An Alternative Approach to the Oblique Derivative Problem in Potential Theory

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

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Vollzug der Promotion: 8. September 2004

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This thesis has evolved with the advice, feedback and help of many people. In particular I would like to express my gratitude to Prof. Dr. W. Freeden for giving me the opportunity to work on this subject and supporting me with advice and suggestions throughout my time. Furthermore I would like to thank HDoz. Dr. V. Michel for valuable discussions and my cooperation partner Dr. P. Schwintzer for answering detailed questions concerning forthcoming satellite missions.

A part of my work is concerning the symbolical solution of partial differential equations. At this point I would like to express my thanks to Dr. habil. W. Seiler, M. Hausdorf, HDoz. Dr. E. Zerz, Dr. A. Quadrat and in particular to V. Levandovskyy for their valuable ideas and directing me to important literature.

Furthermore I would like to especially thank Prof. Dr. S. Pereverzev for giving a very interesting lecture course on inverse problems. This lecture constitutes the basis of my treatment of severely ill-posed problems and gave rise to intense and fertile discussions on this topic. As I am not an expert in stochastics I gratefully acknowledge the patience of Dr. J.-P. Stockis who helped me whenever I had a problem at the borderline between functional analysis and stochastics.

At last I want to thank everybody whom I have not mentioned before including the members of the Geomathematics Group and my family.

The financial support of the Graduiertenkolleg "Mathematik und Praxis" financing my two and a half years of research is gratefully acknowledged.

Contents

Preface

Nowadays one of the major objectives in geosciences is the determination of the gravitational field of our planet, the Earth. A precise knowledge of this physical quantity is not just interesting in its own but it is indeed a key point for a vast number of applications. In particular we want to mention:

- *Geoid.* The geoid is the height of the sea level, i.e., the gravitational force has the same value at each point of this surface. The real height above (or sometimes below) sea level can now be obtained by further measurements like GPS or laser ranging.
- *Prospecting and Exploration.* Natural resources are often accompanied by a different specific weight of the surrounding soil layers. This leaves a kind of fingerprint, small spatial perturbations, in the geopotential field and hence can be detected.
- *Satellite Orbits.* A precise knowledge of the gravitational field enhances the prediction of spacecraft orbits considerably.
- *Solid Earth Physics.* Tectonic processes cause mass inhomogeneities of the lithosphere and as a consequence gravity anomalies which can be measured.
- *Physical Oceanography.* Ocean currents are the source of huge water displacements which result in an actual sea level height which differs from the theoretical sea level determined by the geoid. These height differences enable us to get a better description of these currents.
- *Climate Predictions.* Moving air causes mass anomalies which can be detected with a sufficiently time sensitive measurement of the geopotential field.

This selection of possible applications displays the need for a very accurate model of the geopotential field. However, it is difficult to get information of sufficient accuracy and coverage of the potential directly. Another possible way to retrieve information is measuring the change in the potential, i.e., the gradient or even higher derivatives like the Hesse tensor. Therefore we are facing the question how to obtain this kind of data for a sufficient number of places on the Earth. There are several possibilities which all have their advantages and disadvantages.

- *Terrestrial.* Measurements taken on the ground are the oldest source of information, which locally provides a very dense set of data. However, obstacles are manifold ranging from unsuitable terrain for measurement campaigns over political instabilities to a simple lack of financial resources.

- *Airborne.* Gravitational field determination onboard of a plane is still expensive and also is not capable to provide a sufficient global coverage.

- *Satellite tracks.* Satellites are comparably cheap (taken as a data/cost ratio) and also allow a near to global coverage. One possibility is determining the perturbations of the satellite track due to changes in the gravitational field.

  Satellites have a particular problem. The lower they fly the shorter their life expectance and the higher they fly the bigger the error due to the smoothing of the geopotential field leading to an amplification of the unavoidable measurement errors during the downward continuation process to the Earth's surface. Recent examples are CHAMP (Challenging Minisatellite Payload for Geoscience and Application, launched 2000) and GRACE (Gravity Recovery and Climate Experiment, launched 2003)

- *Spaceborne Gradiometer.* Gradiometer onboard of a satellite enable us to do highly precise measurements but are considerably more expensive than the above variant. The other advantages and disadvantages are right the same. An example is GOCE (Gravity Field and Steady State Ocean Circulation Explorer, launch expected 2006)

Currently one mostly concentrates on getting the geopotential field out of the radial component of the measured derivatives. In principle, this is rather efficient because the reconstruction out of these data is mathematically seen of good nature and the error in this direction is often lower than for the other components. However, just using a relatively small selection of the measured data seems to be a waste. Furthermore an interesting question is how to combine data from completely different sources and positions.

These are exactly the points the following text intends to deal with. We will investigate a sensible possibility to use all obtainable data in a unified setup. Furthermore we will make some improvements at various points.

Introduction and Outline

As we have seen in the preface there is a major interest in a good knowledge of the gravitational field of the Earth. Over the past decades a huge amount of data concerning gravity have been measured out of which one can recover the gravitational field. However, we will not try to tackle this task immediately but take a closer look on the underlying mathematical problems. Actually all of them are special cases of the oblique derivative problem which we want to analyze in this thesis.

First we will give a short mathematical description of the oblique derivative problem. Then we will display some interesting special cases occurring in the geosciences. Afterwards we intend to describe our approach and our results briefly.

1.1 Oblique Derivative Problem

In many fields of geophysics we have the following situation. The behavior of a certain quantity can be described by a differential equation for the whole or a major part of the space. A prominent example is the gravitational field which fulfills the Laplace equation in the outer space of the Earth Σ_{ext}. However we are just able to measure data, e.g., derivatives of the quantity we are interested in, in a very limited area, most of the time just at a surface.

Nevertheless we want to know how the quantity looks like on the whole space. Because we are dealing with a real world situation we are not just interested in existence and uniqueness of our solution but also in how to actually get it and what errors we are facing. This is a physically motivated description of the oblique derivative problem, now we will give a mathematical one.

1.1.1 Definitions

Let V be in an appropriate function space $\mathcal{S}$ defined on $\Sigma_{ext} \subset \mathbb{R}^N$. This V will be the function we are seeking for.

A m^{th} order differential operator $\underline{\Delta}$ in Σ_{ext} is defined as

$$\underline{\Delta} = \sum_{|\mu| \leq m} A_\mu \partial_\mu$$

where the μ are multiindices for an N-dimensional space, ∂_μ the differentials in the corresponding directions and $A_\mu : \Sigma_{ext} \to \mathbb{R}$ smooth functions.

$\Sigma_{ext} \subset \mathbb{R}^N$ is now the set on which V should fulfill the following partial differential equation:

$$\underline{\Delta} V = 0$$

Equivalently one can define differential operators $\{d_k\}_{k\in\{1,\ldots,n\}}$ on Σ_{ext} with smooth functions $D_{k,\mu} : \Sigma_{ext} \to \mathbb{R}$:

$$d_k = \sum_{|\mu|\leq m_k} D_{k,\mu}\partial_\mu$$

which should fulfill the following n equations (side conditions):

$$(d_k V)|_{\Sigma_k} = F_k \qquad \text{for all } \; k \in \{1,\ldots,n\}$$

where the $\Sigma_k \subset \Sigma_{ext}$ and $F_k : \Sigma_k \to \mathbb{R}$ correspond to the input, e.g., measurements. Please note that $(d_k V)|_{\Sigma_k}$ does not mean that d_k is constrained to Σ_k but that this equation just needs to hold on the subset Σ_k

Now we want to know how V looks like on the whole set Σ_{ext}. Therefore we are interested in the following properties:

- Existence of V.
- Uniqueness of V.
- A constructive possibility how to get V out of the F_k.
- An estimate how near we actually get to V, when we work with perturbed data or discrete sets Σ_k.

Usually it is possible to reconstruct V out of one of the equations $d_k V = F_k$ completely or at least to a large amount. Therefore one normally restricts the attention to one side condition $(d_k V)|_{\Sigma_k} = F_k$ at a time and puts together the results later on.

Now we will show two possible specializations of the oblique derivative problem occurring in the geoscientific context. For a much more detailed account on this topic and a vast collection of corresponding literature we want to refer the reader to [Fre99, FGS98, FM03b]. Additionally we will take a more mathematical look on this in the chapter on geoscientifical problems.

1.1.2 Oblique Boundary Value Problem

The first specialization of the oblique derivative problem is the oblique boundary value problem. Using the notation from above we have that Σ_{ext} is the exterior of the Earth including its surface and Σ_k is the Earth's surface. The underlying partial differential equation is the Laplace equation

$$\Delta V = 0$$

Possible terrestrial data available include the gravitational potential itself (Satellite Altimetry), the first derivative (Gravimetry and Geometric-Astronomical Levelling) and the second derivative (Terrestrial Gradiometry) but it should be mentioned that none of the above data is globally available.

