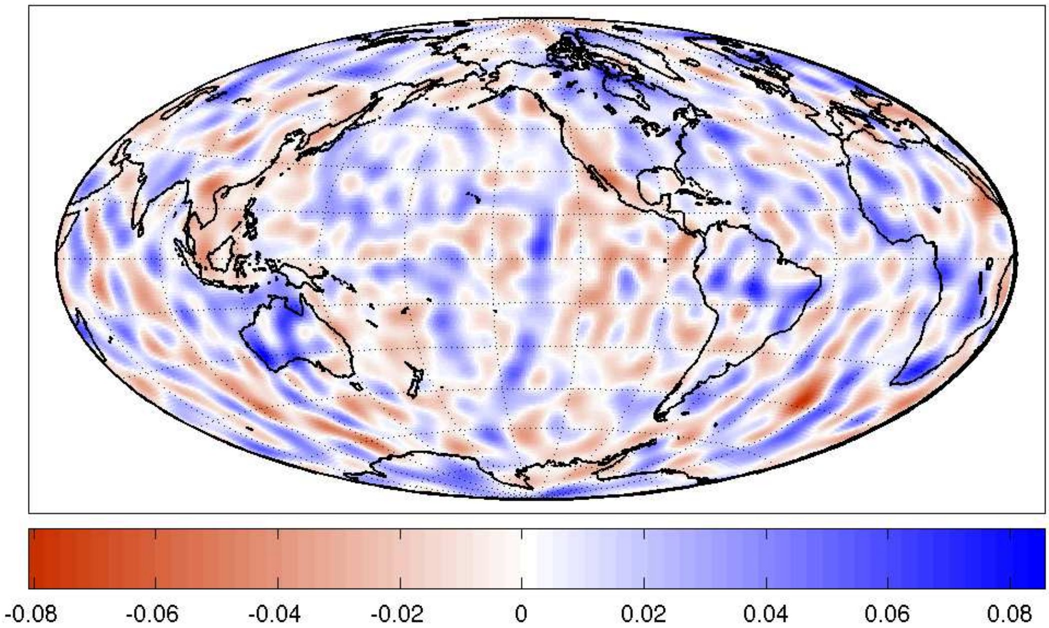


(a) Rayleigh wave phase velocity map at 40 seconds, with $\lambda = 10^{-6}$

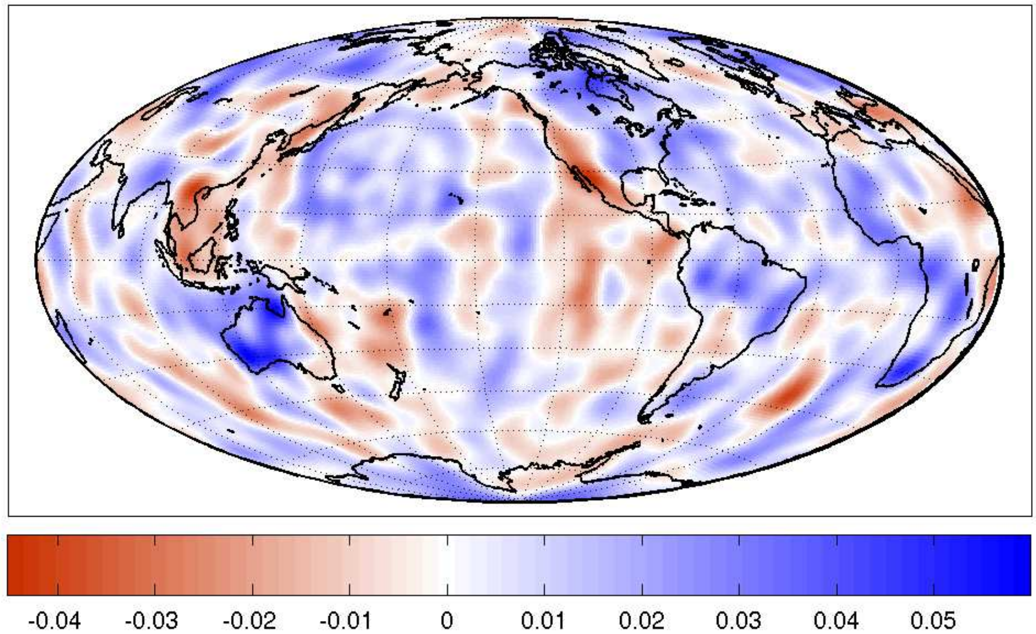


(b) Rayleigh wave phase velocity map at 40 seconds, with $\lambda = 10^{-5}$

Figure 4.13: Rayleigh wave phase velocity maps (with different smoothing parameters) at 40 seconds obtained using the spherical harmonic approximation method

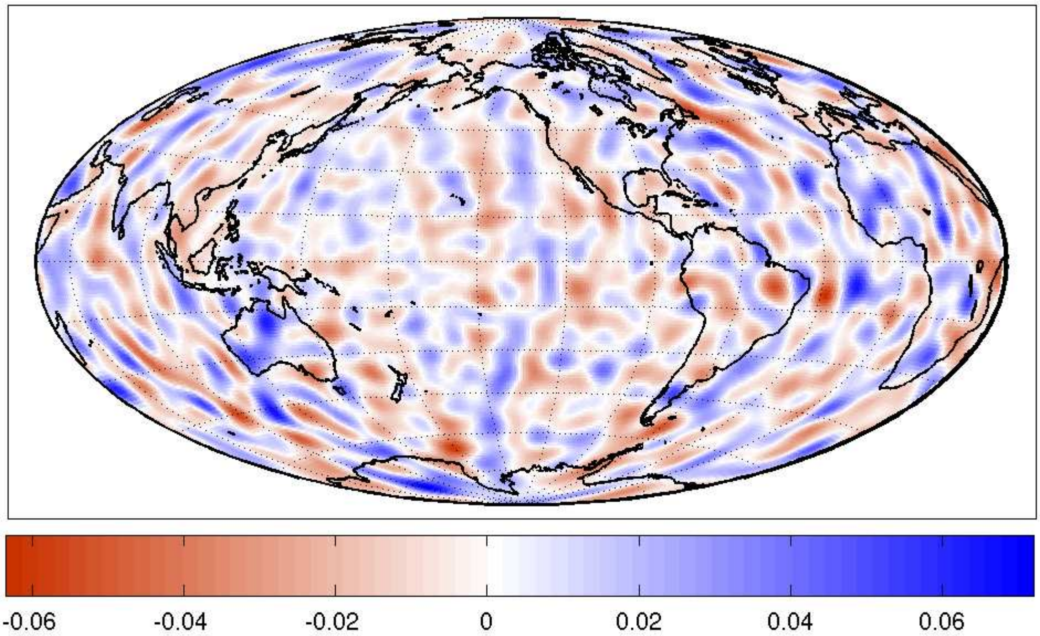


(a) Rayleigh wave phase velocity map at 80 seconds, with $\lambda = 10^{-6}$

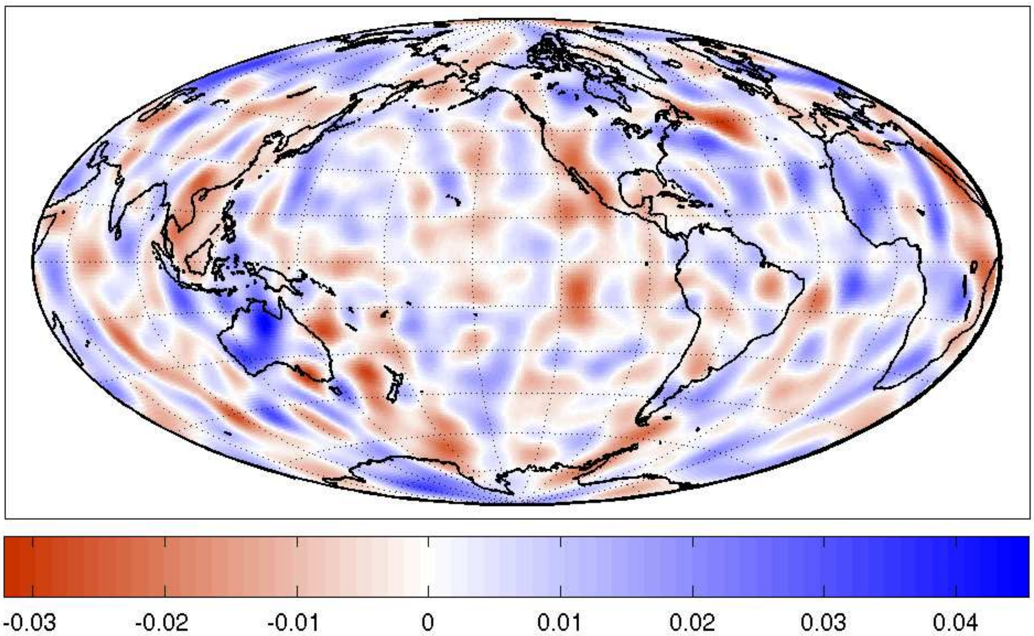


(b) Rayleigh wave phase velocity map at 80 seconds, with $\lambda = 10^{-5}$

Figure 4.14: Rayleigh wave phase velocity maps (with different smoothing parameters) at 80 seconds obtained using the spherical harmonic approximation method

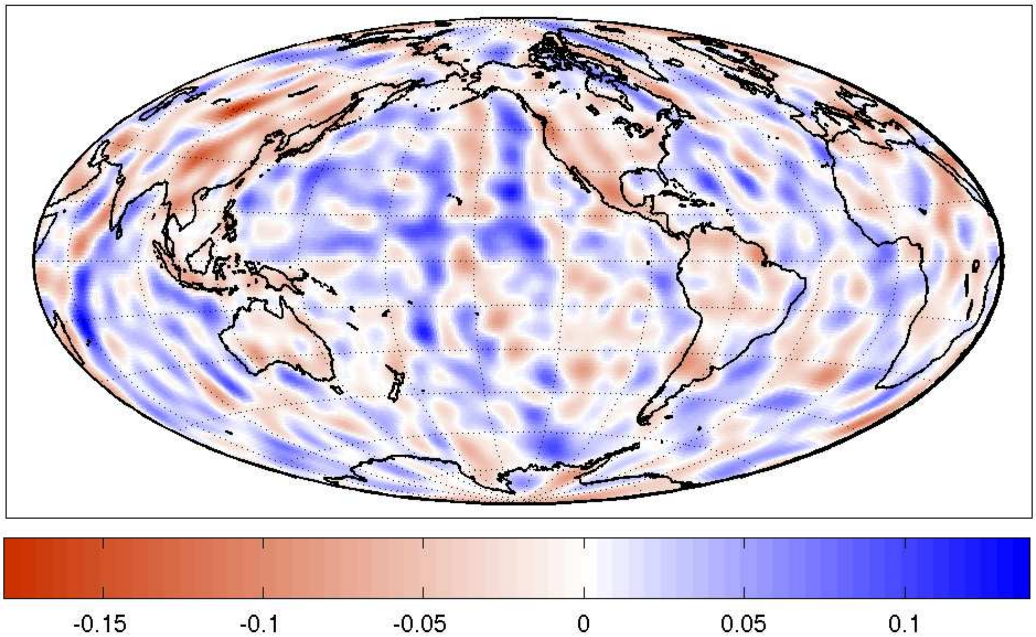


(a) Rayleigh wave phase velocity map at 150 seconds, with $\lambda = 10^{-6}$

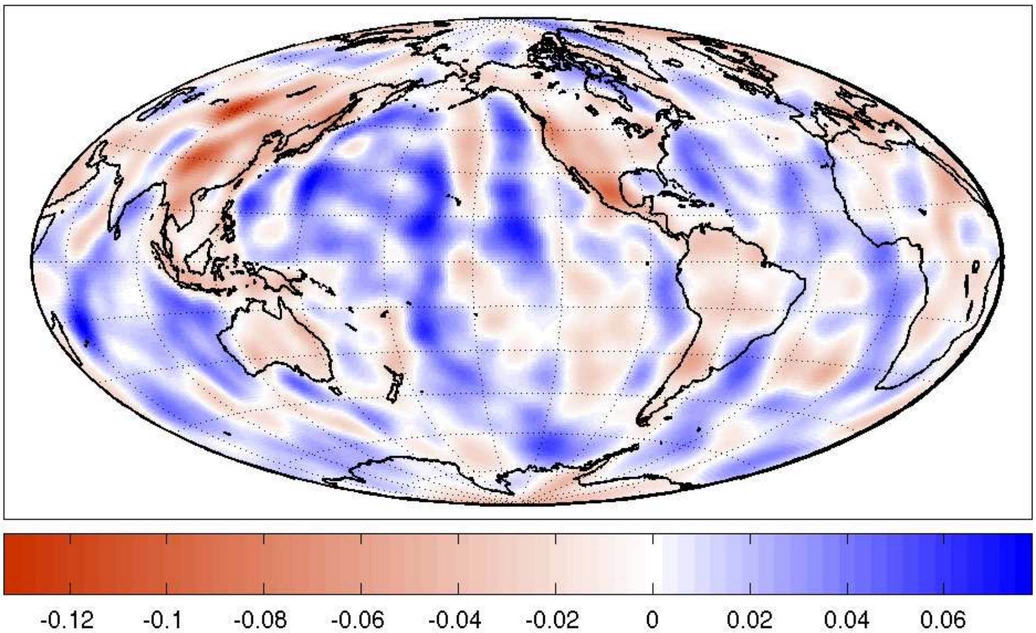


(b) Rayleigh wave phase velocity map at 150 seconds, with $\lambda = 10^{-5}$

Figure 4.15: Rayleigh wave phase velocity maps (with different smoothing parameters) at 150 seconds obtained using the spherical harmonic approximation method