Neglecting the fact that not every derivative allows an exact reconstruction the oblique boundary value problem is of good nature. Possible solution concepts include integral equations [Kel67], pseudo differential equations and mere approximation [FGS98].

In the literature the following cases including solutions have been discussed

- First order differentials, which are not tangential to the boundary, especially [FK81], the references therein and [GT97].
- First and second order radial derivatives in radial direction, e.g., in [FGS98].

Furthermore we know

- For a very limited number which tangential (first or second order) derivatives need to be combined in order to get a complete reconstruction.

Beyond these possibilities we want to consider the much more general case

- First and second order oblique derivatives, i.e., not necessarily non-tangential to the boundary and not just the radial direction.

1.1.3 Oblique Satellite Problem

The second specialization of the oblique derivative problem is the oblique satellite problem. Using the notation from beforehand we again have that Σ_{ext} is the exterior of the Earth including its surface and the Σ_k are satellite tracks. Please note that just in very unusual cases the satellite tracks can be considered as a subset of a surface outside the Earth because normally every satellite track is slightly elliptic and its semimajor axis does not coincide with the rotation axis of the earth.

Again the underlying partial differential equation is the Laplace equation reading

$$\Delta V = 0$$

This time our observables are the first derivatives (Satellite-to-Satellite Tracking) and second derivatives (Satellite Gravity Gradiometry).

This problem is ill-posed, i.e., small perturbations in the input data lead to large differences in the results. The necessary regularization ("downward-continuation") will be described in detail in the chapter concerning Noise and Regularization.

In the literature the following cases including solutions have been discussed

- First and second order radial derivatives in radial direction, e.g., in [Fre99].

Furthermore we know

- For a very limited number which tangential (first or second order) derivatives need to be combined in order to get a complete reconstruction [Sch94].

Beyond these possibilities we want to consider the much more general case

- First and second order oblique derivatives, i.e., derivatives not pointing in the radial direction.

1.2 Outline

Now we want to give a brief outline of the thesis. Our ultimate goal is to provide new tools for getting the gravitational field out of various sources. Therefore we need to consider the next two points in more detail

- Treatment of oblique derivatives.
- Combination of data from different sources.

We will not try to give a completely new solution technique but to enlarge the possibilities and improve the process at several distinct points.

1.2.1 Operator Split Approach for Δ

How can one solve the oblique derivative problem occurring in the geoscientifical context?

This question will be partly answered in Chapter 2 (Split Operators for Δ). Using a more general setup we will classify *all* first order and purely second order differential operators $\mathscr{d}$, where $\Delta(\mathscr{d}V) = 0$. This allows us to solve the oblique derivative problem as if we would just have non-derived data given. So standard methods are applicable. Afterwards we need to invert the differential operator $\mathscr{d}$ to get the final solution, i.e., we have to perform an integration.

In the geo-scientifically relevant case we have the following possibilities for $\mathscr{d}$; the $c_{\boxdot}$ are all real valued constants, x_1, x_2 and x_3 are the variables pointing in the corresponding directions of the Euclidean space, of which we consider the subset Σ_{ext}:

- First order differential operator $\mathscr{d} = \sum_{i=1}^{3} D_i \partial_i + D$.

$$\begin{pmatrix} D_1 \\ D_2 \\ D_3 \end{pmatrix} = \begin{pmatrix} c_r & c_{\neg 3} & c_{\neg 2} \\ -c_{\neg 3} & c_r & c_{\neg 1} \\ -c_{\neg 2} & -c_{\neg 1} & c_r \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

$$D = c$$

- Purely second order differential operator $\mathscr{d} = \sum_{i=1}^{3} \sum_{j=i}^{3} D_{ij} \partial_i \partial_j$.

$$\begin{aligned}
D_{11} =& c_{r,r} x_1^2 + c_{r,\neg 3} x_1 x_2 - c_{r,\neg 2} x_1 x_3 \\
& - c_{\neg 3,1} x_2 + c_{\neg 2,1} x_3 + c_{1,1} \\
D_{22} =& c_{r,r} x_2^2 - c_{r,\neg 3} x_1 x_2 + c_{r,\neg 1} x_2 x_3 \\
& - c_{\neg 3,2} x_1 - c_{\neg 1,2} x_3 + c_{2,2} \\
D_{33} =& c_{r,r} x_3^2 + c_{r,\neg 2} x_1 x_3 - c_{r,\neg 1} x_2 x_3 \\
& - c_{\neg 2,3} x_1 - c_{\neg 1,3} x_2 (+c_{3,3}) \\
D_{12} =& c_{r,\neg 3}(x_2^2 - x_1^2) + 2c_{r,r} x_1 x_2 + c_{r,\neg 1} x_1 x_3 - c_{r,\neg 2} x_3 x_2 \\
& + c_{\neg 3,1} x_1 + c_{\neg 3,2} x_2 - c_{\neg 2,2} x_3 - c_{\neg 1,1} x_3 + c_{1,2} \\
D_{13} =& c_{r,\neg 2}(x_1^2 - x_3^2) - c_{r,\neg 1} x_1 x_2 + 2c_{r,r} x_1 x_3 + c_{r,\neg 3} x_3 x_2 \\
& - c_{\neg 2,1} x_1 + c_{\neg 1,1} x_2 + c_{\neg 2,3} x_3 + c_{1,3} \\
D_{23} =& c_{r,\neg 1}(x_3^2 - x_2^2) + c_{r,\neg 2} x_1 x_2 - c_{r,\neg 3} x_1 x_3 + 2c_{r,r} x_2 x_3 \\
& + c_{\neg 2,2} x_1 + c_{\neg 1,2} x_2 + c_{\neg 1,3} x_3 + c_{2,3}
\end{aligned}$$

The advantage in comparison to other solution methods for the oblique derivative problem is that we can operate as if we actually would not have any oblique derivative. This means that we can rely on standard techniques for solving the oblique derivative problem which have been proven to be reliable in practice.

In particular we do not have any restrictions on our data location, every one which is suitable for the standard problem without derivatives as side conditions does the job. Especially for boundary value problems, where even a small quantity of derivatives which are sufficiently near to the tangent plane pose enormous problems this is really a leap forward. Additionally we can work with standard basis systems and do not have to switch to differentiated (anisotropic) ones.

However the most obvious advantage is that one has a particularly easy solution method for higher derivatives as side conditions. Even for derivatives higher than the second order ones we considered the approach transfers without major problems.

1.2.2 Integration

How does the corresponding integration look like? Do we have uniqueness in the reconstruction or do we have to take care of some kernel spaces?

The necessary computations will be done in Chapter 3 (Integration). We can show that for each of the operators $\mathscr{d}$ proposed above and for spherical harmonics as basis system [FGS98] the integration problem corresponds to solving several band limited systems of linear equations. We explicitly calculate these matrices there.

1.2.3 Geoscientifical Problems

Which mathematical tasks do we have to perform for the oblique boundary value problem and especially for the oblique satellite problem?

In this chapter we will give a more detailed account on the available data and on the mathematical tasks one has to perform for solving this problem.

1.2.4 Noise and Regularization

Does there exist a sensible stopping criterion for the inverse problem “downward-continuation” which allows optimal regularization?
We need to know an approximate error level of our solution after regularization.

This question will be answered in Chapter 5 (Noise and Regularization). In a first part we motivate that the noise model currently in use for ill-posed problems is not appropriate. We replace this noise model with another which seems to fit much better. Regularization under the assumption of this more general noise model is much harder and up till now not known for severely ill-posed problems.

We provide such an optimal regularization procedure using three (two) input data sets.

1.2.5 Unified Setup

How can one combine data from different sources , e.g., different differential components of the satellite and/or different measurement campaigns, in a sensible way? What conditions do we have to impose on the data?

We will answer this question in Chapter 6 (Combining Data in a Unified Setup). We show that from the mathematical point of view the best order for solving our problem is

1. Approximation of the differentiated data with respect to $\mathcal{d}_i$ at the height of the satellite track.
2. Downward-continuation.
3. Data combination and inverting the differential operators $\mathcal{d}_i$ (Integration).

The last point is achieved with a least squares approach on the operators $\mathcal{d}_i$. In particular we obtain that we do not have to care about the non-uniqueness of some of our differential operators $\mathcal{d}_i$ and that we actually minimize the occurring error.

1.2.6 Aspects of Scientific Computing

Does the method proposed in the solutions above actually work on data, derived from a geophysically relevant modell?

We will do the numerical tests in Chapter 7 (Scientific Computing). There we will show that each of the solutions of the above problems actually works in practice. In particular we perform separate tests for

- Downward-continuation.
- Oblique derivative problem.
- Combination of data from completely different data sets.

1.2.7 Remarks

We want to remark that for each of the problems above we will use a completely different strategy to attack it. Therefore some knowledge in the following topics is strongly advisable (ordered by chapter).

- *Chapter 2*
  - (computational) commutative algebra
  - methods for solving PDE's symbolically
- *Chapter 3*
  - basic potential theory
- *Chapter 4*
  - mathematical treatment of gravity data from satellites

- *Chapter 5*
  - stochastical methods
  - advanced knowledge about functional analysis and the theory of inverse problems
- *Chapter 6*
  - basic functional analysis
- *Chapter 7*
  - satellite problems

The following references are just a proposal which were utilized by the author. Any other good books on the mentioned topics should equally provide the background knowledge in a sufficient way: [CLO91, GP02, Sei94], [Wal71], [Fre99, FM03b], [BD96, Per03b], [Rud73] and [Sch97].

Chapter 2

Operator Split Approach for Δ

How can one solve the oblique derivative problem occurring in the geoscientifical context?

In the literature we find solutions for two cases:

- First order differentials, which are not tangential to the boundary (when we have a boundary value problem), e.g., in [FK81, GT97].

- First and second order radial derivatives in radial direction, e.g., in [FGS98].

There are mainly two different ways to classically treat this problem. The first one is an ansatz with an integral equation. The second possibility is an approximation of the given data with an appropriate basis system satisfying the Laplace equation.

Beyond these possibilities we want to consider the much more general case

- First and second order oblique derivatives, i.e., not necessarily non-tangential to the boundary (when we have a boundary value problem) and certainly not just the radial direction.

In order to tackle this problem we will need to introduce a more general setup. Therein we will demand a set of oblique derivatives at a subset which interacts in a special way with the underlying partial differential equation.

This will result in a system of nonlinear partial differential equations which needs to be solved symbolically. It will turn out to be much too complicated to get a general solution and hence we will restrict the attention to the geoscientifically relevant problem with the Laplace operator Δ. Its solution will be obtained for a special case using methods from (non-)commutative algebra.

Please note that our method is a new approach and has the standard teething problems. Although it is general and capable to deal with other operators than the Laplace one we are facing a number of algebraic equations which by now just seem to be solvable under hard restrictions. Furthermore the classification process we do does not return striking new results but "just" tells us that we do not have to do more investigations for the Laplace operator.

2.1 General Problem Setup and Solution Strategy

The oblique derivative problem is a special case of the following very general problem.

Problem 2.1

Let $\mathcal{S}$, $\mathcal{T}_1$ and $\mathcal{T}_2$ be separable normed linear function spaces defined on a domain Σ_{ext} and assume $\Sigma_D \subset \Sigma_{ext} \subset \mathbb{R}^n$. Let $\mathfrak{U} : \mathcal{S} \to \mathcal{T}_1$ and $\mathfrak{D} : \mathcal{S} \to \mathcal{T}_2$ be linear operators. Assume furthermore $T_1 \in \mathcal{T}_1$ and $T_2 \in \mathcal{T}_2$.
We search all $V \in \mathcal{S}$ fulfilling

$$\begin{aligned} \mathfrak{U}V &= T_1 \\ (\mathfrak{D}V)|_{\Sigma_D} &= T_2|_{\Sigma_D} \end{aligned}$$

Remark

Observe that we demand $\mathfrak{D}$ to be defined on the whole function space $\mathcal{S}$ and not just on the space with the functions restricted to Σ_D.

We can simplify the above problem by using the following standard method. If there does not exist at least one solution $\overline{V}$ for the first equation there is nothing to do. Otherwise we can use the linearity of the operator $\mathfrak{U}$ and this solution $\overline{V}$ by substituting V by $V - \overline{V}$ and T_2 by $T_2 - \mathfrak{D}\overline{V}$. Hence we get the following easier configuration:

Problem 2.2 (General Problem)

Let $\mathcal{S}$, $\mathcal{T}_1$ and $\mathcal{T}_2$ be separable normed linear function spaces defined on a domain Σ_{ext} and assume $\Sigma_D \subset \Sigma_{ext} \subset \mathbb{R}^n$. Let $\mathfrak{U} : \mathcal{S} \to \mathcal{T}_1$ and $\mathfrak{D} : \mathcal{S} \to \mathcal{T}_2$ be linear operators. Assume furthermore $T_2 \in \mathcal{T}_2$.
We search all $V \in \mathcal{S}$ fulfilling

$$\begin{aligned} \mathfrak{U}V &= 0 \\ (\mathfrak{D}V)|_{\Sigma_D} &= T_2|_{\Sigma_D} \end{aligned}$$

Remark

This is our oblique derivative problem in the geoscientifical case if we set Σ_{ext} to the exterior of the Earth, Σ_D to the data location, $\mathfrak{U} = \Delta$ and $\mathfrak{D} = d$ to an oblique derivative at Σ_D.

2.1.1 Bidirectional Split Operator

If we take a closer look at the above problem we see that there is just one difference in comparison to a problem with standard side condition. Instead of $V|_{\Sigma_D} = T_2|_{\Sigma_D}$ we have to fulfill $(\mathfrak{D}V)|_{\Sigma_D} = T_2|_{\Sigma_D}$. The problem would simplify considerably if we could remove this additional operator $\mathfrak{D}$.

Definition 2.1 (Bidirectional Split Operator)

$\mathfrak{U}_{\mathfrak{D}} : \mathcal{T}_2 \to \mathcal{T}_1$ *is called* bidirectional split operator *for* $\mathfrak{U}$ *with respect to* $\mathfrak{D}$ *if it fulfills the following property:*

$$\mathfrak{U}V = 0 \Leftrightarrow \mathfrak{U}_{\mathfrak{D}}\mathfrak{D}V = 0 \qquad \textit{for all } V \in \mathcal{S}$$

Remark

Neither existence nor uniqueness of $\mathfrak{U}_{\mathfrak{D}}$ is assured.

The next lemma highlights the significance of this new operator.

Lemma 2.1 (Bidirectional Split lemma)

Let $\mathfrak{U}_{\mathfrak{D}}$ *be a bidirectional split operator for* $\mathfrak{U}$ *with respect to* $\mathfrak{D}$*.*
V *is a solution of the problem*

$$\begin{aligned} \mathfrak{U}V &= 0 \\ (\mathfrak{D}V)|_{\Sigma_D} &= T_2|_{\Sigma_D} \end{aligned}$$

if and only if there exists $V_{\mathfrak{D}} \in \mathcal{T}_2$ *satisfying*

$$\begin{aligned} \mathfrak{U}_{\mathfrak{D}}V_{\mathfrak{D}} &= 0 \\ V_{\mathfrak{D}}|_{\Sigma_D} &= T_2|_{\Sigma_D} \\ \mathfrak{D}V &= V_{\mathfrak{D}} \end{aligned}$$

Proof

Using the definition of the bidirectional split operator we can replace $\mathfrak{U}V = 0$ by $\mathfrak{U}_{\mathfrak{D}}\mathfrak{D}V = 0$. Substituting $\mathfrak{D}V$ by $V_{\mathfrak{D}}$ yields the above result.
Because of the property $\mathfrak{U}V = 0 \;\textit{ iff }\; \mathfrak{U}_{\mathfrak{D}}\mathfrak{D}V = 0$, the "iff" also holds in our proposition. q.e.d.

Instead of solving the original problem we can now restrict ourselves to solving the following problem.

Problem 2.3

We search all $V_{\mathfrak{D}} \in \mathcal{T}_2$ *fulfilling*

$$\begin{aligned} \mathfrak{U}_{\mathfrak{D}}V_{\mathfrak{D}} &= 0 \\ V_{\mathfrak{D}}|_{\Sigma_D} &= T_2|_{\Sigma_D} \end{aligned}$$

After having accomplished this task, we just need to invert the operator $\mathfrak{D}$ in order to get the final result. This means that we split the original problem with a non-standard side condition $(\mathfrak{D}V)|_{\Sigma_D} = T_2|_{\Sigma_D}$ into a problem with a standard side condition $V_{\mathfrak{D}}|_{\Sigma_D} = T_2|_{\Sigma_D}$ and an additional integration problem $\mathfrak{D}V = V_{\mathfrak{D}}$. This was the motivation for calling $\mathfrak{U}_{\mathfrak{D}}$ bidirectional split operator.

Obviously this approach just makes sense if $\mathfrak{U}_{\mathfrak{D}}$ exists and if we can compute it. This will turn out to be a very hard problem.

2.1.2 Relaxations

The constraint $\mathfrak{U}V = 0 \Leftrightarrow \mathfrak{U}_{\mathfrak{D}}\mathfrak{D}V = 0$ is too strict in most cases. Obviously we require that there is no nonzero function V fulfilling $\mathfrak{U}V = 0$ which is mapped to 0 by $\mathfrak{D}$. Therefore we rule out a lot of possible candidates for $\mathfrak{D}$. So we need to relax the conditions imposed on the bidirectional split operator.