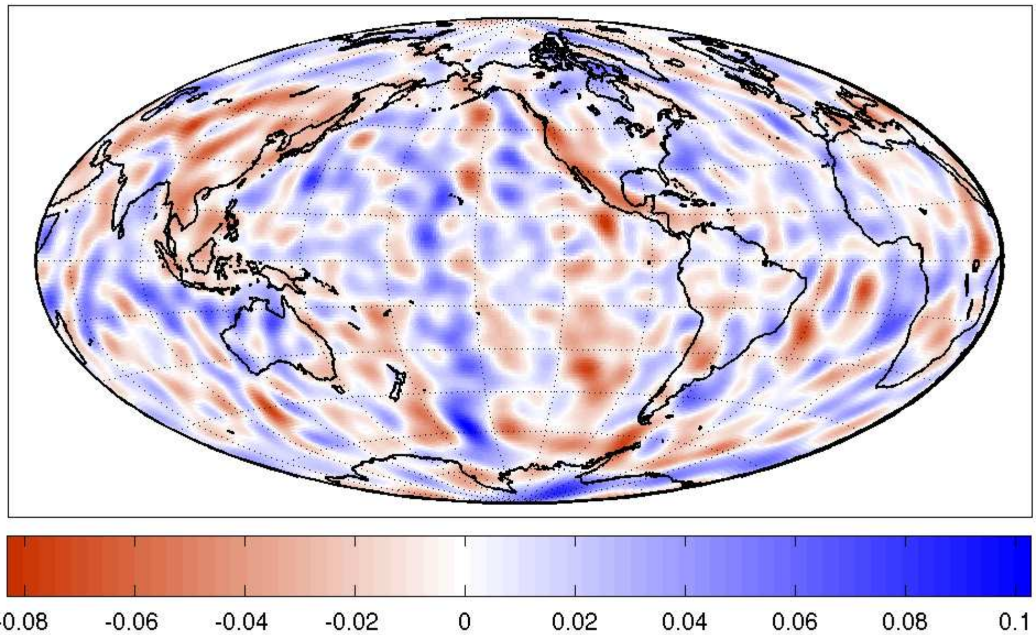


(a) Love wave phase velocity map at 40 seconds, with $\lambda = 10^{-6}$

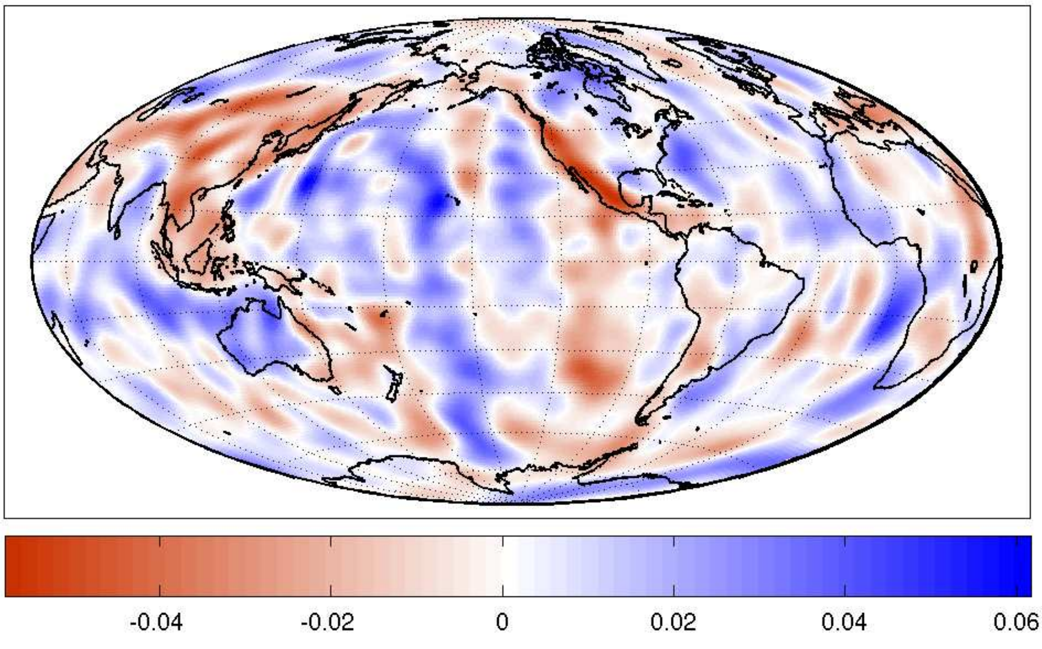


(b) Love wave phase velocity map at 40 seconds, with $\lambda = 10^{-5}$

Figure 4.16: Love wave phase velocity maps (with different smoothing parameters) at 40 seconds obtained using the spherical harmonic approximation method

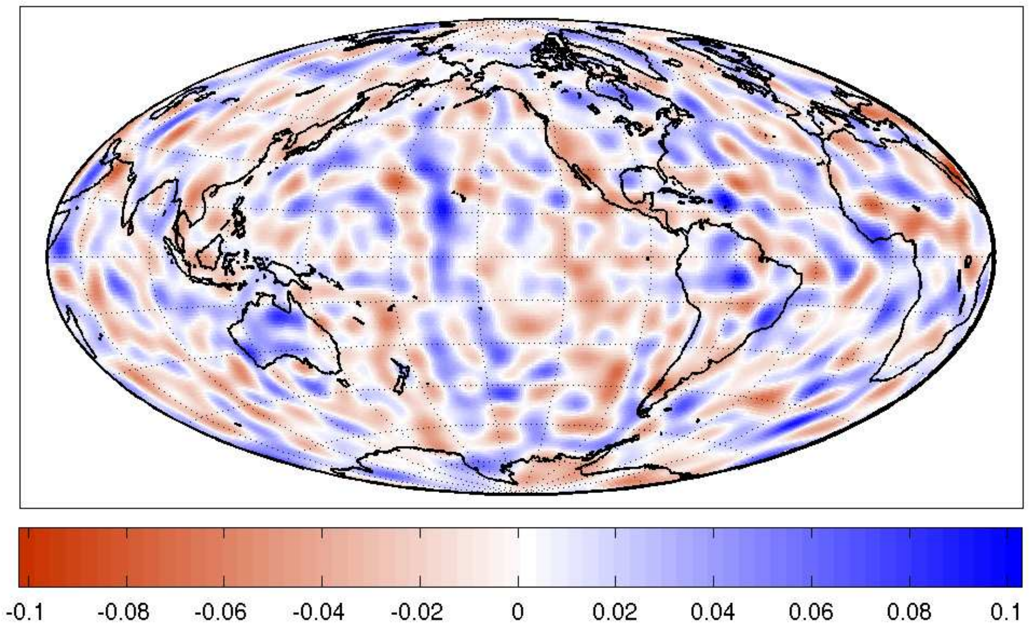


(a) Love wave phase velocity map at 80 seconds, with $\lambda = 10^{-6}$

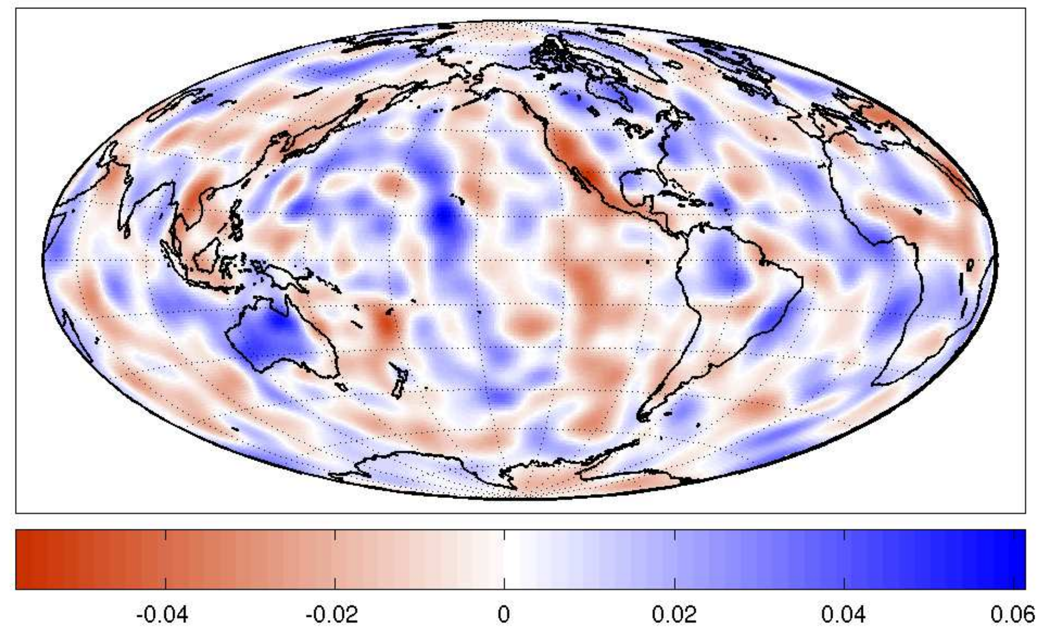


(b) Love wave phase velocity map at 80 seconds, with $\lambda = 10^{-5}$

Figure 4.17: Love wave phase velocity maps (with different smoothing parameters) at 80 seconds obtained using the spherical harmonic approximation method



(a) Love wave phase velocity map at 150 seconds, with $\lambda = 10^{-6}$



(b) Love wave phase velocity map at 150 seconds, with $\lambda = 10^{-5}$

Figure 4.18: Love wave phase velocity maps (with different smoothing parameters) at 150 seconds obtained using the spherical harmonic approximation method

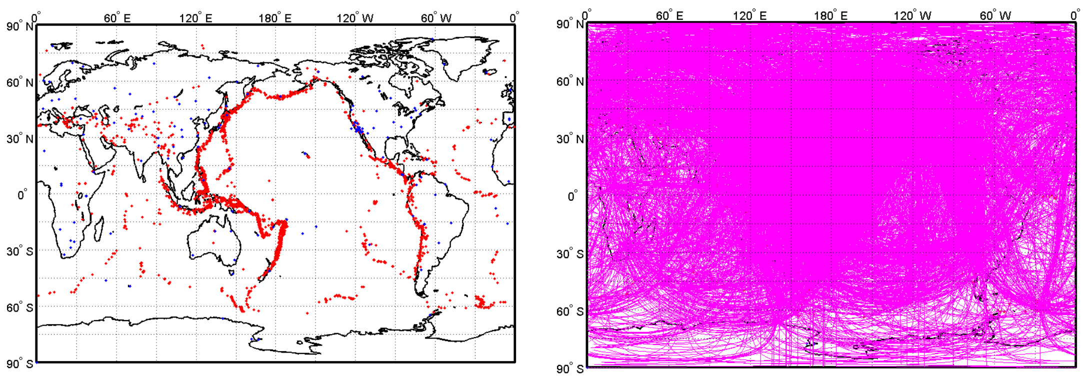
To verify our spline method some tests with synthetic data sets, namely the so-called checkerboard tests, a test by adding random noise to the initial traveltime data and a test with a so-called hidden object, have been done as well.
All these tests have been done using spline and spherical harmonic approximation methods. The results show that in all cases (in particular for reconstructions of local/localized models) the spline approximation is more accurate in the sense that the so-called root-mean-square (RMS) of the difference of the initial model and the reconstruction via splines is smaller than the RMS for the corresponding reconstruction via spherical harmonics (see Figures 4.23, 4.25 to 4.29 and 4.32). It should be mentioned that here all functions are calculated and plotted such that one point corresponds to each pair of colatitude and longitude, i.e. for example global maps are calculated and plotted on a 180×360 point grid. Hence, we obtain the difference of the initial model and the reconstruction (i.e. the reconstruction error) in a matrix form. Note that for a matrix $A = \{a_{i,j}\}_{i=1,\dots,n; j=1,\dots,m}$ the RMS is calculated by the following formula

$$RMS(A) = \frac{\sqrt{\sum_{i=1}^{n} \sum_{j=1}^{m} a_{i,j}^2}}{\sqrt{nm}}.$$

Tests with the checkerboard models include the reconstruction of the model presented in Figure 4.21(a) using the rays in Figure 4.19 (global case) (see Figure 4.22) and the reconstruction of the model presented in Figure 4.21(b) at Australia and the neighborhood using rays in Figure 4.20 (local case) (see Figure 4.24), via splines and spherical harmonics. For the spherical harmonic reconstruction we took the smoothing parameter λ such that the corresponding RMS of the reconstruction error is minimal (see Table 4.3).
To see how the measurement errors affect the result, we add a random error of one percent to the traveltimes used to obtain the models in Figure 4.22 and recalculate the corresponding maps using spline (Figures 4.26 and 4.27) and spherical harmonic (Figures 4.28 and 4.29) approximation methods. The spline as well as the spherical harmonic reconstruction is presented for two different smoothing parameters, $\rho = 0.06$, $\rho = 0.25$, and respectively $\lambda = 10^{-5}$, $\lambda = 10^{-6}$. For the reconstructions with a bigger smoothing parameter the obtained maps (Figures 4.26 and 4.28) visually are closer to the original (Figure 4.21(a)), while for the reconstructions with a smaller smoothing parameter (Figures 4.27 and 4.29) the

corresponding RMS of the reconstruction error is smaller (see also Table 4.3). These results demonstrate that the "sensitivity" of our spline method to the measurement errors, at least, is not more than the corresponding "sensitivity" of the spherical harmonic approximation method.

Next we want to see how the changes of a model in some area affect the model elsewhere. For this purpose we obtain reconstructions of the velocity model in Figure 4.30 using spline (see Figures 4.31(a) and 4.32(a)) and spherical harmonic (see Figures 4.31(b) and 4.32(b)) approximation methods. Here also for the spherical harmonic reconstruction we took the smoothing parameter λ such that the corresponding RMS of the reconstruction error is minimal (see Table 4.3). As we can see from Figure 4.32, comparing with the spherical harmonic reconstruction, in case of spline reconstruction the error is more concentrated around the "hidden object". Moreover, for the spline reconstruction the corresponding RMS is smaller than for the spherical harmonic reconstruction.



(a) ray sources (red) and receivers (blue) (b) ray paths

Figure 4.19: ray sources, receivers and paths used for the calculations for Figure 4.5(a)

(a) global case

λ	$RMS(\Delta)$
10^{-5}	0.0563
10^{-6}	0.0504
10^{-7}	0.0483
10^{-8}	0.0497
10^{-9}	0.0539

(b) local case

λ	$RMS(\Delta)$
10^{-5}	0.0907
10^{-6}	0.0634
10^{-7}	0.0336
10^{-8}	0.0273
10^{-9}	0.0271
10^{-10}	0.0276
10^{-12}	0.0295

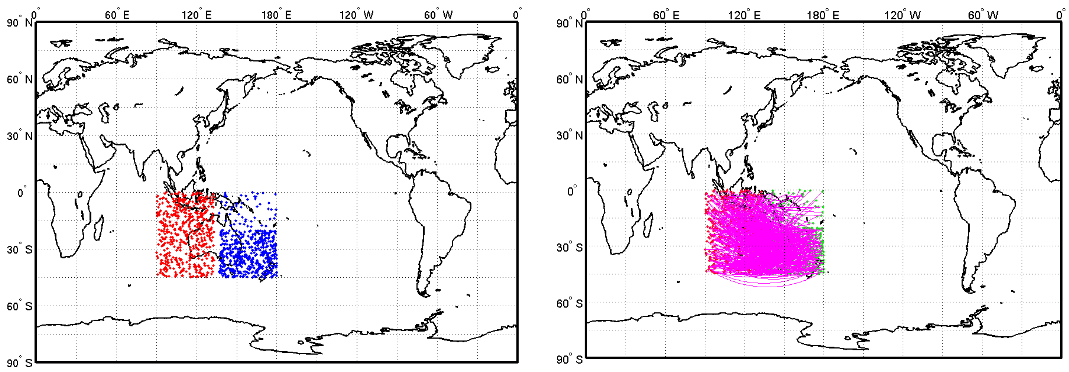
Table 4.1: RMS table for the spherical harmonic reconstruction of checkerboard models in Figure 4.21(a) (left) and in Figure 4.21(b) (right), where λ is the smoothing parameter, and Δ is the reconstruction error

λ	$RMS(\Delta)$
10^{-3}	0.0881
10^{-4}	0.0704
10^{-5}	0.0580
10^{-6}	0.0554
10^{-7}	0.0646
10^{-8}	0.1493

Table 4.2: RMS table for the spherical harmonic reconstruction of the checkerboard model in Figure 4.21(a), where a random error of 1% has been added to the corresponding traveltimes

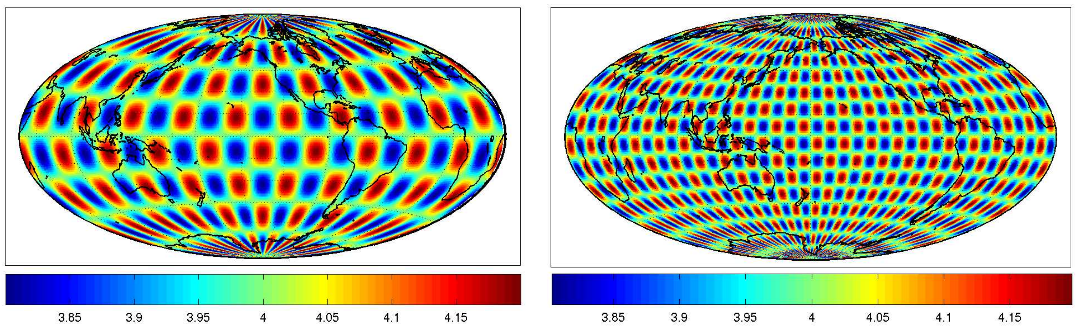
λ	$RMS(\Delta)$
10^{-3}	0.0406
10^{-4}	0.0341
10^{-5}	0.0321
10^{-6}	0.0324
10^{-7}	0.0382

Table 4.3: RMS table for the spherical harmonic reconstruction of the velocity model in Figure 4.30



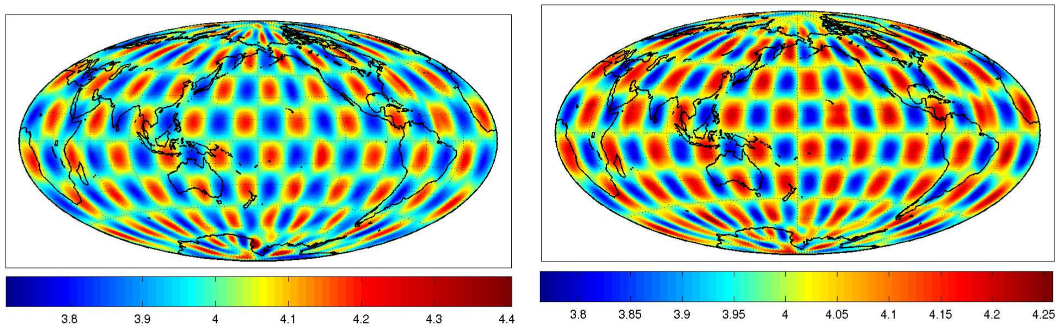
(a) ray sources (red) and receivers (blue) (b) ray paths

Figure 4.20: sources, receivers and paths of 500 synthetic rays



(a) $a = 8$, $b = 10$ (b) $a = 16$, $b = 20$

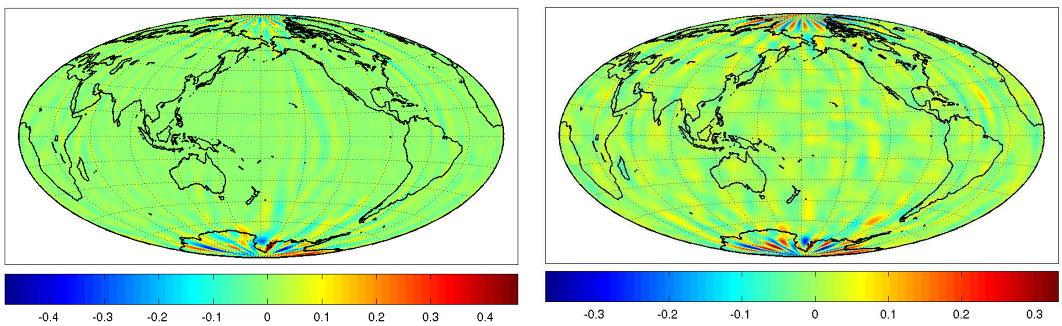
Figure 4.21: synthetic (checkerboard) velocity model given by the formula $F(\theta, \phi) = 4 + 0.2 \sin(a\theta) \sin(b\phi)$, with $\theta \in [0, \pi]$, $\phi \in [0, 2\pi)$



(a) spline reconstruction with $\rho = 10^{-4}$.

(b) spherical harmonic reconstruction with $\lambda = 10^{-7}$

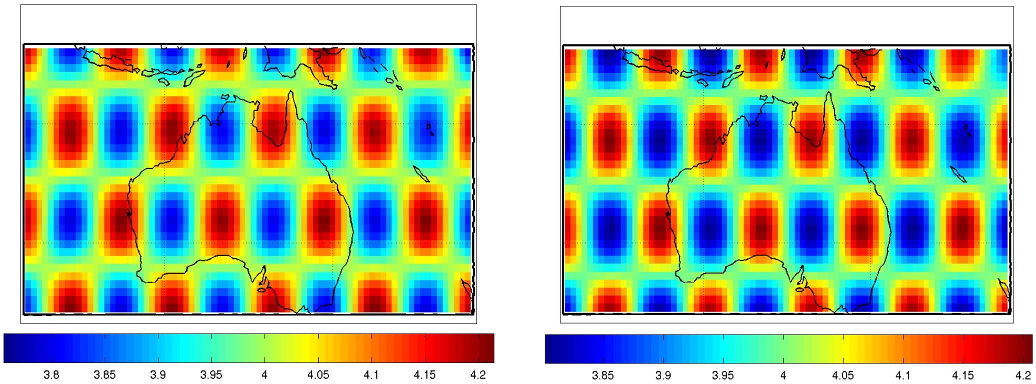
Figure 4.22: reconstructions of the synthetic velocity model presented in Figure 4.21(a) (global case) by the spline (left) and the spherical harmonic (right) approximation method, respectively



(a) error of spline reconstruction, where $RMS(\Delta) = 0.0438$

(b) error of spherical harmonic reconstruction, where $RMS(\Delta) = 0.0483$

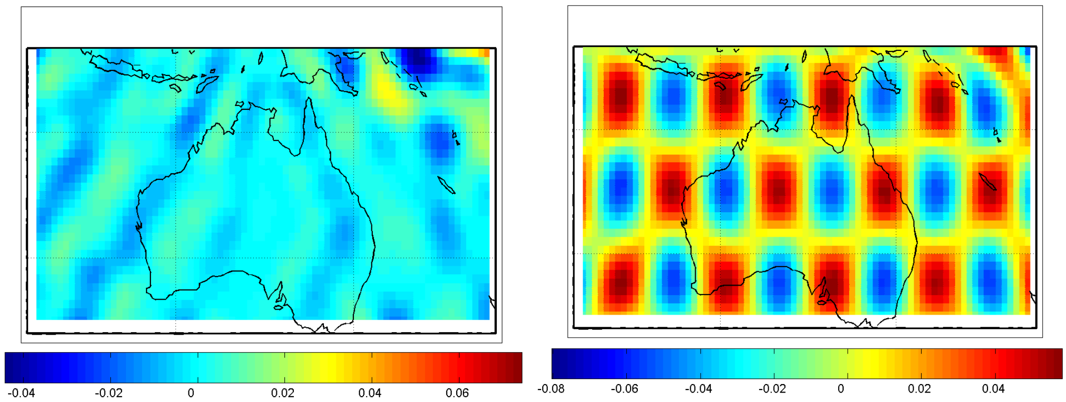
Figure 4.23: errors of the reconstructions presented in Figure 4.22



(a) spline reconstruction with $\rho = 10^{-5}$

(b) spherical harmonic reconstruction with $\lambda = 10^{-9}$

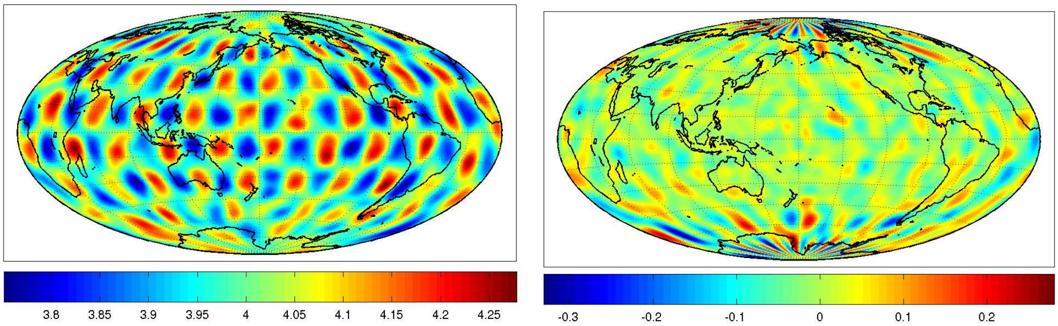
Figure 4.24: reconstructions of the synthetic velocity model presented in Figure 4.21(b) (local case) by the spline (left) and the spherical harmonic (right) approximation method, respectively



(a) error of spline reconstruction, where $RMS(\Delta) = 0.005$

(b) error of spherical harmonic reconstruction, where $RMS(\Delta) = 0.0271$

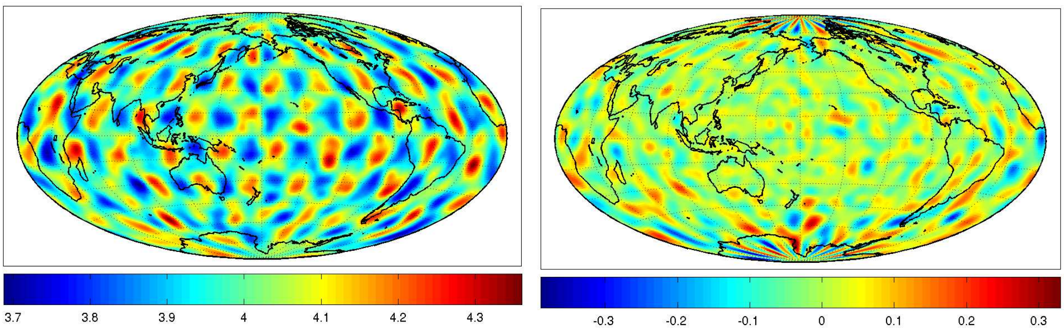
Figure 4.25: errors of the reconstructions presented in Figure 4.24



(a) spline reconstruction with $\rho = 0.25$

(b) error of spline reconstruction where $RMS(\Delta) = 0.0568$

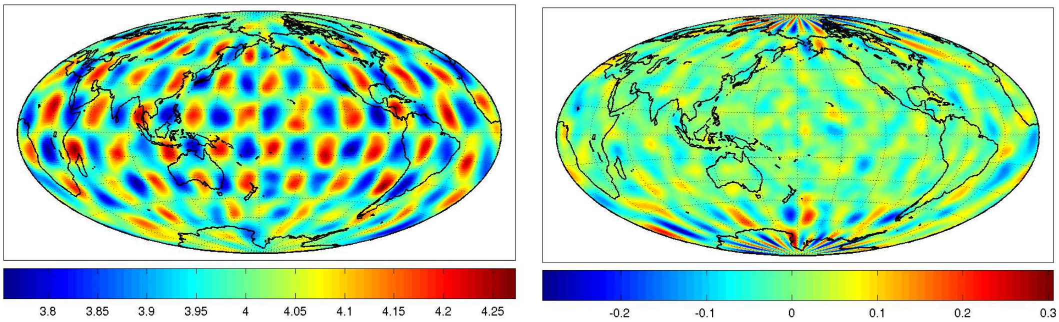
Figure 4.26: spline reconstruction (left) with $\rho = 0.25$, and corresponding error (right), of the velocity model in Figure 4.21, with 1% random error in the traveltimes



(a) spline reconstruction, with $\rho = 0.06$

(b) error of spline reconstruction, where $RMS(\Delta) = 0.0542$

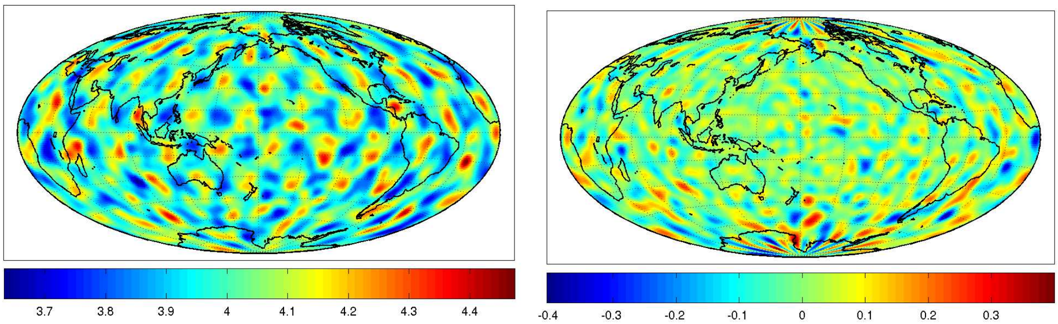
Figure 4.27: spline reconstruction (left) with $\rho = 0.06$, and corresponding error (right) of the velocity model in Figure 4.21, with 1% random error in the traveltimes



(a) spherical harmonic reconstruction with $\lambda = 10^{-5}$

(b) error of spline reconstruction where $RMS(\Delta) = 0.0580$

Figure 4.28: spherical harmonic reconstruction (left) with $\lambda = 10^{-5}$, and corresponding error (right), of the velocity model in Figure 4.21, with 1% random error in the traveltimes



(a) spherical harmonic reconstruction with $\lambda = 10^{-6}$

(b) error of spline reconstruction where $RMS(\Delta) = 0.0554$

Figure 4.29: spherical harmonic reconstruction (left) with $\lambda = 10^{-6}$, and corresponding error (right), of the velocity model in Figure 4.21, with 1% random error in the traveltimes

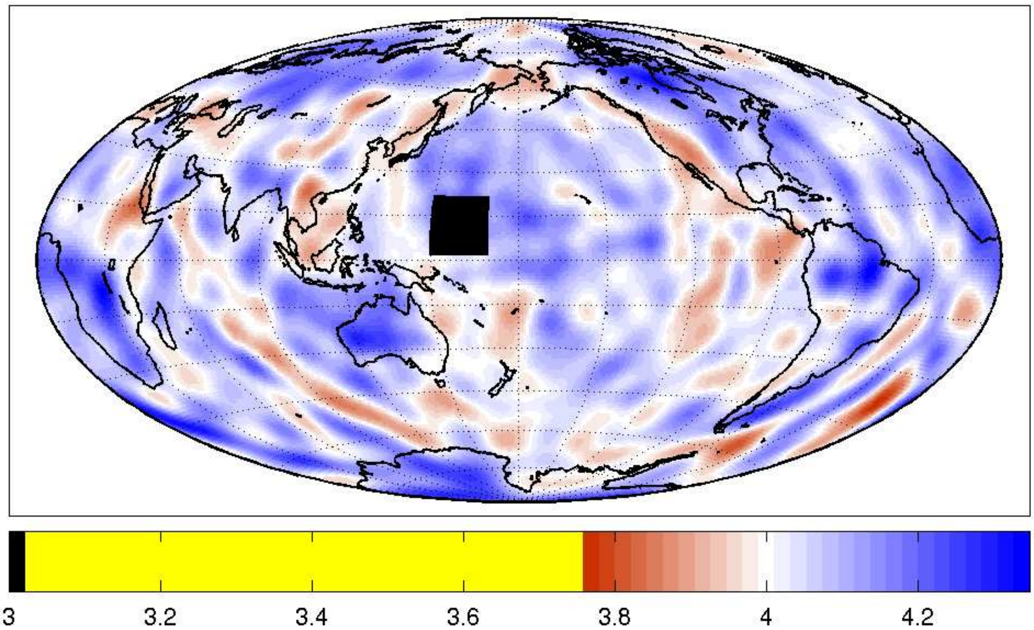
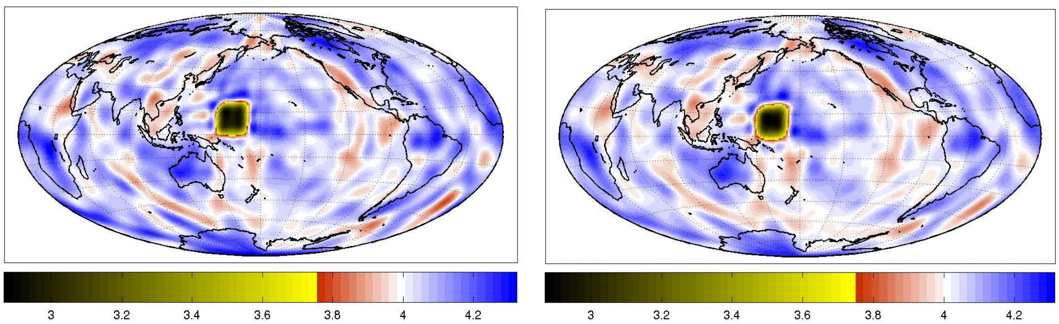
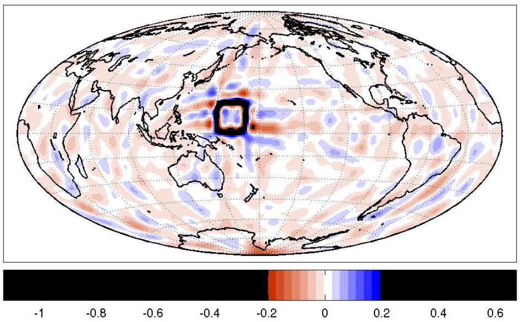