Definition 2.2 (Split Operator)

$\mathfrak{U}_{\mathfrak{D}} : \mathcal{T}_2 \to \mathcal{T}_1$ *is called* split operator *for* $\mathfrak{U}$ *with respect to* $\mathfrak{D}$ *if it fulfills the following property:*

$$\mathfrak{U}V = 0 \Rightarrow \mathfrak{U}_{\mathfrak{D}}\mathfrak{D}V = 0 \qquad \textit{for all } V \in \mathcal{S}$$

Remark

Observe that every bidirectional split operator is also a split operator. The opposite does not hold because $\mathfrak{U}_{\mathfrak{D}} = 0$ is a split operator but not a bidirectional one.

We also get a weaker version of the bidirectional split lemma which exactly has the same proof as this one:

Lemma 2.2 (Split Lemma)

Let $\mathfrak{U}_{\mathfrak{D}}$ *be a split operator for* $\mathfrak{U}$ *with respect to* $\mathfrak{D}$.
If V *is a solution of the problem*

$$\begin{aligned} \mathfrak{U}V &= 0 \\ (\mathfrak{D}V)|_{\Sigma_D} &= T_2|_{\Sigma_D} \end{aligned}$$

then it is also a solution of the problem

$$\begin{aligned} \mathfrak{U}_{\mathfrak{D}}V_{\mathfrak{D}} &= 0 \\ V_{\mathfrak{D}}|_{\Sigma_D} &= T_2|_{\Sigma_D} \\ \mathfrak{D}V &= V_{\mathfrak{D}} \end{aligned}$$

This relaxation is at some point a trade. On the one hand we are gaining a larger number of possible operators and an easier job to show that $\mathfrak{U}_{\mathfrak{D}}$ is fulfilling the requirements. On the other hand we have to check every solution of our new problem if it is really a solution of the old one. Hence we have to choose among the possible solutions V the ones which fulfill $\mathfrak{U}V = 0$.

Considering this problem the kernel of $\mathfrak{D}$ and $\mathfrak{U}_{\mathfrak{D}}$ are of high importance, they are the source of candidates for solutions. For example, if $\mathfrak{U}_{\mathfrak{D}} = 0$ we will not gain any valuable information out of the solution of the new problem although 0 is a split operator. So we will restrict ourselves to split operators which do not behave too badly in this respect.

2.1.3 Composition and Linearity

As remarked in the introduction we will have to deal with second order derivatives as side conditions. Quite a lot of second order differential operators can be seen as a composition of two first order differential operators. Using split operators we can attack this problem directly. The proof works exactly the same way as the split lemma.

Lemma 2.3 (Composition of Split Operators)

Assume $\mathfrak{D} = \mathfrak{D}_2\mathfrak{D}_1$ and let $\mathfrak{U}_{\mathfrak{D}_2}$ and $\left(\mathfrak{U}_{\mathfrak{D}_2}\right)_{\mathfrak{D}_1}$ be the corresponding (bidirectional) split operators.

V is a solution of the problem

$$\begin{aligned} \mathfrak{U}V &= 0 \\ (\mathfrak{D}V)|_{\Sigma_D} &= T_2|_{\Sigma_D} \end{aligned}$$

(iff) then it is also a solution of the problem

$$\begin{aligned} \left(\mathfrak{U}_{\mathfrak{D}_2}\right)_{\mathfrak{D}_1} V_{\mathfrak{D}} &= 0 \\ V_{\mathfrak{D}}|_{\Sigma_D} &= T_2|_{\Sigma_D} \\ \mathfrak{D}V &= V_{\mathfrak{D}} \end{aligned}$$

In other words, we have the equality

$$\left(\mathfrak{U}_{\mathfrak{D}_2}\right)_{\mathfrak{D}_1} = \mathfrak{U}_{(\mathfrak{D}_2\mathfrak{D}_1)} = \mathfrak{U}_{\mathfrak{D}}$$

Thus, by composition, we are able to handle any finite compositions of operators $\mathfrak{D}$. In particular, the second derivatives we observe as data in our satellite problem are covered.

Furthermore we can consider the following situation whose proof is straightforward, again.

Lemma 2.4 (Linearity of Split Operators)

Assume $\mathfrak{U}_{\mathfrak{D}_1} = \mathfrak{U}_{\mathfrak{D}_2}$ are (bidirectional) split operators with respect to $\mathfrak{D}_1$ and $\mathfrak{D}_2$ respectively.

Then $\mathfrak{U}_{\mathfrak{D}} := \mathfrak{U}_{\mathfrak{D}_1}$ is a split operator with respect to the operator

$$\mathfrak{D} = \alpha_1\mathfrak{D}_1 + \alpha_2\mathfrak{D}_2 \qquad \textit{where} \quad \alpha_1, \alpha_2 \in \mathbb{R}$$

2.1.4 Kernels

Now we will consider some further properties concerning the (algebraic) kernels (i.e., nullspace) of our operators. First we will rewrite our definition of a (bidirectional) split operator in an algebraic way.

Lemma 2.5

$\mathfrak{U}_{\mathfrak{D}}$ is a bidirectional split operator of $\mathfrak{U}$ with respect to $\mathfrak{D}$ iff

$$\ker(\mathfrak{U}) = \ker(\mathfrak{U}_{\mathfrak{D}}\mathfrak{D})$$

$\mathfrak{U}_{\mathfrak{D}}$ is a split operator of $\mathfrak{U}$ with respect to $\mathfrak{D}$ iff

$$\ker(\mathfrak{U}) \subset \ker(\mathfrak{U}_{\mathfrak{D}}\mathfrak{D})$$

This is a trivial consequence of $\mathfrak{U}V = 0$ iff $V \in \ker(\mathfrak{U})$.

Obviously it does not make too much sense if $\ker(\mathfrak{U}_{\mathfrak{D}}\mathfrak{D})$ is getting much bigger than $\ker(\mathfrak{U})$ because we would need to check much more solutions if they really fulfill the requirements. In particular, it is not useful if $\mathfrak{U}_{\mathfrak{D}}\mathfrak{D} = 0$ or even $\mathfrak{U}_{\mathfrak{D}} = 0$ because we would not gain anything.

In order to classify the set of solutions we will introduce the following notation:

Definition 2.3 (Subset Kernel)

Using the notation from the problems above we define the subset kernel *as*

$$\operatorname{sker}(\mathfrak{D}) = \left\{ V \in \mathcal{S} \mid \left. (\mathfrak{D}V)\right|_{\Sigma_D} = 0 \right\}$$

Observe that $\operatorname{sker}(\mathfrak{D}) \supset \ker(\mathfrak{D})$. As we will see later on, we will actually get $\operatorname{sker}(\mathfrak{D}) = \ker(\mathfrak{D})$ for a wide class of geoscientifically relevant problems.

Using this new definition we may rewrite our original problem algebraically:

Lemma 2.6

The set of all solutions of the general problem *is* $\ker(\mathfrak{U}) \cap \operatorname{sker}(\mathfrak{D}) + \overline{V}$*, where* $\overline{V}$ *is one solution of the problem.*

In particular existence of a solution means that such a $\overline{V}$ *exists, uniqueness means that* $\ker(\mathfrak{U}) \cap \operatorname{sker}(\mathfrak{D}) = \{0\}$.

Lemma 2.7

The set of solutions we get when applying the split operator is $\ker(\mathfrak{U}_{\mathfrak{D}}\mathfrak{D}) \cap \operatorname{sker}(\mathfrak{D}) + \overline{V}$*, where* $\overline{V}$ *is one solution of the problem.*

The set of all solutions can be found by intersecting with $\ker(\mathfrak{U})$.

Note that for none of the solution procedures the operator $\mathfrak{D}$ is required to be one-to-one and onto.

2.1.5 Application

Now we want to turn our attention to the geo-scientifically relevant case of the Laplace operator Δ.

Problem 2.4

Let $\overline{\Sigma_{ext}} \subset \mathbb{R}^3$ be a domain and Σ_{Data} in its interior. Assume furthermore $\mathscr{d}$ to be a smooth first order or second order differential operator on Σ_{ext}. Let Data be a smooth function on Σ_{Data}.

We search all harmonic [FGS98] functions $V : \overline{\Sigma_{ext}} \to \mathbb{R}$ fulfilling

$$\begin{aligned}(\Delta V)|_{\Sigma_{ext}} &= 0 \\ (\mathscr{d} V)|_{\Sigma_{Data}} &= Data\end{aligned}$$

Remark

The notation "smooth differential operator" is meant as an abbreviation for a differential operator with smooth coefficient functions.