Figure 4.30: velocity model with a hidden object

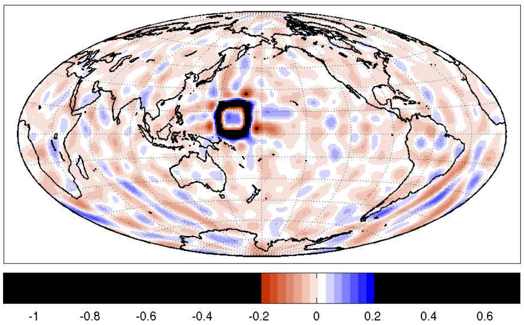


(a) reconstruction via splines (b) reconstruction via spherical harmonics

Figure 4.31: reconstruction of the velocity model in Figure 4.30 using the ray system in Figure 4.19 via splines with $\rho = 0.05$ (left) and spherical harmonics with $\lambda = 10^{-5}$ (right), respectively



(a) error of the reconstruction via splines



(b) error of the reconstruction via spherical harmonics

Figure 4.32: errors of the reconstructions presented in Figure 4.31, where for the spline reconstruction $RMS(\Delta) = 0.0288$ and for spherical harmonic reconstruction $RMS(\Delta) = 0.0321$

4.4 On Uniqueness and Convergence Results

As we have seen in case of seismic surface wave tomography with PREM as a reference model for any $\nu_1, \nu_2 \in \Omega$ the seismic ray $\gamma(\nu_1, \nu_2)$ between ν_1 and ν_2 is the arc of the great circle connecting these points. In this case we obtain the following new result.

Theorem 4.4.1 *Let $S \subset \Omega$ be an open set in Ω-topology, i.e. for any $x \in S$ there exists $\delta = \delta(x) > 0$ such that $\{y \in \Omega \, : \, d(y,x) < \delta\} \subset S$, where $d(x,y)$ is the spherical distance between x and y. Let also $A, B \subset S$ be non-empty sets with $\overline{A \cup B} = \overline{S}$ and $\Gamma := \{\gamma(\nu_1, \nu_2); \, \nu_1 \in A, \nu_2 \in B\}$. Then for any function $F \in \mathrm{C}(\Omega)$, from*

$$\mathcal{F}_\gamma := \int_\gamma F(\xi) d\sigma(\xi) = 0, \quad \textit{for any} \quad \gamma \in \Gamma \tag{4.11}$$

follows that $F \equiv 0$ on S.

First let us prove the following lemma.

Lemma 4.4.2 *Let $F \in \mathrm{C}(\Omega)$ be a given function and P, Q_0, with $Q_0 \neq P$ and $Q_0 \neq -P$ be arbitrary points on Ω. Then for any $\varepsilon > 0$ there exists $\delta > 0$ such that for any $Q \in \Omega \setminus \{-P\}$, with $|Q_0 - Q| < \delta$,*

$$\left| \int_{\gamma(P,Q_0)} F(\xi) d\sigma(\xi) - \int_{\gamma(P,Q)} F(\xi) d\sigma(\xi) \right| \leq \varepsilon, \tag{4.12}$$

where $\gamma(P, Q_0)$ and $\gamma(P,Q)$ are the minimal spherical arcs between P and Q_0 and respectively P and Q.

Proof: Take an arbitrary $\varepsilon > 0$. Let $g_0(t)$ and $g(t)$ be the parametric equations of $\gamma(P, Q_0)$ respectively $\gamma(P,Q)$. Then (see (4.7))

$$\begin{aligned} g_0(t) &= \cos(t)P + \sin(t)Q_{P0}, \quad t \in [0, d_0], \\ g(t) &= \cos(t)P + \sin(t)Q_P, \quad t \in [0, d], \end{aligned}$$

where $d_0 := \arccos(P \cdot Q_0)$, $d := \arccos(P \cdot Q)$, $Q_{P0} := w_0/\|w_0\|$, $Q_P := w/\|w\|$, with $w_0 := Q_0 - (P \cdot Q_0)P$ and $w := Q - (P \cdot Q)P$.

Since $F \in \mathrm{C}(\Omega)$ and Ω is compact, F is uniformly continuous on Ω, and there exists a constant $M > 0$ such that $|F(\xi)| \le M$, for any $\xi \in \Omega$. Let $\varepsilon_0 := \varepsilon/(2\pi)$. It follows that there exists a constant δ_{ε_0} with $0 < \delta_{\varepsilon_0} \le \varepsilon/(2M)$ such that

$$|F(\xi) - F(\eta)| \le \varepsilon_0, \quad \text{whenever} \quad |\xi - \eta| \le \delta_{\varepsilon_0}. \tag{4.13}$$

From the definition of Q_P follows that it can be considered as a continuous function of Q on $\Omega \setminus (\{P\} \cup \{-P\})$.
Now let $Q \in \Omega \setminus (\{P\} \cup \{-P\})$. Hence there exists a constant $\delta_1 > 0$ such that

$$|Q_{P0} - Q_P| \le \delta_{\varepsilon_0}, \quad \text{whenever} \quad |Q_0 - Q| \le \delta_1. \tag{4.14}$$

Moreover, since $P \cdot Q \in [-1, 1]$ and the function $\arccos(\cdot)$ is continuous on $[-1, 1]$, d also can be considered as a continuous function of Q. Therefore, there exists a constant $\delta_2 > 0$ such that

$$|d_0 - d| \le \delta_{\varepsilon_0}, \quad \text{whenever} \quad |Q_0 - Q| \le \delta_2. \tag{4.15}$$

Now let $\delta_3 := \min(\delta_1, \delta_2)$, $\bar{d} := \min(d_0, d)$ and $|Q_0 - Q| \le \delta_3$.
Hence, from (4.14) follows that for all $t \in [0, \bar{d}]$

$$\begin{aligned} |g_0(t) - g(t)| &= |\cos(t)P + \sin(t)Q_{P0} - \cos(t)P - \sin(t)Q_P| \\ &= |\sin(t)(Q_{P0} - Q_P)| \le |Q_{P0} - Q_P| \le \delta_{\varepsilon_0}. \end{aligned} \tag{4.16}$$

Combining (4.13),(4.15) and (4.16) we obtain that
if $d_0 \le d$ then

$$\begin{aligned} &\left| \int_{\gamma(P,Q_0)} F(\xi) d\sigma(\xi) - \int_{\gamma(P,Q)} F(\xi) d\sigma(\xi) \right| = \left| \int_0^{d_0} F(g_0(t))dt - \int_0^{d} F(g(t))dt \right| \\ &\left| \int_0^{d_0} (F(g_0(t)) - F(g(t)))dt - \int_{d_0}^{d} F(g(t))dt \right| \le \left| \int_0^{d_0} (F(g_0(t)) - F(g(t)))dt \right| \\ &+ \left| \int_{d_0}^{d} F(g(t))dt \right| \le \sup_{t \in [0,d_0]} |F(g_0(t)) - F(g(t))|\, d_0 + \sup_{\xi \in \Omega} |F(\xi)|\, |d_0 - d| \\ &\le \varepsilon_0 d_0 + M|d_0 - d| \le \varepsilon/2 + \varepsilon/2 = \varepsilon, \end{aligned}$$

otherwise

$$\left|\int_{\gamma(P,Q_0)} F(\xi)d\sigma(\xi) - \int_{\gamma(P,Q)} F(\xi)d\sigma(\xi)\right| = \left|\int_0^{d_0} F(g_0(t))dt - \int_0^{d} F(g(t))dt\right|$$
$$= \left|\int_0^{d} (F(g(t)) - F(g_0(t)))dt - \int_d^{d_0} F(g_0(t))dt\right| \leq \left|\int_0^{d} (F(g(t)) - F(g_0(t)))dt\right|$$
$$+ \left|\int_d^{d_0} F(g_0(t))dt\right| \leq \sup_{t\in[0,d]} |F(g(t)) - F(g_0(t))|\, d + \sup_{\xi\in\Omega} |F(\xi)|\, |d_0 - d|$$
$$\leq \varepsilon_0 d + M|d_0 - d| \leq \varepsilon/2 + \varepsilon/2 = \varepsilon.$$

Note that since $Q_0 \neq P$ we can choose $\delta_0 > 0$ sufficiently small such that $|Q - Q_0| < \delta_0$ implies $Q \neq P$. Hence, for the given $\varepsilon > 0$, the corresponding δ can be taken as $\delta := \min(\delta_1, \delta_2, \delta_0)$. ■

Proof of Theorem 4.4.1: Suppose there exists $x_0 \in S$ such that $F(x_0) \neq 0$. Let $F(x_0) > 0$ (otherwise instead of F we will take $-F$). Since F is continuous on Ω, there exists $U(x_0)$, an open ball with center x_0, such that $F(x) > 0$, $x \in U(x_0)$. Now, there are only two possible cases:
1. $U(x_0) \cap A \neq \emptyset$ and $U(x_0) \cap B \neq \emptyset$.
2. $U(x_0) \cap A = \emptyset$ or $U(x_0) \cap B = \emptyset$.
The first case implies that there exists $\gamma(x_0', x_0'') \in \Gamma$ such that $x_0' \in A \cap U(x_0)$ and $x_0'' \in B \cap U(x_0)$, hence, $\gamma(x_0', x_0'') \subset U(x_0)$. However, from (4.11) we have that

$$\int_{\gamma(x_0',x_0'')} F(\xi)d\sigma(\xi) = 0$$

which is a contradiction to the fact that $F(x) > 0$, $x \in U(x_0)$ and F is continuous on $U(x_0)$.
In the second case: let $U(x_0) \cap B = \emptyset$ (the case $U(x_0) \cap A = \emptyset$ is analogous). It follows that $U(x_0) \subset \bar{A}$. Take any $y_1 \in B \setminus (\partial U(x_0) \cup (-\partial U(x_0))$ (if $B \setminus (\partial U(x_0) \cup (-\partial U(x_0)) = \emptyset$ then decrease the radius of $U(x_0)$). Denote the great circle connecting x_0 and y_1 by l_0. l_0 will intersect the boundary of $U(x_0)$ in two points: x_1^0 and x_2^0. Now let $\varepsilon > 0$ be arbitrary. Since $U(x_0) \subset \bar{A}$, for arbitrarily small $\delta > 0$ there exists $x_1, x_2 \in A \cap U(x_0)$ such that $x_1 \neq -y_1$, $x_2 \neq -y_2$, $|x_1 - x_1^0| < \delta$ and $|x_2 - x_2^0| < \delta$ (see Figure 4.33). But since $x_1, x_2 \in A$ and

$y_1 \in B$, there exist $\gamma(x_1, y_1), \gamma(x_2, y_1) \in \Gamma$ and therefore

$$\int_{\gamma(x_1,y_1)} F(\xi) d\sigma(\xi) = 0 \quad \text{and} \quad \int_{\gamma(x_2,y_1)} F(\xi) d\sigma(\xi) = 0.$$

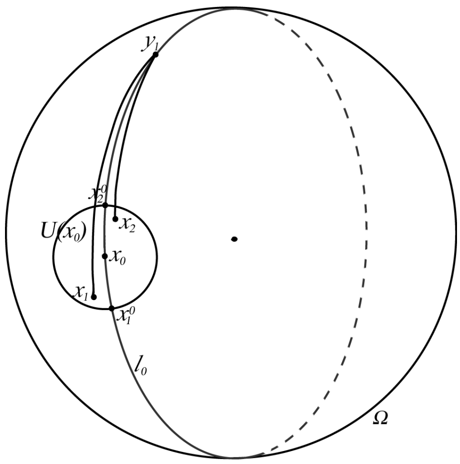


Figure 4.33: illustration of $U(x_0)$, l_0, $\gamma(x_1, y_1)$, $\gamma(x_2, y_1)$

In this case from Lemma 4.4.2 follows that we can choose δ such that

$$\left| \int_{\gamma(x_1^0,y_1)} F(\xi) d\sigma(\xi) \right| \leq \left| \int_{\gamma(x_1,y_1)} F(\xi) d\sigma(\xi) \right| + \frac{\varepsilon}{2},$$
$$\left| \int_{\gamma(x_2^0,y_1)} F(\xi) d\sigma(\xi) \right| \leq \left| \int_{\gamma(x_2,y_1)} F(\xi) d\sigma(\xi) \right| + \frac{\varepsilon}{2}.$$

Therefore,

$$\begin{aligned} \left| \int_{\gamma(x_1^0,x_2^0)} F(\xi) d\sigma(\xi) \right| &= \left| \int_{\gamma(x_1^0,y_1)} F(\xi) d\sigma(\xi) - \int_{\gamma(x_2^0,y_1)} F(\xi) d\sigma(\xi) \right| \\ &\leq \left| \int_{\gamma(x_1^0,y_1)} F(\xi) d\sigma(\xi) \right| + \left| \int_{\gamma(x_2^0,y_1)} F(\xi) d\sigma(\xi) \right| \\ &\leq \left| \int_{\gamma(x_1,y_1)} F(\xi) d\sigma(\xi) \right| + \left| \int_{\gamma(x_2,y_1)} F(\xi) d\sigma(\xi) \right| + \frac{\varepsilon}{2} + \frac{\varepsilon}{2} \\ &= \varepsilon. \end{aligned}$$

From the arbitrariness of ε follows that

$$\int_{\gamma(x_1^0, x_2^0)} F(\xi) d\sigma(\xi) = 0, \tag{4.17}$$

which is again a contradiction to the fact that $F(x) > 0$, $x \in U(x_0)$ and F is continuous on $U(x_0)$. ■

Hence, this result can be applied for local as well as global approximation problems. More precisely, it follows that for any open in Ω-topology set $S \subset \Omega$, if the union of the sets of the given seismic sources and receivers is dense on S then Problem 4.0.2 (in continuous case) in S has no more than one solution. In particular by taking $S = \Omega$ we obtain that if the union of the sets of the given seismic sources and receivers is dense on Ω then Problem 4.0.2 (in continuous case) has no more than one solution. Moreover, it follows that in this case the system of linear bounded functionals corresponding to our spline interpolation problem is complete and therefore (see Theorem 3.7.5), the sequence of approximating splines converges to the initial function in the sense of strong $\mathcal{W}$ convergence.

A question arises whether it is not sufficient for the unique determination of a continuous function on the sphere that the corresponding system of rays covers the sphere, in the sense that the union of the images of the rays gives the sphere. The following example shows that although the system of corresponding rays covers the domain, we have non-uniqueness in the determination of the function.

Let Ω_1 be a spherical cap which in the spherical coordinates can be written as $\Omega_1 := \{\xi = \bar{\xi}(1, \theta, \phi) \in \Omega \,|\, \theta \leq \pi/4\}$, where $\bar{\xi}(1, \theta, \phi)$, with $\theta \in [0, \pi]$ and $\phi \in [0, 2\pi)$, is the representation of $\xi \in \Omega$ in the spherical coordinates. For any $\phi \in [0, \pi]$ by γ_ϕ we denote the minimal spherical arc between the points $E_\phi = \bar{\xi}(1, \pi/4, \phi)$ and $R_\phi = \bar{\xi}(1, \pi/4, \phi + \pi)$ (see Figure 4.34).
Let also $\Gamma_1 := \bigcup_{\phi \in [0,\pi]} \gamma_\phi$ *. Clearly $\Gamma_1 = \Omega_1$. And if we set

$$f_1(\xi) = f_1(\bar{\xi}(1, \theta, \phi)) = \sin(8\theta), \quad \xi \in \Omega_1,$$

then it is not hard to check that

$$\int_\gamma f_1(\xi) d\sigma(\xi) = 0, \quad \text{for all} \quad \gamma \in \Gamma_1. \tag{4.18}$$

* γ_ϕ is understood here as a set of points

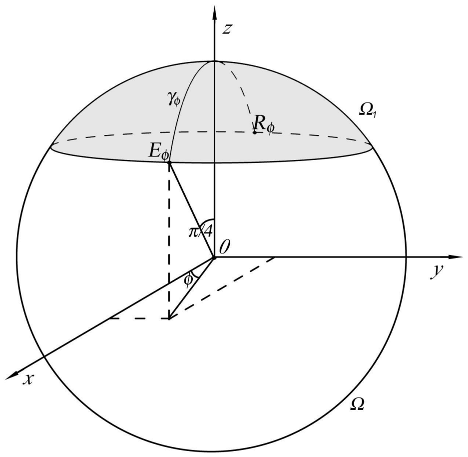


Figure 4.34: Plot of Ω_1 and γ_ϕ.

In fact $E_\phi = \bar{\xi}(1, \pi/4, \phi)$ and $R_\phi = \bar{\xi}(1, \pi/4, \phi+\pi)$ can be written in the cartesian coordinates as

$$\begin{aligned} E_\phi &= \left(\frac{\cos(\phi)}{\sqrt{2}}, \frac{\sin(\phi)}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right) \\ R_\phi &= \left(-\frac{\cos(\phi)}{\sqrt{2}}, -\frac{\sin(\phi)}{\sqrt{2}}, \frac{1}{\sqrt{2}}\right). \end{aligned}$$

We see that $E_\phi \cdot R_\phi = 0$ for all $\phi \in [0, \pi]$, therefore the parametric equation of γ_ϕ, $\phi \in [0, \pi]$, $r_\phi(\cdot)$, can be written as (see (4.7))

$$r_\phi(t) = (x_\phi(t), y_\phi(t), z_\phi(t)) = \cos(t)E_\phi + \sin(t)R_\phi, \quad t \in [0, \pi/2].$$

Hence

$$z_\phi(t) = \frac{\cos(t)}{\sqrt{2}} + \frac{\sin(t)}{\sqrt{2}} = \cos(\pi/4 - t), \quad t \in [0, \pi/2].$$

Therefore if $\bar{\xi}(1, \theta_\phi(t), \varphi_\phi(t))$ is the representation of $r_\phi(t)$ in the spherical coordinates, then

$$\theta_\phi(t) = \arccos(z_\phi(t)) = \begin{cases} \frac{\pi}{4} - t, & \text{if} \quad t \in [0, \frac{\pi}{4}], \\ t - \frac{\pi}{4}, & \text{if} \quad t \in [\frac{\pi}{4}, \frac{\pi}{2}]. \end{cases} \tag{4.19}$$

Hence, (4.18) is true since, for any $\phi \in [0, \pi]$ and the corresponding γ_ϕ

$$\begin{aligned}\int_{\gamma_\phi} f_1(\xi) d\sigma(\xi) &= \int_{\gamma_\phi} f_1(\bar{\xi}(1,\theta,\varphi)) d\sigma(\bar{\xi}(1,\theta,\varphi)) = \int_0^{\pi/2} \sin(8\theta_\phi(t))dt \\ &= \int_0^{\pi/4} \sin(2\pi - 8t)dt + \int_{\pi/4}^{\pi/2} \sin(8t - 2\pi)dt \\ &= -\int_0^{\pi/4} \sin(8t)dt + \int_{\pi/4}^{\pi/2} \sin(8t)dt = 0.\end{aligned}$$

Furthermore, we denote

$$f(\xi) = \begin{cases} f_1, & \text{if} \quad \xi \in \Omega_1, \\ 0, & \text{if} \quad \xi \in \Omega \setminus \Omega_1. \end{cases} \tag{4.20}$$

Clearly $f \in \mathrm{C}(\Omega)$. Let also Γ_2 be a system of rays such that it covers $\Omega \setminus \Omega_1$ but has no intersection with Ω_1, i.e. $\Gamma_2 = \Omega \setminus \Omega_1$ (such a set of rays can be constructed in an analogous way to Γ_1). Then clearly by taking $\Gamma := \Gamma_1 \cup \Gamma_2$ we obtain a set of rays that covers Ω, i.e. $\Gamma = \Omega$, and

$$\int_\gamma f(\xi) d\sigma(\xi) = 0, \quad \text{for all} \quad \gamma \in \Gamma. \tag{4.21}$$

However $f \not\equiv 0$ (see Figure 4.35).

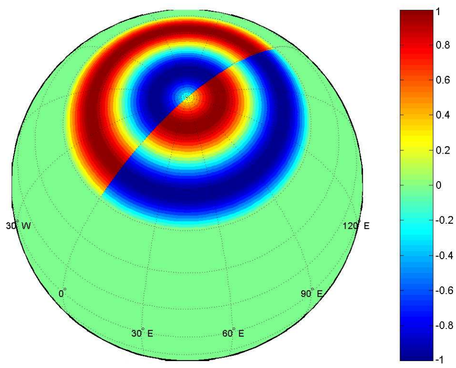


Figure 4.35: Plot of the function $f(\xi)$, $\xi \in \Omega$ defined by (4.20)

.

From the constructions above we see that this counterexample also works for local approximation problems.

Chapter 5

Application to Seismic Body Wave Tomography

In this chapter we present an application of the spline approximation method, described in Chapter 3, to the seismic body wave traveltime tomography.
Following the considerations in Chapter 2 we will discuss the linearized inverse problem which can be formulated as follows (see Problem 2.2.5):

Problem 5.0.3 *Given real numbers* $T_q; q = 1, ..., N$ *and pairs of points* $(E_q, R_q) \in \Omega \times \Omega$. *Find a function* $\tilde{S} \in \mathrm{C}(B)$ *such that*

$$T_q = \int_{\gamma_q} \tilde{S}(x)\, d\sigma(x), \quad q = 1, ..., N, \tag{5.1}$$

where $\gamma_q; q = 1, ..., N$, *are given curves/raypaths (defined according to the reference model* S_0*) between* E_q *and* R_q.

Here we will also take PREM ([16]) as a reference model, or more precisely for a simpler numerics an approximation to PREM.

Assumption 5.0.4 *We assume that* $\gamma_i \neq \gamma_j$, *if* $i \neq j$, $i, j = 1, ..., N$.

5.1 Initial Constructions

Since here the function $\tilde{S}$ which needs to be approximated is defined on a unit ball, we will take the unit ball $B = \{x \in \mathbb{R}^3 \,|\, |x| \leq 1\}$ as an initial set (see Section 3.1).

As an initial basis system on B we will take the system $\{W^B_{k,n,j}\}_{k,n\in\mathbb{N}_0;j=-n,\dots,n}$ defined in Section 1.5 (see also Section 3.1.2 and Section 3.2.2). Note that here $W^B_{k,n,j} \in \mathrm{C}_\Theta(B)$, with $\Theta = \{0\}$, $k,n \in \mathbb{N}_0; j = -n,...,n$, i.e. any $W^B_{k,n,j}$ is continuous on $B \setminus \{0\}$ and bounded on B.

The results of Section 3.1 and Section 3.2 will be summarized briefly here for a special case of initial set and initial basis system.

If $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ is an arbitrary real sequence, with $A_{k,n} \neq 0$ for all $k,n \in \mathbb{N}_0$, then $\mathcal{E} := \mathcal{E}(\{A_{k,n}\}; B)$ denotes the space of all functions $F \in \mathrm{L}^2(B)$, satisfying

$$\sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{j=-n}^{n} A_{k,n}^{-2} \left| \left(F, W^B_{k,n,j}\right)^2_{\mathrm{L}^2(B)} \right| < +\infty$$

This space is a pre-Hilbert space if it is equipped with the inner product

$$(F,G)_{\mathcal{H}(\{A_{k,n}\};B)} := \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{j=-n}^{n} A_{k,n}^{-2} \left(F, W^B_{k,n,j}\right)_{\mathrm{L}^2(B)} \left(G, W^B_{k,n,j}\right)_{\mathrm{L}^2(B)} \quad F,G \in \mathcal{E},$$

which is always finite due to the Cauchy–Schwarz inequality. The Hilbert space $\mathcal{H} := \mathcal{H}(\{A_{k,n}\}; B)$ is defined as the completion of $\mathcal{E}(\{A_{k,n}\}; B)$ with respect to $(.,.)_\mathcal{H}$. The induced norm is denoted by $\|F\|_\mathcal{H} := \sqrt{(F,F)_\mathcal{H}}$.

As we have already seen in Section 3.1.2, here $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ will be summable if

$$\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} A_{k,n}^2 k^5 n < \infty.$$

And if $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ is summable, then this Sobolev space $\mathcal{H}$ possesses a unique reproducing kernel $K_\mathcal{H} : B \times B \to \mathbb{R}$ given by

$$K_\mathcal{H}(x,y) = \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{j=-n}^{n} A_{k,n}^2 W^B_{k,n,j}(x) W^B_{k,n,j}(y).$$

Moreover, the summability also implies that $\mathcal{H}(\{A_{k,n}\}; B) \subset \mathrm{C}_\Theta(B)$ and

$$\|F\|_\infty \leq \|F\|_\mathcal{H} \left(\sum_{k=0}^{\infty}\sum_{n=0}^{\infty} A_{k,n}^2 \left(\sqrt{2k+3} \left\| P_k^{(0,2)} \right\|_{\mathrm{C}[-1,1]} \right)^2 \frac{2n+1}{4\pi} \right)^{1/2} \qquad (5.2)$$

for all $F \in \mathcal{H}$.

5.2 Application

We define functionals $\mathcal{F}_q : \mathcal{H} \to \mathbb{R}$, $q = 1, ..., N$ as path integrals of a function in $\mathcal{H}$ over γ_q, i.e. for any $F \in \mathcal{H}$

$$\mathcal{F}_q F := \int_{\gamma_q} F(x)\, \mathrm{d}\sigma(x), \quad q = 1, ..., N.$$

The discussed functionals $\mathcal{F}_q$ are obviously linear, due to the linearity of the integral, and continuous on $\mathcal{H} \subset \mathrm{C}_\Theta(B)$ since

$$\begin{aligned} |\mathcal{F}_q F| &\leq \|F\|_\infty \cdot \text{length}\,(\gamma_q) \\ &\leq \|F\|_{\mathcal{H}} \left(\sum_{k=0}^{\infty} \sum_{n=0}^{\infty} A_{k,n}^2 \left(\sqrt{2k+3} \left\| P_k^{(0,2)} \right\|_{\mathrm{C}[-1,1]} \right)^2 \frac{2n+1}{4\pi} \right)^{1/2} M^{S_0}, \end{aligned}$$

for all $F \in \mathcal{H}$, where we have used Equation (5.2) and Assumption 2.2.10.

Theorem 5.2.1 *From Assumption 5.0.4 follows that the system of functionals* $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$ *is linearly independent.*

Proof: Let Assumption 5.0.4 hold, i.e. $\gamma_i \neq \gamma_j$, if $i \neq j$, $i, j = 1, ..., N$, but $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$ is linearly dependent. That is there exist coefficients $a_1, ..., a_N$ where at least one of them is not 0, such that $\sum_{k=1}^{N} a_k \mathcal{F}_k = 0$. However, this means that for any $F \in \mathcal{H}$

$$\sum_{k=1}^{N} a_k \mathcal{F}_k F = 0. \tag{5.3}$$

Let $a_{i_0} \neq 0$. Assume without loss of generality that $a_{i_0} > 0$. We will construct a function in $\mathcal{H}$ for which (5.3) does not hold. As we have already mentioned by r_x and ξ_x we will always denote the norm and the unit vector of $x \in \mathbb{R}^3 \setminus \{0\}$ respectively. Clearly, from Assumption 5.0.4 and Assumption 2.2.9 follows that there exists $x_0 \in \gamma_{i_0}$, with $x_0 \neq 0$ and $\varepsilon > 0$ such that $x_0(\varepsilon) \cap \gamma_i = \emptyset$ if $i \neq i_0$, where $x_0(\varepsilon)$ is the ε-neighborhood of x_0. Now, it is not hard to check that for an arbitrary real $M_0 > 0$ we can construct $u_1 \in \mathrm{C}[0,1]$ and $v_1 \in \mathrm{C}(\Omega)$ such that for $F_1(x) = F_1(r_x \xi_x) := u_1(r_x) v_1(\xi_x)$, $x \in B \setminus \{0\}$ we have that $F_1(x) \geq 0$, $x \in B$ and

$$F_1(x) = \begin{cases} M_0, & \text{if} \quad x \in x_0(\varepsilon/n_0) \\ 0, & \text{if} \quad x \in B \backslash x_0(\varepsilon), \end{cases} \tag{5.4}$$

where n_0 is some fixed integer.
Hence,

$$\lambda_1 := \sum_{k=1}^{N} a_k \int_{\gamma_k} F_1(x)\mathrm{d}\sigma(x) = a_{i_0} \int_{\gamma_{i_0}} F_1(x)\mathrm{d}\sigma(x) > \frac{a_{i_0} M_0 \varepsilon}{2n_0} =: M_1 > 0. \quad (5.5)$$