Please note that we do not require that we can make a complete reconstruction of the geopotential V out of the data for the derivative $\mathscr{d}$.

Now we will turn our attention to the problem of actually obtaining the necessary split operators for this problem. First we will attack the problem for first order differential operators, afterwards for purely second order differential operators $\mathscr{d}$.

Our goal is to classify which side conditions $\mathscr{d}$ possess a split operator in the form of another differential operator of maximal degree 2.

2.2 Split Operators with Respect to a First Order Operator Condition

Because of the mere impossibility to compute these split operators in general, we will just try to get a solution for our problem. On the other hand we can keep the problem at some points a little bit more general than described beforehand.

However, due to our algebraic approach and the fact that we use the cartesian coordinate system to tackle the problem we face another kind obstacle:

- The function V we search for has to be smooth in the domain we consider, i.e., $V \in C^\infty\left(\overline{\Sigma_{ext}}\right)$.
- We need the underlying differential operator $\overline{\Delta}$ to be defined and smooth on $\overline{\Sigma_{ext}}$.
- We need the side condition $\mathscr{d}$ to be defined and smooth on $\overline{\Sigma_{ext}}$.

In order to keep the notation simple $A_\boxdot$ should incorporate the whole family of possible A, A_i, A_{ij} and so on. The same notation will be used for other variables if appropriate, too. We want to mention again that we denote the derivative in the Euclidean direction x_i by ∂_i.

As we are normally concerned with the three-dimensional space we will restrict our attention to this special case. In particular this implies for our notation that all indices in sums are assumed to reach from 1 to 3, e.g., $\sum_i = \sum_{i=1}^3$ if not stated otherwise.

Problem 2.5

Assume

$$\overline{\Delta} = \sum_{i \le j} A_{ij} \partial_i \partial_j + \sum_i A_i \partial_i + A$$

where the $A_{\boxdot} \in C^\infty\left(\overline{\Sigma_{ext}}\right)$ *denote smooth functions and all matrices* $\mathbf{a}_{ij} = \left(\begin{smallmatrix} A_{ii} & A_{ij} \\ 0 & A_{jj} \end{smallmatrix}\right)$ *are definite. (I.e.,* $\left(v^T \mathbf{a}_{ij} v\right)(x) \neq 0$ *for all* $v \in \mathbb{R}^2 \setminus \{0\}$ *for all* $x \in \overline{\Sigma_{ext}}$*)*
Additionally $\overline{\Delta}$ *should fulfill the following* technical condition*. For all differential operators* $\{1, \partial_i, \partial_j\partial_k, \partial_i\partial_j\partial_k\}$ *with* $1 \le i \le j \le k \le 3$ *and* $j \neq 3$ *there should exist an half order* $\blacktriangleright$ *on the multi-indices and functions* H, H_i, H_{ij}, H_{ijk} *which fulfill for all values (*ν*,* μ *are multi-indices):*

- $H_\mu \in C^3\left(\overline{\Sigma_{ext}}\right)$ *for all* μ
- $\overline{\Delta} H_\mu = 0$ *for all* μ
- $\partial_\nu H_\mu = 0$ *for all* $\nu \blacktriangleright \mu$
- $\partial_\nu H_\nu = \overline{H}_\nu \neq 0$ *for all* ν

Assume furthermore

$$\not{d} = \sum_k D_k \partial_k + D$$

where the $D_{\boxdot} \in C^\infty\left(\overline{\Sigma_{ext}}\right)$ *are smooth functions and at every point at least one of the* $D_i \neq 0$*.*
Does there exist a sensible (non-zero) split operator $\overline{\Delta}_{\not{d}}$ *for* $\overline{\Delta}$ *with respect to* $\not{d}$*? How does it look like? Which conditions does* $\not{d}$ *have to fulfill?*

Note that in terms of the operator notation in the last section we would have $\mathfrak{U} = \overline{\Delta}$, $\mathfrak{D} = \not{d}$ and hence $\mathfrak{U}_{\mathfrak{D}} = \overline{\Delta}_{\not{d}}$.

Remark

Because we assume all of our functions to be sufficiently smooth we have $\partial_i\partial_j = \partial_j\partial_i$ and hence can assume $A_{ij} = 0$ for $i > j$.
Every elliptic or hyperbolic differential operator fulfills the above requirement beside the technical condition of the existence of the half order $\blacktriangleright$ and the corresponding functions $H_{\boxdot}$.
Alternatively to $1 \le i \le j \le k \le 3$ and $j \neq 3$ we could require μ not equalling $(1,1,1)$, $(2,2,2)$, $(3,3,3)$ or $(3,3)$ depending on what simplification is actually the easiest to perform. Note that this is a minor alteration which does not change the problem but just slightly how we deal with it.

Lemma 2.8

The Laplace operator $\Delta = \sum_i \partial_i \partial_i$ fulfills the requirements imposed by the above problem.

Proof

Using the notation of the above problem we have $A_{ij} = \delta_{ij}$ and $A = A_i = 0$ for all possible i and j. This means that $\mathbf{a}_{ij} = \left(\begin{smallmatrix} 1 & 0 \\ 0 & 1 \end{smallmatrix}\right) > 0$ as required.

As order on the multi-index ν we choose the standard lexicographical order. Then the technical condition, the existence of particular H_ν, is fulfilled by the homogeneous harmonic polynomials up to degree 3 , namely [FGS98].

$$
\begin{array}{lll}
{}^0H_0^0 = 1 & & \\
{}^0H_1^1 = x_1 & {}^0H_1^0 = x_2 & {}^1H_1^0 = x_3 \\
{}^0H_2^2 = x_1^2 - x_3^2 & {}^0H_2^1 = x_1 x_2 & {}^0H_2^0 = x_2^2 - x_3^2 \\
{}^1H_2^1 = x_1 x_3 & {}^1H_2^0 = x_2 x_3 & \\
{}^0H_3^3 = x_1^3 - 3x_1 x_3^2 & {}^0H_3^2 = x_1^2 x_2 - x_2 x_3^2 & {}^0H_3^1 = x_1 x_2^2 - x_1 x_3^2 \\
{}^0H_3^0 = x_2^3 - 3x_2 x_3^2 & & \\
{}^1H_3^2 = x_1^2 x_3 - \dfrac{x_3^3}{3} & {}^1H_3^1 = x_1 x_2 x_3 & {}^1H_3^0 = x_2^2 x_3 - \dfrac{x_3^3}{3}
\end{array}
$$

This yields the proposition both for $1 \le i \le j \le k \le 3$ and $j \neq 3$ or ν not equalling $(1,1,1)$, $(2,2,2)$, $(3,3,3)$ or $(3,3)$. q.e.d.

2.2.1 First Order Split Operators

Now we want to analyze possible split operators systematically. The first idea is taking $\overline{\Delta}_{\mathscr{d}}$ to be a first order differential operator, i.e., $\overline{\Delta}_{\mathscr{d}}\,\mathscr{d}$ has second order. This search will return a negative result.

Lemma 2.9

Let $\overline{\Delta}$ and $\mathscr{d}$ be as defined in the above problem.

Then there does not exist a nontrivial split operator in the form $\overline{\Delta}_{\mathscr{d}} = \sum_i B_i \partial_i + B$, where the B_i and B denote smooth functions, i.e., $B_\boxdot \in C^\infty(\overline{\Sigma_{ext}})$.

Proof

Without loss of generality we will assume D_3 to be nonzero at the particular point considered. Any other configuration could be obtained by mere permutation.

First we need to compute $\overline{\Delta}_{\mathscr{d}}\,\mathscr{d}$. Using the chain rule we obtain:

$$
\begin{aligned}
\overline{\Delta}_{\mathscr{d}}\,\mathscr{d} &= \sum_i B_i \sum_j \left(\left(\partial_i D_j \right) \partial_j + D_j \partial_i \partial_j \right) \\
&\quad + \sum_j B D_j \partial_j + \sum_i B_i \left(\partial_i D + D \partial_i \right) + BD \\
&= \sum_{i,j} B_i D_j \partial_i \partial_j \\
&\quad + \sum_i \left(\left(\sum_j B_i \partial_j D_j \right) + B D_i + B_i D \right) \partial_i \\
&\quad + BD + \sum_i B_i \partial_i D
\end{aligned}
$$

Now we want to use the technical condition concerning the functions $H_{\boxdot}$. As we see we do not have a statement for $\partial_3 \partial_3$. Therefore we have to do the following consideration.