Now since length(γ_i), $i = 1, ..., N$ is bounded

$$M_2 := \sum_{k=1}^{N} |a_k| \operatorname{length}(\gamma_k) < \infty.$$

Let $p := \max(\|u_1\|_\infty, \|v_1\|_\infty)$ and $g_k(r) := \tilde{G}_k(3,3,r)$, $k \in \mathbb{N}$, $r \in [0,1]$. Since the system $\{g_k\}_{k\in\mathbb{N}_0}$ is closed in C[0, 1] (see Section 1.3) and the system $\{Y_{n,j}\}_{n\in\mathbb{N}_0; j=-n,...,n}$ is closed in C(Ω) (see Theorem 1.4.10), for $\delta := M_1/(2M_2)$ and for $\delta_1 < \min(p, \delta/(3p))$ there exist linear combinations

$$\tilde{g} := \sum_{k=0}^{k_0} b_k g_k \quad \text{and} \quad \tilde{Y} := \sum_{n=0}^{n_0} \sum_{j=-n}^{n} c_{n,j} Y_{n,j}$$

such that

$$\|u_1 - \tilde{g}\|_\infty \le \delta_1,$$
$$\|v_1 - \tilde{Y}\|_\infty \le \delta_1.$$

Hence, if we denote $F_2(x) = F_2(r_x\xi_x) = \tilde{g}(r_x)\tilde{Y}(\xi_x)$, $x \in B \setminus \{0\}$ and $F_2(0)$ appropriate, then clearly, $F_2 \in \mathcal{H}$ and

$$\begin{aligned}
&\sup_{x\in B\setminus\{0\}} |F_2(x) - F_1(x)| = \sup_{x\in B\setminus\{0\}} \left|\tilde{g}(r_x)\tilde{Y}(\xi_x) - u_1(r_x)v_1(\xi_x)\right| \\
&= \sup_{x\in B\setminus\{0\}} \Big|(\tilde{g}(r_x) - u_1(r_x))(\tilde{Y}(\xi_x) - v_1(\xi_x)) \\
&\quad + v_1(\xi_x)(\tilde{g}(r_x) - u_1(r_x)) + u_1(r_x)(\tilde{Y}(\xi_x) - v_1(\xi_x))\Big| \\
&\le \sup_{r\in(0,1]} |\tilde{g}(r) - u_1(r)| \sup_{\xi\in\Omega} \left|\tilde{Y}(\xi) - v_1(\xi)\right| \\
&\quad + \sup_{\xi\in\Omega} |v_1(\xi)| \sup_{r\in(0,1]} |\tilde{g}(r) - u_1(r)| + \sup_{r\in(0,1]} |u_1(r)| \sup_{\xi\in\Omega} \left|\tilde{Y}(\xi) - v_1(\xi)\right| \\
&\le \delta_1^2 + 2p\delta_1 \le 3p\delta_1 \\
&\le \delta.
\end{aligned}$$

Thus, if we denote

$$\lambda_2 := \sum_{k=1}^{N} a_k \mathcal{F}_k F_2 = \sum_{k=1}^{N} a_k \int_{\gamma_k} F_2(x) \mathrm{d}\sigma(x),$$

then using in the case of $0 \in \gamma_k$ the fact that path integrals are invariant w.r.t. changes of the function at one single point

$$\begin{aligned} |\lambda_1 - \lambda_2| &= \left| \sum_{k=1}^{N} a_k \int_{\gamma_k} (F_1 - F_2)(x) \mathrm{d}\sigma(x) \right| \\ &\leq \sup_{x \in B \setminus \{0\}} |F_1(x) - F_2(x)| \sum_{k=1}^{N} |a_k| \, \mathrm{length}(\gamma_k) \\ &\leq \delta M_2 = \frac{M_1}{2}. \end{aligned}$$

That is

$$\lambda_1 - M_1/2 \leq \lambda_2 \leq \lambda_1 + M_1/2,$$

such that using (5.5) we obtain that

$$\sum_{k=1}^{N} a_k \mathcal{F}_k F_2 = \lambda_2 > M_1 - \frac{M_1}{2} = \frac{M_1}{2} > 0.$$

However, this is a contradiction to (5.3), hence, $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$ is linearly independent. ■

The idea that we follow here is to approximate $\tilde{S}$ by a spline $S \in \mathcal{H}$ based on a system $\{\mathcal{F}_1, \mathcal{F}_2, ..., \mathcal{F}_N\}$, i.e. by a spline of the form

$$S(x) = \sum_{k=1}^{N} a_k \mathcal{F}_k K_{\mathcal{H}}(., x), \quad x \in B.$$

It is known that if L is a curve parameterized by a $\mathrm{C}^{(1)}([a, b], \mathbb{R}^3)$–function l, and F is a continuous scalar field, then

$$\int_L F(x) \, \mathrm{d}\sigma(x) = \int_a^b F(l(t)) \, |l'(t)| \, \mathrm{d}t \, .$$

Hence, knowing parametric equations of raypaths $\gamma_q; q = 1, ..., N$ we can calculate the matrix components corresponding to our spline interpolation problem:

$$(\mathcal{F}_l)_x \, (\mathcal{F}_q)_y \, K_{\mathcal{H}}(y, x) = \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} A_{k,n}^2 \sum_{j=-n}^{n} \int_{\gamma_l} W_{k,n,j}^B(x) \, \mathrm{d}\sigma(x) \int_{\gamma_q} W_{k,n,j}^B(y) \mathrm{d}\sigma(y).$$

And by solving the linear equation system

$$\sum_{q=1}^{N} a_q \, (\mathcal{F}_l)_x \, (\mathcal{F}_q)_y \, K_{\mathcal{H}}(y,x) = T_l \text{ for all } l = 1, ..., N$$

we obtain the coefficients $(a_q)_{q=1,\ldots,N}$ of the spline

$$S(x) \;=\; \sum_{q=1}^{N} a_q \, (\mathcal{F}_q)_y \, K_{\mathcal{H}}(y,x) = \sum_{q=1}^{N} a_q \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} A_{k,n}^2 \sum_{j=-n}^{n} \int_{\gamma_q} W_{k,n,j}^B(y) \, \mathrm{d}\sigma(y) \, W_{k,n,j}^B(x)$$

approximating the function $\tilde{S}$.
Methods of determining the parametric equations of the raypaths $\gamma_q; q = 1, ..., N$ are described in Appendix A.

5.3 Numerical Tests

Let V_0 be the P-wave velocity function according to PREM. In numerical tests we take $S_1 := 1/V_1$ as a reference slowness model , where V_1 is an approximation to V_0 with a function which stepwise is of the form (see Figures 5.1 and 5.2):

$$V(r) = A \, r^{(1-b)}, \quad r \in [0,1], \quad A, b = \text{const.} \tag{5.6}$$

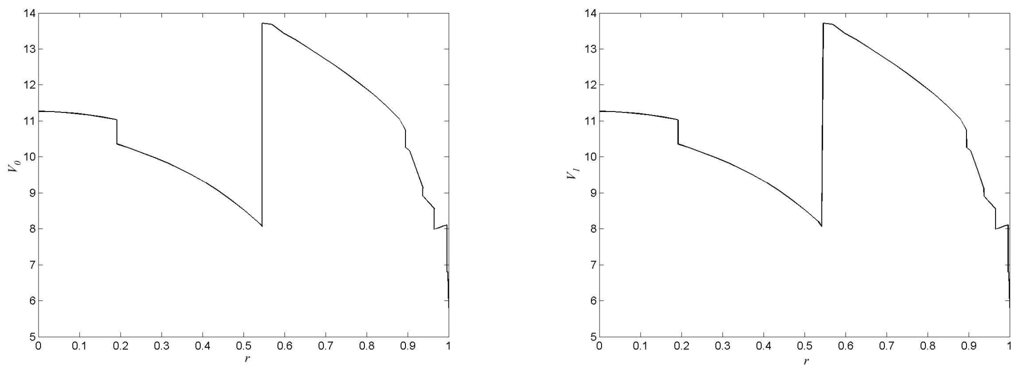


Figure 5.1: P-Wave velocity V_0 (according to PREM) (left), approximation of V_0, with a function V_1 which stepwise is of the form (5.6) (right).

r	$V_0(r)$		r	$V_0(r)$
0.00000	11.26620		0.62784	13.24532
0.03139	11.25593		0.65924	13.01579
0.06278	11.23712		0.69063	12.78389
0.09418	11.20576		0.72202	12.54466
0.12557	11.16186		0.75341	12.29316
0.15696	11.10542		0.78481	12.02445
0.18835	11.03643		0.81620	11.73357
0.19173	11.02827		0.84759	11.41560
0.19173	10.35568		0.87898	11.06557
0.21975	10.24959		0.89484	10.75131
0.25114	10.12291		0.89484	10.26622
0.28253	9.98554		0.90582	10.15782
0.31392	9.83496		0.92152	9.64588
0.34531	9.66865		0.93722	9.13397
0.37671	9.48409		0.93722	8.90522
0.40810	9.27876		0.95134	8.73209
0.43949	9.05015		0.96547	8.55896
0.47088	8.79573		0.96547	7.98970
0.50228	8.51298		0.97646	8.03370
0.53367	8.19939		0.98744	8.07688
0.54623	8.06482		0.99617	8.11061
0.54623	13.71660		0.99617	6.80000
0.56506	13.68753		0.99765	6.80000
0.56977	13.68041		1.00000	5.80000
0.59645	13.44742			

Table 5.1: The values of $V_0(r)$ for different $r \in [0, 1]$

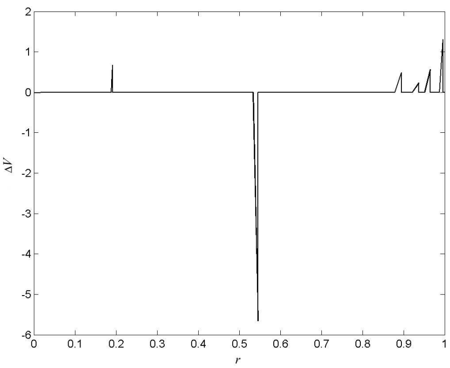


Figure 5.2: Difference of V_1 and V_0, $\Delta V = V_1 - V_0$.

More precisely, we get V_1 by dividing [0,1] into 48 parts (according to Table 5.1) and in each of these parts approximating V_0 with a function of a form (5.6). Thus, rays should be generated according to the slowness model S_1. In this case the parametric equations of the raypaths $\gamma_q; q = 1, ..., N$ can be written in a simple analytic form (see Section A.2).

As a sequence $\{A_{k,n}\}_{k,n\in\mathbb{N}_0}$ we took $A^2_{k,n} = B^2_k C^2_n$, $k, n \in \mathbb{N}_0$, where $B^2_k = e^{-\lambda_1 k(k+1)}$ is the Gauß–Weierstraß symbol, and $C^2_n = e^{-\lambda_2 n}$ is the Abel-Poisson symbol (see Section 3.1.2 and Section 3.2.2). In this case our reproducing kernel $K_{\mathcal{H}}(\cdot,\cdot)$ can be written as (see (1.11) and [24], p. 45)

$$\begin{aligned} K_{\mathcal{H}}(x,y) &= \sum_{k=0}^{\infty}\sum_{n=0}^{\infty}\sum_{j=-n}^{n} A^2_{k,n} W^B_{k,n,j}(x) W^B_{k,n,j}(y) \qquad (5.7) \\ &= \frac{1}{4\pi}\frac{1-h^2}{(1+h^2-2h(\frac{x}{|x|}\cdot\frac{y}{|y|}))^{(3/2)}} \\ &\quad \times \sum_{k=0}^{\infty} B^2_k (2k+3) P^{(0,2)}_k\left(2|x|-1\right) P^{(0,2)}_k\left(2|y|-1\right) \\ &= K_1\left(x/|x|, y/|y|\right) K_2\left(|x|,|y|\right), \end{aligned}$$

where

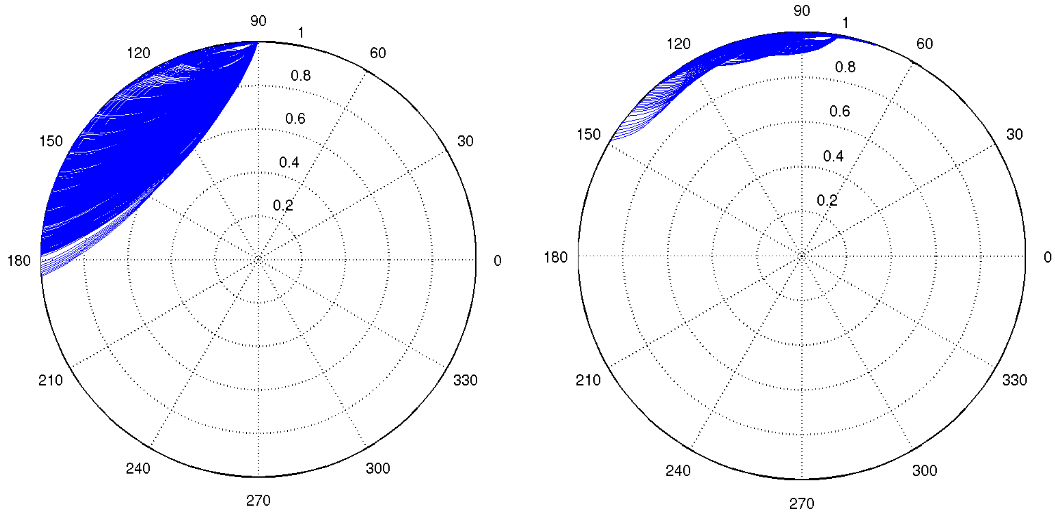
$$K_1\left(x/|x|, y/|y|\right) = K_1\left(\xi_x, \xi_y\right) := \frac{1}{4\pi}\frac{1-h^2}{(1+h^2-2h(\xi_x\cdot\xi_y))^{(3/2)}}, \qquad (5.8)$$

with $h := C_1^2 = e^{-\lambda_2}$ and

$$K_2\left(|x|,|y|\right) = K_2\left(r_x, r_y\right) := \sum_{k=0}^{\infty} B_k^2(2k+3)P_k^{(0,2)}(2r_x-1)P_k^{(0,2)}(2r_y-1). \quad (5.9)$$

We see that for fixed $x_0 \in B$, K_1 only depends on ξ_y, i.e. on the unit vector of y, and K_2 only depends on r_y, i.e. on the radius of y. This suggests that we can choose parameters λ_1, λ_2 independently to control the localization character (hat-width) of $K_{\mathcal{H}}$ in the direction of r_y and ξ_y respectively. The last point is particularly important in body wave tomography, since here the unknown (velocity) function has strong variations in the direction of r_y and relatively small variations in the direction of ξ_y.

The representation of $x \in B$ in the spherical coordinates will be denoted by $\bar{x}(r,\theta,\phi)$, where $r \in [0,1], \theta \in [0,\pi]$ and $\phi \in [0,2\pi)$.