We are just interested in solutions obeying $\overline{\Delta} V = 0$ and hence $\overline{\Delta}_{\mathscr{d}}\,\mathscr{d}\, V = 0$. So subtracting $\frac{D_3 B_3}{A_{33}} \overline{\Delta}$ ($A_{33} \neq 0$ because $\mathbf{a}_{13}$ is definite) does not change the set of solutions and additionally will remove the $\partial_3 \partial_3$ term. Cleaning up the resulting equation yields:

$$
\begin{aligned}
0 &= \left(\overline{\Delta}_{\mathscr{d}}\,\mathscr{d} - \frac{D_3 B_3}{A_{33}} \overline{\Delta} \right) V \\
&= \Bigg(\sum_i \left(D_i B_i - \frac{D_3 B_3}{A_{33}} A_{ii} \right) \partial_i \partial_i \\
&\quad + \sum_{i<j} \left(D_j B_i + D_i B_j - \frac{D_3 B_3}{A_{33}} A_{ij} \right) \partial_i \partial_j \\
&\quad + \sum_i \left(\left(\sum_j B_j \partial_j D_i \right) + B D_i + B_i D - \frac{D_3 B_3}{A_{33}} A_i \right) \partial_i \\
&\quad + BD + \sum_i B_i \partial_i D - \frac{D_3 B_3}{A_{33}} A \Bigg) V
\end{aligned}
$$

Now we can apply the technical condition we required to hold. Namely for all differential operators $\{1, \partial_i, \partial_i \partial_j\}$ with $1 \leq i \leq j \leq 3$ and $j \neq 3$ there exists a half order $\blacktriangleright$ on the multi-indices and functions H_0, H_i, H_{ij} which fulfill for all values (ν, μ are multi-indices):

- $\overline{\Delta} H_\mu = 0$ for all μ
- $\partial_\nu H_\mu = 0$ for all $\nu \blacktriangleright \mu$
- $\partial_\nu H_\nu = \overline{H}_\nu \neq 0$

Using $\nu_1 \blacktriangleleft \nu_2 \blacktriangleleft \ldots \blacktriangleleft \nu_9$ (there are nine differentials of the above form left) we can rewrite the above equation in the following terms:

$$\left(\sum_{i=1}^{9} C_{\nu_i}\partial_{\nu_i}\right) V = 0$$

where the C_{ν_i} are appropriate smooth functions.
Now inserting the H_{ν_k} in the above equation yields the following 9 equations:

$$\begin{aligned}
0 &= \left(\sum_{i=1}^{9} C_{\nu_i}\partial_{\nu_i}\right) H_{\nu_k}\\
&= \left(\sum_{i<k} C_{\nu_i}\partial_{\nu_i} H_{\nu_k}\right) + C_{\nu_k}\overline{H}_{\nu_k} + \left(\sum_{i>k} C_{\nu_i}\partial_{\nu_i} H_{\nu_k}\right)\\
&= \left(\sum_{i<k} C_{\nu_i}\partial_{\nu_i} H_{\nu_k}\right) + C_{\nu_k}\overline{H}_{\nu_k}
\end{aligned}$$

which is structurally seen a triangular homogeneous linear system of linear equations. Using $\overline{H}_{\nu_k} \neq 0$ for all ν_k we immediately get $C_{\nu_k} = 0$ for all ν_k.
Expanding the C_ν again we get the following four sets of equations:

$$\begin{aligned}
0 =& BD + \sum_i B_i\partial_i D - \frac{D_3B_3}{A_{33}} A \\
0 =& \left(\sum_j B_j\partial_j D_i\right) + BD_i + B_iD - \frac{D_3B_3}{A_{33}} A_i && \text{for all } i\\
0 =& B_iD_j + B_jD_i - \frac{D_3B_3}{A_{33}} A_{ij} && \text{for all } i<j\\
0 =& B_iD_i - \frac{D_3B_3}{A_{33}} A_{ii} && \text{for all } i
\end{aligned}$$

Using the last two sets of equations we get:

$$\begin{aligned}
0 =& D_iD_j\left(B_iD_j + B_jD_i - \frac{D_3B_3}{A_{33}} A_{ij}\right)\\
=& B_iD_iD_j^2 + B_jD_jD_i^2 - D_iD_j\frac{D_3B_3}{A_{33}} A_{ij}\\
=& \frac{D_3B_3}{A_{33}}\left(A_{ii}D_j^2 + A_{jj}D_i^2 - A_{ij}D_iD_j\right)\\
=& -\frac{D_3B_3}{A_{33}}\begin{pmatrix} -D_j & D_i\end{pmatrix}\begin{pmatrix} A_{ii} & A_{ij}\\ 0 & A_{jj}\end{pmatrix}\begin{pmatrix} -D_j\\ D_i\end{pmatrix}\\
=& -\frac{D_3B_3}{A_{33}}\begin{pmatrix} -D_j & D_i\end{pmatrix}\mathbf{a}_{ij}\begin{pmatrix} -D_j\\ D_i\end{pmatrix}
\end{aligned}$$

We assumed every matrix of the type $\mathbf{a}_{ij}$ to be definite. In particular this means that $0 = \frac{D_3B_3}{A_{33}}$ because we assumed $D_3 \neq 0$ and therefore $(-D_j \;\; D_3) \neq 0$. As $\frac{D_3}{A_{33}} \neq 0$ we get $B_3 = 0$.

Using the third set of equations this immediately yields $B_i D_3 = 0$ and hence $B_i = 0$ for all i. Then the second set of equations also yields $BD_3 = 0$ and thus $B = 0$. These arguments hold for all points in $\overline{\Sigma_{ext}}$ and hence the operator $\overline{\Delta}_d = 0$ is the trivial operator. q.e.d.

2.2.2 Second Order Split Operators

As we have seen, first order differential operators are not appropriate candidates for (bidirectional) split operators. Therefore we will try second order differential operators.

Definition 2.4

The second order differential operator $\widetilde{\Delta}$ is defined as

$$\widetilde{\Delta} = \sum_{i \le j} B_{ij} \partial_i \partial_j + \sum_i B_i \partial_i + B$$

The $B_{\boxdot} \in C^\infty(\overline{\Sigma_{ext}})$ are assumed to be smooth functions.

$\widetilde{\Delta}$ shall be our candidate for the (bidirectional) split operator $\overline{\Delta}_d$ as described in the last problem.

Now we want to classify as many cases as possible. Therefore we will do the necessary computations in several steps. For all steps we will use one of the computer algebra systems *Maple 7* with the *PDEtools* package or *Singular*, according to which one is more appropriate.

Because of its length we have not included the whole calculations into this text and we will just give the most important steps. The scripts itself may be requested electronically from the author.

2.2.3 First Computations

Like beforehand our first task is applying our functions $H_{\boxdot}$ to get a set of conditions for our coefficients. Thus we will subtract a multiple of $\overline{\Delta}$ in order to cancel the $\partial_1\partial_1\partial_1$, $\partial_2\partial_2\partial_2$, $\partial_3\partial_3\partial_3$ and $\partial_3\partial_3$ terms.

$$\begin{aligned}
\widetilde{\Delta}_d - \Bigg(& \sum_i \frac{B_{ii}}{A_{ii}} D_i \partial_i \overline{\Delta} \\
& + \frac{1}{A_{33}} \Bigg(\Bigg(\sum_i B_{3i} \partial_i D_3 - \frac{B_{ii}}{A_{ii}} D_i \partial_i A_{33} \Bigg) \\
& \qquad + B_{33}\partial_3 D_3 - \frac{B_{33}}{A_{33}} D_3 A_3 + B_3 D_3 + B_{33} D \Bigg) \overline{\Delta} \Bigg) \\
= + & \left(B_{11} D_2 - A_{11} \frac{B_{22}}{A_{22}} D_2 + B_{12} D_1 - A_{12} \frac{B_{11}}{A_{11}} D_1 \right) \partial_1\partial_1\partial_2 \\
+ & \left(B_{22} D_1 - A_{22} \frac{B_{11}}{A_{11}} D_1 + B_{12} D_2 - A_{12} \frac{B_{22}}{A_{22}} D_2 \right) \partial_1\partial_2\partial_2
\end{aligned}$$

$$
\begin{aligned}
&+\left(B_{11}D_3 - A_{11}\frac{B_{33}}{A_{33}}D_3 + B_{13}D_1 - A_{13}\frac{B_{11}}{A_{11}}D_1\right)\partial_1\partial_1\partial_3 \\
&+\left(B_{33}D_1 - A_{33}\frac{B_{11}}{A_{11}}D_1 + B_{13}D_3 - A_{13}\frac{B_{33}}{A_{33}}D_3\right)\partial_1\partial_3\partial_3 \\
&+\left(B_{22}D_3 - A_{22}\frac{B_{33}}{A_{33}}D_3 + B_{23}D_2 - A_{23}\frac{B_{22}}{A_{22}}D_2\right)\partial_2\partial_2\partial_3 \\
&+\left(B_{33}D_2 - A_{33}\frac{B_{22}}{A_{22}}D_2 + B_{23}D_3 - A_{23}\frac{B_{33}}{A_{33}}D_3\right)\partial_2\partial_3\partial_3 \\
&+\Bigg(B_{23}D_1 - A_{23}\frac{B_{11}}{A_{11}}D_1 + B_{13}D_2 - A_{13}\frac{B_{22}}{A_{22}}D_2 \\
&\qquad\qquad\qquad + B_{12}D_3 - A_{12}\frac{B_{33}}{A_{33}}D_3\Bigg)\partial_1\partial_2\partial_3 \\
&+\text{lower order parts}
\end{aligned}
$$

Note that $A_{ii} \neq 0$ because of the definiteness of $\mathbf{a}_{ij}$.

The subtraction of a multiple of $\overline{\Delta}$ enabled us to reduce all occurring coefficients to the ones covered by the technical condition given in our problem setup. We did not write down the result completely because it would cover roughly three pages right now.

Now we will apply the same strategy as shown beforehand. We will insert all different H_ν consecutively and hence get that all of the remaining coefficients in front of the ∂_ν are zero as shown in the last lemma.

2.2.4 Second Order Terms

First we will just take a look at the seven equations generated by the third order terms in the above operator which are manageable because of their minor size:

$$
\begin{aligned}
0 =& B_{ii}D_j - \frac{B_{jj}}{A_{jj}}A_{ii}D_j + B_{ij}D_i - \frac{B_{ii}}{A_{ii}}A_{ij}D_i \qquad \text{for all } i,j \\
0 =& B_{23}D_1 - \frac{B_{11}}{A_{11}}A_{23}D_1 + B_{13}D_2 - \frac{B_{22}}{A_{22}}A_{13}D_2 + B_{12}D_3 - \frac{B_{33}}{A_{33}}A_{12}D_3
\end{aligned}
$$

Now we want to take a closer look at these equations. Like in the preceding section we can extract quite a lot of information out of them:

Lemma 2.10

Let $\overline{\Delta}$, $\not{d}$ and $\widetilde{\Delta}$ be as defined beforehand. Then the second order parts of $\overline{\Delta}$ and $\widetilde{\Delta}$ are essentially the same. (In these terms essentially means "up to a factor".)

Proof

Again all the considerations are made pointwise. We will use the first set of equations to get our results. As we can assume without loss of generality that $D_1 \neq 0$ we will just consider the pair $(1,2)$. However, all the arguments would be the same for any other pair.

Consider the two equations

$$\begin{aligned}
0 =& B_{11}D_2 - \frac{B_{22}}{A_{22}}A_{11}D_2 + B_{12}D_1 - \frac{B_{11}}{A_{11}}A_{12}D_1 \\
0 =& B_{22}D_1 - \frac{B_{11}}{A_{11}}A_{22}D_1 + B_{12}D_2 - \frac{B_{22}}{A_{22}}A_{12}D_2
\end{aligned}$$

As $D_1 \neq 0$ we can isolate B_{12} out of the first equation.

$$B_{12} = A_{12}\frac{B_{11}}{A_{11}} - A_{11}\frac{D_2}{D_1}\left(\frac{B_{11}}{A_{11}} - \frac{B_{22}}{A_{22}}\right)$$

Substituting this result in the second one and multiplying with D_1 yields:

$$\begin{aligned}
0 =& B_{22}D_1^2 - \frac{B_{11}}{A_{11}}A_{22}D_1^2 - B_{11}D_2^2 \\
&+ \frac{B_{22}}{A_{22}}A_{11}D_2^2 + \frac{B_{11}}{A_{11}}A_{12}D_1D_2 - \frac{B_{22}}{A_{22}}A_{12}D_1D_2 \\
=& -\left(\frac{B_{11}}{A_{11}} - \frac{B_{22}}{A_{22}}\right)\left(A_{11}D_2^2 - A_{12}D_1D_2 + A_{22}D_1^2\right) \\
=& -\left(\frac{B_{11}}{A_{11}} - \frac{B_{22}}{A_{22}}\right)\begin{pmatrix} -D_2 & D_1 \end{pmatrix}\begin{pmatrix} A_{11} & A_{12} \\ 0 & A_{22} \end{pmatrix}\begin{pmatrix} -D_2 \\ D_1 \end{pmatrix} \\
=& -\left(\frac{B_{11}}{A_{11}} - \frac{B_{22}}{A_{22}}\right)\begin{pmatrix} -D_2 & D_1 \end{pmatrix}\mathbf{a}_{12}\begin{pmatrix} -D_2 \\ D_1 \end{pmatrix}
\end{aligned}$$

Using $D_1 \neq 0$ and the matrix $\mathbf{a}_{12}$ to be definite we get

$$\frac{B_{11}}{A_{11}} = \frac{B_{22}}{A_{22}} =: C$$

where C denotes a smooth function. Hence

$$B_{11} = A_{11}\frac{B_{11}}{A_{11}} = CA_{11} \qquad \text{and} \quad B_{22} = A_{22}\frac{B_{22}}{A_{22}} = CA_{22}$$

Using this relation for the equation derived for B_{12} we get

$$B_{12} = CA_{12}$$

As we could apply this method for the pair $(1,3)$ as well, we can finally derive

$$B_{ij} = CA_{ij} \qquad \text{for all } \ (i,j) \quad \text{without} \quad (2,3)$$

The equivalent equation for the last pair can be derived out of the equation $B_{23}D_1 - \frac{B_{11}}{A_{11}}A_{23}D_1 + B_{13}D_2 - \frac{B_{22}}{A_{22}}A_{13}D_2 + B_{12}D_3 - \frac{B_{33}}{A_{33}}A_{12}D_3 = D_1\left(B_{23} - CA_{23}\right) = 0$.
In order that our split operator makes any sense it is reasonable to assume $C \neq 0$. (Otherwise $\widetilde{\Delta}$ is a first order operator which has to be zero by the last subsection.

Hence $\widetilde{\Delta}$ would be trivial in this case.) Thus by substituting $B_{\boxdot} = B_{\boxdot}/C$ we can assume $C = 1$. As the considerations were independent of the particular point considered the second order part of $\overline{\Delta}$ and $\widetilde{\Delta}$ are identical up to a common factor.

q.e.d.

This result simplifies our operator considerably. However the equations we can derive are still too complicated to have a chance of computing a symbolical solution.

2.2.5 Restriction to $\overline{\Delta} = \Delta$

We have seen that the second order part of $\overline{\Delta}$ does not change considerably. Thus we can restrict our attention on $\overline{\Delta} = \Delta$, even if we want to use compositions of oblique derivatives. This means in particular $B_{ij} = A_{ij} = \delta_{ij}$ and $A_i = A = 0$ for all combinations i and j, i.e., $\widetilde{\Delta} = \Delta + \sum_i B_i\partial_i + B$

Hence our differential operator looks:

$$
\begin{aligned}
\widetilde{\Delta}\mathcal{d} - &\left(\sum_i D_i\partial_i\Delta + \left(\left(\sum_i B_{3i}\partial_i D_3\right) + \partial_3 D_3 - D_3 A_3 + B_3 D_3 + D\right)\Delta\right)\\
= &+ \left(2\partial_1 D_1 + B_1 D_1 - 2\partial_3 D_3 - B_3 D_3\right)\partial_1\partial_1\\
&+ \left(2\partial_2 D_2 + B_2 D_2 - 2\partial_3 D_3 - B_3 D_3\right)\partial_2\partial_2\\
&+ \left(2\partial_2 D_1 + B_2 D_1 + 2\partial_1 D_2 + B_1 D_2\right)\partial_1\partial_2\\
&+ \left(2\partial_3 D_1 + B_3 D_1 + 2\partial_1 D_3 + B_1 D_3\right)\partial_1\partial_3\\
&+ \left(2\partial_3 D_2 + B_3 D_2 + 2\partial_2 D_3 + B_2 D_3\right)\partial_2\partial_3\\
&+ \left(\widetilde{\Delta} D_1 + 2\partial_1 D + B_1 D\right)\partial_1\\
&+ \left(\widetilde{\Delta} D_2 + 2\partial_2 D + B_2 D\right)\partial_2\\
&+ \left(\widetilde{\Delta} D_3 + 2\partial_3 D + B_3 D\right)\partial_3\\
&+ \left(\widetilde{\Delta} D\right)
\end{aligned}
$$

2.2.6 Further Conditions

Now we can extract further equations by the usage of the technical condition as shown beforehand. Hence we end up at the following system of equations:

$$
\begin{aligned}
0 =& \widetilde{\Delta} D_i + 2\partial_i D + B_i D && \text{for all } i\\
0 =& 2\partial_i D_j + B_i D_j + 2\partial_j D_i + B_j D_i && \text{for all } i \neq j\\
0 =& 2\partial_i D_i + B_i D_i - 2\partial_j D_j - B_j D_j && \text{for all } i \neq j\\
0 =& \widetilde{\Delta} D
\end{aligned}
$$

Introducing the differential operators $\mathscr{b}_i = 2\partial_i + B_i$ we get the following much more simple form:

$$
\begin{aligned}
0 =& \widetilde{\Delta} D_i + \mathscr{b}_i D && \text{for all } i \\
0 =& \mathscr{b}_i D_j + \mathscr{b}_j D_i && \text{for all } i \neq j \\
0 =& \mathscr{b}_i D_i - \mathscr{b}_j D_j && \text{for all } i \neq j \\
0 =& \widetilde{\Delta} D
\end{aligned}
$$

We have tried to translate the system in the language of *non-commutative algebra*. This was done in collaboration with. V. Levandovskyy (Univ. of Kaiserslautern) using a beta version of Singular [GPS01] which is capable of handling non-commutative problems [Lev03].