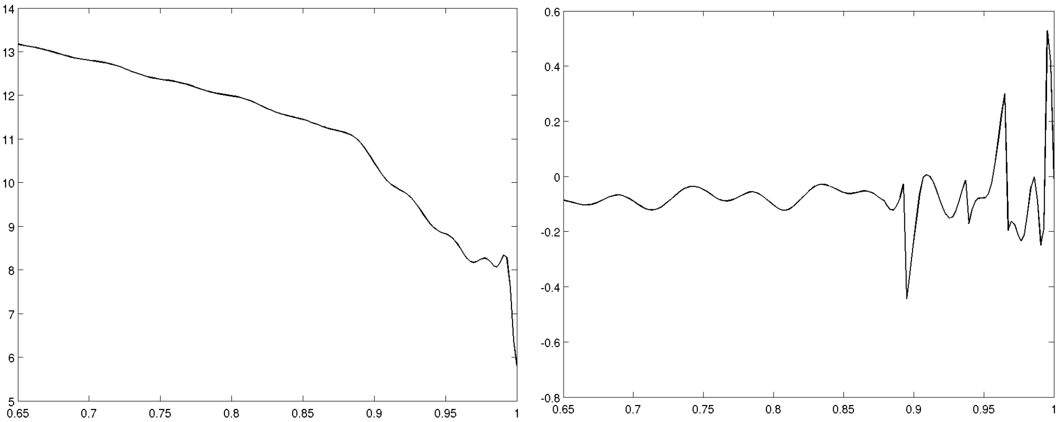
(a) paths of 360 synthetic rays (b) paths of 300 synthetic rays

Figure 5.3: paths of synthetic rays generated according to V_1 and plotted on the plane $\phi = 90°$

Here we run two numerical tests. In the first one we reconstruct $V_1(r)$ in the segment $r \in [0.65, 1]$ with $\theta = 120°$ and $\phi = 90°$ (see Figures 5.4 and 5.5) using the synthetic ray system presented in Figure 5.3(a), while in the second one we approximate the function $V_2(\bar{x}(r,\theta,\phi)) := 5 + 0.1\,\sin(5r)\cos(20\theta)$ at $r = 0.98$,

$r = 0.99$, $\theta \in [100°, 125°]$ and $\phi = 90°$ (see Figures 5.6 and 5.7) using the synthetic ray system presented in Figure 5.3(b). The integral terms representing the matrix components and the spline basis have been calculated approximately with the trapezoidal rule, where the series in (5.9) has been truncated at level 50. Moreover, a smoothing (regularization) of the linear equation system, with a smoothing parameter ρ, has been done.

The results show that with our spline method we are able to obtain a good approximation for a relatively smooth model (see Figures 5.6 and 5.7) as well as for a model with a rather big variations (see Figures 5.4 and 5.5). Hence, the described spline approximation method proved to be an alternative to the existing methods in seismic body wave tomography.



(a) reconstruction of V_1 (b) error of the reconstruction of V_1

Figure 5.4: reconstruction and corresponding error of V_1 using the rays in Figure 5.3(a), with $\lambda_1 = 0.001$, $\lambda_2 = 10$, $\rho = 10^{-6}$

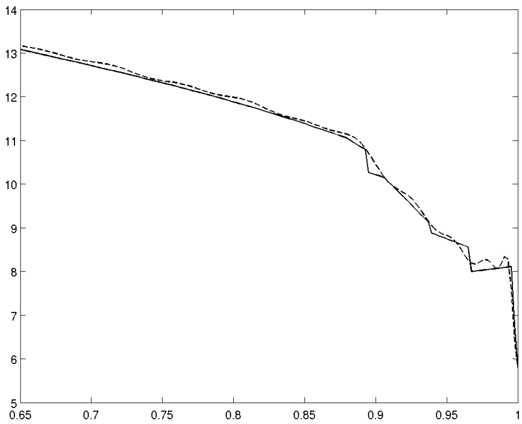
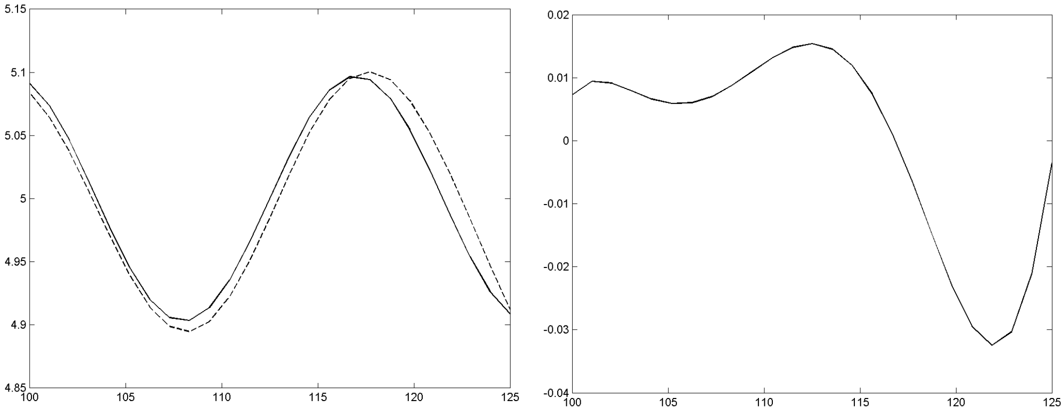


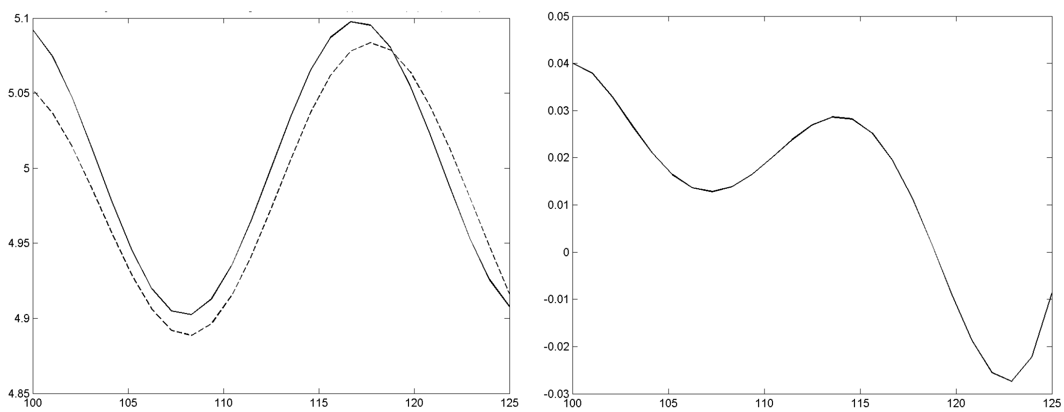
Figure 5.5: comparison of the profiles of V_1 (solid line) and its reconstruction (dashed line)



(a) comparison of the profiles of V_2 (solid line) and its reconstruction (dashed line)

(b) error of the reconstruction of V_2

Figure 5.6: reconstruction of $V_2(r, \theta)$ using the rays in Figure 5.3(b), with $\lambda_1 = 0.2$, $\lambda_2 = 0.3, \rho = 0.04$ at $r = 0.99$, $\theta \in [100°, 125°]$ and $\phi = 90°$



(a) comparison of the profiles of V_2 (solid line) and its reconstruction (dashed line)

(b) error of the reconstruction of V_2

Figure 5.7: reconstruction of $V_2(r, \theta)$ using the rays in Figure 5.3(b), with $\lambda_1 = 0.2$, $\lambda_2 = 0.3, \rho = 0.04$ at $r = 0.98$, $\theta \in [100°, 125°]$ and $\phi = 90°$

5.4 On Uniqueness and Convergence Results

If the reference slowness model S_0 depends only on the radius r, i.e. $S_0 = S_0(r)$ $r = |x|$, $x \in B$, then the rays are planar (see e.g. [1], [12]) and Problem 2.2.6 can be considered separately in each cross-section of B by the plane of a great circle. Hence, the problem of finding the function $\mathcal{S}$ becomes planar, and can be formulated as follows.

Problem 5.4.1 *Given a function $\tau(u) = \tau(\nu_1, \nu_2)$, $u = (\nu_1, \nu_2) \in \Omega_2 \times \Omega_2$, find a continuous function S on B_2 such that*

$$\tau(\nu_1, \nu_2) = \int_{\gamma_{S_0}(u)} S(x) d\sigma(x), \tag{5.10}$$

where Ω_2 and B_2 are the unit circle and respectively the unit disk in $\mathbb{R}^2$.

For this problem V. Romanov (see [61]) obtained the following uniqueness result.

Theorem 5.4.2 *Let $r_0 > 0$ and the function $m(r) = rS_0(r)$ satisfy the conditions*

$$m(r) > 0, m'(r) > 0, m(r) \in \mathrm{C}^{(2)}[r_0, 1]. \tag{5.11}$$

in the domain $D = \{x : r_0 \leq |x| \leq 1\}$. In this case the continuous function S is uniquely defined in the domain D by the function $\tau(\nu_1, \nu_2)$ for those $\nu_1, \nu_2 \in \Omega_2$ for which the rays $\gamma(\nu_1, \nu_2)$ are contained in D.

In our case of the reference velocity function V_0 defined in the previous section, we see that $S_0 = 1/V_0$ is a piecewise smooth (continuously differentiable) function, and therefore can be arbitrarily well approximated by a smooth function, which again will be denoted by S_0. So, we can assume that $S_0 \in \mathrm{C}^{(2)}[0, 1]$. Hence, $m(r) = rS_0(r)$ is in $\mathrm{C}^{(2)}[0, 1]$, too.

As we can see from Figure 5.8, $m'(r) > 0$ for $r \in [d_2, 1]$. Hence, from Theorem 5.4.2 follows that (5.10) uniquely determines S in $\{x : d_2 \leq |x| \leq 1\}$. However, we will see that in the whole B_2 the solution of Problem 5.4.1 in general can be non-unique.

Let $S_1 : B_2 \to \mathbb{R}$ be a solution of Problem 5.4.1. We present a procedure to construct a function $S_2 \in \mathrm{C}(B_2)$ which differs from S_1 and which solves Problem

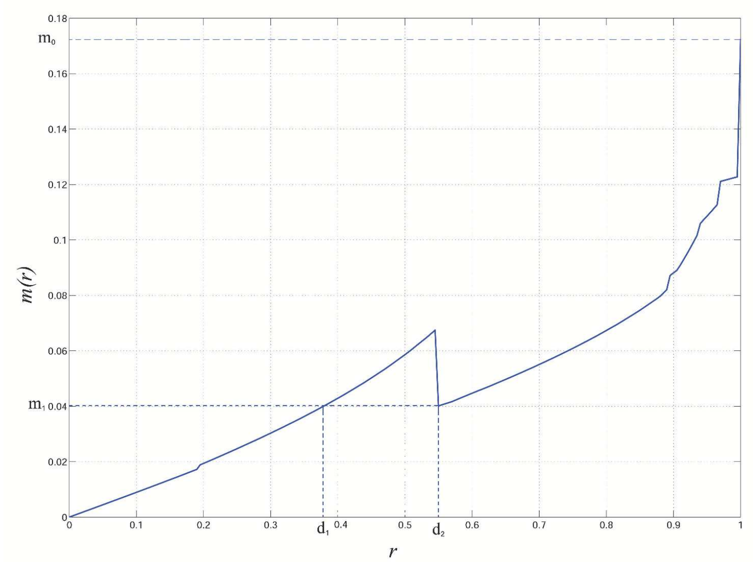


Figure 5.8: Plot of $m(r) = rS_0(r)$

5.4.1. From Figure 5.8 we can see that $m(r)$ monotonically decreases from m_0 to m_1 with the decreasing r in $[d_2, 1]$. In $[d_1, d_2]$ it increases then again decreases with the decreasing r, such that $m(d_1) = m(d_2) = m_1$. In this case it can be shown that there is no ray with the *turning point* (see Section A.2) in $[d_1, d_2]$ (see e.g. [1], [12]).
Denote $D_1 := \{x \in \mathbb{R}^2 : |x| \leq d_1\}$, $D_2 := \{x \in \mathbb{R}^2 : d_1 \leq |x| \leq d_2\}$ and $D_3 := \{x \in \mathbb{R}^2 : d_2 \leq |x| \leq 1\}$. Take $F_1 \in \mathrm{C}(D_2 \cup D_3)$ such that $F_1 = S_1$ on D_3 but $F_1 \neq S_1$ on D_2. For any seismic ray $\gamma(\nu_1, \nu_2)$, $\nu_1, \nu_2 \in \Omega_2$ that intersects D_1, denote by $\gamma'(\nu_1, \nu_2)$ the part of $\gamma(\nu_1, \nu_2)$ whose image is in D_1, by $\gamma''(\nu_1, \nu_2)$ the part of $\gamma(\nu_1, \nu_2)$ whose image is in $D_2 \cup D_3$ (see Figure 5.9), and denote

$$\tau'(\nu_1, \nu_2) := \tau(\nu_1, \nu_2) - \int_{\gamma''(\nu_1,\nu_2)} F_1(x) d\sigma(x).$$

Discuss now the problem of finding a function S which is given on D_1 by the equation

$$\tau'(\nu_1, \nu_2) = \int_{\gamma'(\nu_1,\nu_2)} S(x) d\sigma(x). \qquad (5.12)$$

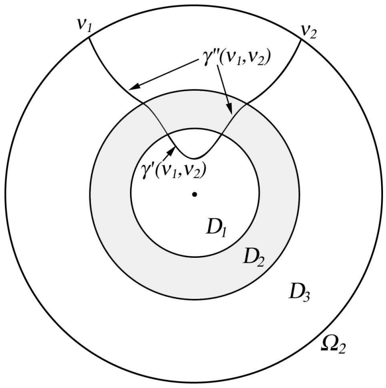


Figure 5.9: illustration of D_1, D_2, D_3 and $\gamma(\nu_1, \nu_2)$

If we suppose that there exists $F_2 \in \mathrm{C}(D_1)$ such that it solves (5.12) and $F_2 = F_1$ on the boundary of D_1, then it is easy to check that the function

$$S_2(x) = \begin{cases} F_1(x), & x \in D_2 \cup D_3, \\ F_2(x), & x \in D_1, \end{cases}$$

will be a solution of Problem 5.4.1 which differs from S_1.
Clearly, the existence of such an F_2 depends on F_1, in particular it depends on the values of F_1 on D_2. We shall mention that the problem of describing the set of such functions, i.e. the problem of describing the set of non-uniqueness of the solution of Problem 5.4.1 is still open.
For the one-dimensional and non-linear analog of Problem 5.4.1 the nature of the non-uniqueness of the solution was studied by M. Gerver and V. Markushevich (see [29], [30]).
Taking into account facts mentioned above, from Assumption 2.2.8 follows that if the sets of the given seismic sources and receivers are dense in Ω, then the function $\tau(\cdot, \cdot)$ uniquely determines the function S in D_3. However, in this case the corresponding system of functionals need not to be complete in whole $\mathcal{W}$, and thus, the convergence Theorem 3.7.5 can be invalid. Note that it is possible to develop the described spline approximation concept in a closed spherical shell as well. The closed spherical shell is compact and thus, can be considered as an initial set. Hence, here the problem is the choice of the corresponding initial basis system. For similar bases see e.g. [76] and the references therein.

Chapter 6

Conclusions and Outlook

The main aim of this work was to obtain an approximate solution of the seismic traveltime tomography problems with the help of splines based on reproducing kernel Sobolev spaces. It was shown that the seismic traveltime tomography problem is ill-posed and regularization can be constructed with the help of such splines. In order to be able to apply the spline approximation concept to surface wave as well as to body wave tomography problems, the spherical spline approximation concept was extended for the case where the domain of the function to be approximated is an arbitrary compact set in $\mathbb{R}^n$ and a finite number of discontinuity points is allowed. This concept was discussed in details for the case of the unit ball and the unit sphere. Furthermore, we presented applications of such spline interpolation/approximation method to seismic surface wave as well as body wave tomography, and discussed the theoretical and numerical aspects of such applications. It has been shown that the question of uniqueness of the seismic traveltime tomography problem and the question of convergence of the interpolating spline sequence have close relationship; more precisely the sequence of interpolating splines converges if and only if the corresponding system of functionals is complete in a corresponding space. In other words in that case if the corresponding system of functionals is complete then the constructed spline method enables a well-posed determination of an arbitrarily good approximation to the solution of the seismic traveltime tomography problem. It also has been shown that in the case of surface wave tomography for that completeness it is enough that the union of the sets of given seismic sources and receivers is dense

on the sphere.
The results of numerous numerical tests have been presented in this work as well. For the surface wave tomography the numerical tests include the reconstruction of the Rayleigh and Love wave phase velocity at 40, 50, 60, 80, 100, 130 and 150 seconds and comparison (for some phases) with the corresponding maps obtained with the well-known spherical harmonics approximation method. Moreover, some tests with synthetic data sets including the so-called checkerboard tests, a test by adding random noise to the initial traveltime data and a test with a so-called hidden object have been presented as well. It has been observed that the phase velocity maps obtained via splines have similar structure as the corresponding maps obtained via the spherical harmonic approximation method. However, in the tests with the synthetic data sets it was shown that splines (in particular in case of local/localized models) allow more accurate reconstruction. For the body wave tomography numerical tests include a partial reconstruction of the P-wave velocity function (according to PREM) and its perturbation with the use of synthetic data sets.
These results demonstrate that the spline interpolation or approximation method indeed represents an alternative to the present methods in seismic tomography. It was shown that this spline method can be used for global velocity determination as well as for local calculations. The advantage of the method should be the localizing character of the spline basis functions, which becomes clearly visible in case of local data sets or regional disturbances.
The disadvantage of the method is that it requires relatively large computational time, in particular for the calculation of the matrix $\mathbf{k}_N$ (see (3.15)), with a relatively big N. Moreover, since $\mathbf{k}_N$ has N^2 elements one requires $\mathcal{O}(N^2)$ operations for the necessary calculations. For some inverse problems there are algorithms which reduce the computational costs to, for example, $\mathcal{O}(N^\alpha)$, $1 \leq \alpha < 2$ or $\mathcal{O}(N \log N)$ (see e.g. [23], [31], [35]). This motivates further research on finding such a procedure for our problem. From the practical point of view, of course, it is interesting to obtain velocity models for body wave tomography, using real data sets, too. In this context the test calculations in Section 5.3 show promising results. The problem of choosing an "optimal" sequence $\{A_k\}_{k\in\mathbb{N}_0}$ (see Section 3.1) for each special approximation problem is also a topic of further research.

Appendix A

On Seismic Ray Theory

In this appendix, we shall present, without derivation or proofs, a brief introduction into the seismic ray theory in the context of this work. This introduction is based on [12] where further details can be found.

A.1 Seismic Rays

The waves that arise in earthquakes are called seismic waves. These waves propagate in the elastic body of the Earth according to the laws of geometric seismology which are altogether analogous to the laws of propagation of a light ray. The trajectories, which are orthogonal to the wave fronts, are here called *seismic rays*, by analogy with a light ray.

The study on seismic rays can be divided into two parts: *kinematic* and *dynamic*. The computation of seismic rays, wave fronts, and traveltimes are subject of the kinematic part, while the computation of synthetic seismograms, particle ground motion diagrams and the vectorial amplitudes of the displacement vector are subject of the dynamic part. These both parts can be investigated by the application of so-called asymptotic high-frequency methods to the elastodynamic equations. The kinematic part, however, may also be developed by some simple approaches, for example, by Fermat principle. In this work we are interested only in the kinematic part of seismic ray theory.

Let $v(\cdot)$ be the propagation speed of the seismic wave. Since in the body of the Earth v is not constant but varies from point to point, seismic rays are not straight lines. Fermat's principle from variational calculus (see e.g. [12], [18]) states: *a ray joining any pair of points x_0, x is an extremal of the functional*

$$J(l) = \int_{l(x_0,x)} \frac{1}{v(y)} d\sigma(y), \tag{A.1}$$

where $l(x_0, x)$ is an arbitrary sufficiently smooth curve joining the pair of points x_0, x; $d\sigma(x)$ is the element of its length in the Euclidean metric.

Clearly, from (A.1) follows that $J(l)$ gives the time a wave takes to travel from the point x_0 to x over the curve $l(x_0, x)$. Thus, a seismic ray is a curve $l(x_0, x)$ on which the traveltime of the wave is a minimum. Actually, for rather complex media where the function v differs strongly from a constant, the pair of points x_0, x can be joined by several rays (or even an uncountable set of rays), where on each of these rays the functional $J(\cdot)$ has a minimum. In this case we will take as a seismic ray any particular one of them.

We denote the seismic ray joining the points x_0 and x by $\gamma(x_0, x)$. So, the traveltime $\tau(x_0, x)$ of the wave along this ray or so-called first-arrival traveltime between x_0 and x is calculated by the formula

$$\tau(x_0, x) = \int_{\gamma(x_0,x)} \frac{1}{v(y)} d\sigma(y). \tag{A.2}$$

The wave front at $T =$ const is the surface defined by the equality $\tau(x_0, x) = T$, where x_0 is fixed. Let $\nu(x_0, x)$ be the unit vector tangential to the ray $\gamma(x_0, x)$ at the point x directed to the side of increasing τ. Then (A.2) implies that

$$\nabla_x \tau(x_0, x) = \frac{1}{v(x)} \nu(x_0, x) =: \mathbf{s}(x_0, x),$$

where $\nabla_x \tau$ denotes the gradient of the function τ computed with respect to the variable x and $\mathbf{s}$ is the slowness vector. We denote also $s = |\mathbf{s}|$, i.e. $s(x) = 1/v(x)$. Hence, we arrive at the so-called *Eikonal equation*

$$|\nabla_x \tau(x_0, x)|^2 = s^2(x). \tag{A.3}$$

As is demonstrated in the variational calculus (see e.g. [12]) the *characteristics* of this nonlinear first-order partial differential equation are precisely the rays, i.e. the extremals of the functional in (A.1).

Let the distance of the ray path measured along the ray be σ, and the length of the ray path be L. Let also the parametric equation of the ray path be written as $\mathbf{x} = \mathbf{x}(\sigma)$, $\sigma \in [0, L]$. In this case from the Eikonal equation (A.3) using the method of characteristics one can derive the so-called *ray tracing system*

$$\frac{\partial \mathbf{x}}{\partial \sigma} = v\,\mathbf{s}, \quad \frac{\partial \mathbf{s}}{\partial \sigma} = \nabla \left(\frac{1}{v} \right). \tag{A.4}$$

These equations give a system of six first order ordinary differential equations which in general must be integrated numerically to find the ray path $\mathbf{x} = \mathbf{x}(\sigma)$ (for more see e.g. [12]). In some special cases it is also possible to find an analytical solution of the system (A.4).

A.2 Mohorovičić velocity distribution

Let the unit ball $B = \{x \in \mathbb{R}^3 : |x| \leq 1\}$ be an approximation to the Earth. In the spherical coordinates B can be represented as $B = \{(r, \theta, \phi) : r \in [0,1], \theta \in [0, \pi], \phi \in [0, 2\pi)\}$. Assume that a wave velocity function v is depends only on the radius r, i.e. $v = v(r)$, $r \in [0,1]$. Moreover, suppose that B can be divided into N layers defined by spherical surfaces $r_0 = 0, r_1, r_2, ..., r_N = 1$, where in the layer i, i.e. when $r_{i-1} \leq r < r_i$ the velocity function v can be represented as

$$v(r) = A_i\, r^{(1-C_i)}, \quad A_i, C_i = \text{const.} \tag{A.5}$$

Velocity distribution (A.5) is known as the Mohorovičić velocity law (see [11]) or also as Bullen's velocity law. Following [12] we present here an analytical solution of the ray tracing system (A.4), in case of v being given by (A.5).
Since the velocity v is depends only on r, a ray as a whole is situated in a plane passing through the origin of B, the start and the end point of the ray in question. So, any point of a ray can be represented by two coordinates, say (r, θ). It should be mentioned also that in this case a ray is symmetric with respect to the line passing through the origin of B and the mid-point of the part of the great circle connecting the start and the end points of the ray in question (see e.g. [1], [12]).
Let now γ be an arbitrary ray with start point $P = (r_P, \theta_P)$ and end point $Q = (r_Q, \theta_Q)$. The traveltime corresponding to γ will be denoted by T_γ, i.e.

$$\int_\gamma \frac{1}{v(x)} d\sigma(x) =: T_\gamma.$$

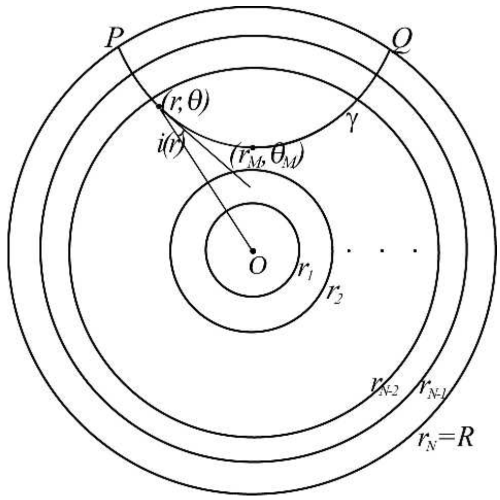


Figure A.1: illustration of a ray path

Let (r, θ) be an arbitrary point on γ. The acute angle between the radius vector of (r, θ) and the tangent vector of γ at (r, θ) is denoted by $i(r)$ (see Figure A.1). Here, we have that

$$p := \frac{r \sin i(r)}{v(r)} = \text{const.} \tag{A.6}$$

In seismology p is usually called the *ray parameter*, and (A.6) is the *generalized Snell's law* for a radially symmetric medium (see e. g. [1], [11]).
Denote the coordinate r of the *turning point* of γ (i.e. the point on γ with the minimal radius vector) by r_M (see Figure A.1), i.e. $i(r_M) = \pi/2$, and $r_M/v(r_M) = p$. Moreover,

$$w(r) := \sqrt{\frac{r^2}{v^2(r)} - p^2}, \quad r \in [0, 1],$$

and

$$r(t) := a\, t^2 + b\, t + 1, \quad t \in [0, T_\gamma], \tag{A.7}$$

where $a := 4(1 - r_M)/T_\gamma^2$ and $b := -4(1 - r_M)/T_\gamma$.
Choose $j \in \mathbb{N}$ such that $r_{j-1} \le r_M < r_j$, i.e. r_M is in the j-th layer.
Take any $t \in [0, T_\gamma]$ and let $r(t)$ be in the k-th layer, i.e. $r_{k-1} \le r(t) < r_k$.
Now

(i) if $t \le T_\gamma/2$ then denote

$$\theta(t) := \theta_P + \sum_{i=k+1}^{N} \left(\frac{-1}{C_{i-1}}\right)\left(\arctan\left(\frac{w(r_{i-1})}{p}\right) - \arctan\left(\frac{w(r_i)}{p}\right)\right)$$
$$+ \left(\frac{-1}{C_{k-1}}\right)\left(\arctan\left(\frac{w(r(t))}{p}\right) - \arctan\left(\frac{w(r_k)}{p}\right)\right),$$

(ii) if $t > T_\gamma/2$ and $k = j$ then

$$\theta(t) := \theta(T_\gamma/2) + \left(\frac{-1}{C_{k-1}}\right)\left(\arctan\left(\frac{w(r(t))}{p}\right) - \arctan\left(\frac{w(r_M)}{p}\right)\right),$$

(iii) otherwise, i. e. if $t > T_\gamma/2$ and $k > j$ then

$$\theta(t) := \theta(T_\gamma/2) + \left(\frac{-1}{C_{k-1}}\right)\left(\arctan\left(\frac{w(r(t))}{p}\right) - \arctan\left(\frac{w(r_M)}{p}\right)\right)$$
$$+ \sum_{i=j}^{k-1} \left(\frac{-1}{C_i}\right)\left(\arctan\left(\frac{w(r_{i+1})}{p}\right) - \arctan\left(\frac{w(r_i)}{p}\right)\right)$$
$$+ \left(\frac{-1}{C_{k-1}}\right)\left(\arctan\left(\frac{w(r(t))}{p}\right) - \arctan\left(\frac{w(r_k)}{p}\right)\right).$$

Finally, from [12] pp. 177 follows that γ can be parameterized by the equation

$$x(t) = (r(t), \theta(t)), \quad t \in [0, T_q],$$

where $r(t)$ and $\theta(t)$ are defined above.
It is easy to check that in this case $x(\cdot) \in \mathrm{C}^1[0, T_\gamma]$, i.e. $x'(\cdot)$ is a continuous function on $[0, T_q]$. Note that actually in [12] the parametrization of γ is given using r as a parameter, in which case $\theta'(r)$ is not continuous at r_M, that is why, to avoid that discontinuity, we introduced the parameter t.

A.3 The Linearized Eikonal Equation

Equation (A.3) is nonlinear. To linearize it we assume that an initial estimate s_0 of the slowness function s is available. The traveltime corresponding to s_0 will be denoted by τ_0. From (A.3) we have

$$|\nabla \tau_0|^2 = s_0^2. \tag{A.8}$$

Denote also $\tau_1 := \tau - \tau_0$, and $s_1 := s - s_0$. With these definitions, we can rewrite Equation (A.3) in the form

$$(\nabla\tau_0+\nabla\tau_1)^2 = (\nabla\tau_0)^2+2\nabla\tau_0\cdot\nabla\tau_1+(\nabla\tau_1)^2 = (s_0+s_1)^2 = s_0^2+2s_0s_1+s_1^2, \quad \text{(A.9)}$$

or, taking into account the Equation (A.8),

$$2\nabla\tau_0\cdot\nabla\tau_1 + (\nabla\tau_1)^2 = 2s_0s_1 + s_1^2. \quad \text{(A.10)}$$

Neglecting the squared terms, we arrive at the equation

$$\nabla\tau_0\cdot\nabla\tau_1 = s_0s_1, \quad \text{(A.11)}$$

which is the linearized version of the eikonal equation (A.3). The accuracy of the linearization depends on the relative ratio of the slowness perturbation s_1 and the true slowness model s. Although it is difficult to give a quantitative estimate, in seismology the ratio of 10% is generally assumed to be a safe upper bound.

We can rewrite Equation (A.11) in the form

$$\nu_0\cdot\nabla\tau_1 = s_1, \quad \text{(A.12)}$$

where ν_0 is the unit vector, pointing in the gradient direction for the initial traveltime τ_0. The integral solution of Equation (A.12) takes the form

$$\tau_1(x_0,x) = \int_{\gamma_0(x_0,x)} s_1(x)d\sigma(x), \quad \text{(A.13)}$$

which states that the traveltime perturbation τ_1 can be computed by integrating the slowness perturbation s_1 along the ray γ_0 defined by the initial slowness model s_0 (see e.g. [12], [42], [61]). This is the basic principle of traveltime linearized tomography.

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Eidesstattliche Erklärung

Hiermit erkläre ich an Eides statt, dass ich die vorliegende Arbeit selbst und nur unter Verwendung der in der Arbeit genannten Hilfen und Literatur angefertigt habe.

Kaiserslautern, 22. November 2006