However, up till now we were not able to get sufficient results this way. This seems to be due to the fact that the above equations are extraordinarily symmetric. The underlying Gröbner Basis approaches to solve such a problem basically work by breaking the symmetries resulting in very bad results, if at all.

Therefore we will restrict our attention to the commutative case (i.e., the $B_{\boxdot}$ and the differential operators ∂_i commute). This means in particular $B_i = 2\overline{b}_i$ and $B = \overline{b}$, where $\overline{b}_{\boxdot} \in \mathbb{R}$ which results in the following system:

$$
\begin{aligned}
0 =& \sum_j (\partial_j \partial_j D_i + 2\overline{b}_j \partial_j D_i) + \overline{b} D_i + 2\partial_i D + 2\overline{b}_i D && \text{for all } i \\
0 =& \partial_i D_j + \overline{b}_i D_j + \partial_j D_i + \overline{b}_j D_i && \text{for all } i \neq j \\
0 =& \partial_i D_i + \overline{b}_i D_i - \partial_j D_j + \overline{b}_j D_j && \text{for all } i \neq j \\
0 =& \sum_j (\partial_j \partial_j D + 2\overline{b}_j \partial_j D) + \overline{b} D
\end{aligned}
$$

2.2.7 Solving the System

We need to do some preparatory steps to solve this system using a method proposed in [Sei94]. We transform the system of partial differential equations into a system of polynomial equations, i.e., changing the language from PDE's to commutative algebra. In this case the differentials ∂_i get the new variables which will be denoted by `si` from now on. The other coefficients stay right the same. In particular we will write the real variables $\texttt{bi} = \overline{b}_i$).

Now we are ready to solve the problem. We will order the different functions in the following vector: (D_1, D_2, D_3, D). The equations we derived now describe an ideal in a four dimensional polynomial ring with the vector of variables $(\texttt{s1}, \texttt{s2}, \texttt{s3}, \texttt{b1}, \texttt{b2}, \texttt{b3}, \texttt{b})$. Alternatively we can consider them as generators of a module with respect to the one dimensional polynomial ring in the same variables. In order to get solutions to our problem we will now compute a standard basis to this particular ideal/module. The method of choice is Buchberger's algorithm to obtain a Gröbner Basis [GP02], the program used is *Singular* [GPS01].

When we transfer this standard basis back in the language of PDE's we obtain a system without hidden integrability conditions [Sei94].

We are mainly interested in solutions which are ordered in the different functions D_i and then according to the differentiations. Therefore we chose the order $(c, dp(3), dp(4))$ for our problem. For further instructions on the possible orderings, their advantages and disadvantages we want to refer the reader to [GP02].

```
ring r=0,(s1,s2,s3,b1,b2,b3,b),(c,dp(3),dp(4));
vector v1=[s2+b2,s1+b1,0,0];
vector v2=[s3+b3,0,s1+b1,0];
vector v3=[0,s3+b3,s2+b2,0];
vector v4=[s1+b1,-s2-b2,0,0];
vector v5=[s1+b1,0,-s3-b3,0];
vector v6=[s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3+b,0,0,2*b1+2*s1];
vector v7=[0,s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3+b,0,2*b2+2*s2];
vector v8=[0,0,s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3+b,2*b3+2*s3];
vector v9=[0,0,0,s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3+b];
module m = v1,v2,v3,v4,v5,v6,v7,v8,v9;
std(m);
```

The first line of our result looks the following way:

```
_[1]= [0,0,0,b1^4+2*b1^2*b2^2+b2^4+2*b1^2*b3^2+2*b2^2*b3^2+b3^4
      -2*b1^2*b -2*b2^2*b-2*b3^2*b+b^2]
```

Hence we have the equation

$$\begin{aligned} 0 =& \overline{b}_1^4 + 2\overline{b}_1^2\overline{b}_2^2 + \overline{b}_2^4 + 2\overline{b}_1^2\overline{b}_3^2 + 2\overline{b}_2^2\overline{b}_3^2 + \overline{b}_3^4 - 2\overline{b}_1^2\overline{b} - 2\overline{b}_2^2\overline{b} - 2\overline{b}_3^2\overline{b} + \overline{b}^2 \\ =& (\overline{b}_1^2 + \overline{b}_2^2 + \overline{b}_3^2 - \overline{b})^2 \end{aligned}$$

which immediately implies $\overline{b} = \overline{b}_1^2 + \overline{b}_2^2 + \overline{b}_3^2$. Using this result we can run *Singular* again.

```
ring r=0,(s1,s2,s3,b1,b2,b3),(c,dp(3),dp(3));
vector v1= [s2+b2,s1+b1,0,0];
vector v2= [s3+b3,0,s1+b1,0];
vector v3= [0,s3+b3,s2+b2,0];
vector v4= [s1+b1,-s2-b2,0,0];
vector v5= [s1+b1,0,-s3-b3,0];
vector v6= [s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3
             +(b1^2+b2^2+b3^2),0,0,2*b1+2*s1];
vector v7= [0,s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3
              +(b1^2+b2^2+b3^2),0,2*b2+2*s2];
vector v8= [0,0,s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3
                +(b1^2+b2^2+b3^2),2*b3+2*s3];
```

```
vector v9= [0,0,0,s1^2+s2^2+s3^2+2*b1*s1+2*b2*s2+2*b3*s3
                              +(b1^2+b2^2+b3^2)];
module m = v1,v2,v3,v4,v5,v6,v7,v8,v9;
std(m);
```

Running this script we get the following result:

```
_[1]=[0,0,0,s3^2+2*s3*b3+b3^2]
_[2]=[0,0,0,s2*s3+s2*b3+s3*b2+b2*b3]
_[3]=[0,0,0,s1*s3+s1*b3+s3*b1+b1*b3]
_[4]=[0,0,0,s2^2+s3^2+2*s2*b2+2*s3*b3+b2^2+b3^2]
_[5]=[0,0,0,s1*s2+s1*b2+s2*b1+b1*b2]
_[6]=[0,0,0,s1^2+s2^2+s3^2+2*s1*b1+2*s2*b2+2*s3*b3+b1^2+b2^2+b3^2]
_[7]=[0,0,s3^2+2*s3*b3+b3^2,-2*s3-2*b3]
_[8]=[0,0,s2*s3+s2*b3+s3*b2+b2*b3,-2*s2-2*b2]
_[9]=[0,0,s1*s3+s1*b3+s3*b1+b1*b3,-2*s1-2*b1]
_[10]=[0,0,s2^2+s3^2+2*s2*b2+2*s3*b3+b2^2+b3^2]
_[11]=[0,0,s1*s2+s1*b2+s2*b1+b1*b2]
_[12]=[0,0,s1^2+s2^2+s3^2+2*s1*b1+2*s2*b2+2*s3*b3+b1^2+b2^2+b3^2
          ,2*s3+2*b3]
_[13]=[0,s3+b3,s2+b2]
_[14]=[0,s2+b2,-s3-b3]
_[15]=[0,s1^2+s2^2+s3^2+2*s1*b1+2*s2*b2+2*s3*b3+b1^2+b2^2+b3^2,0
          ,2*s2+2*b2]
_[16]=[s3+b3,0,s1+b1]
_[17]=[s2+b2,s1+b1]
_[18]=[s1+b1,0,-s3-b3]
```

This result tells a lot about the different possible solutions. The number of solutions can now be derived by a comprehensive method out of such an algebraic standard basis [Sei94].

Therefore we will determine the corresponding Cauchy data set Γ; i.e., if $\{\mu_1, ..\mu_n\}$ are the degrees of the leading monomials, then

$$\Gamma := \mathbb{N}^3 \setminus \left(\bigcup_{i=1}^{n} \mu_i + \mathbb{N}^3 \right).$$

The cardinality $|\Gamma|$ returns the dimension of the vector space of solutions. In order to be able to count easily, we will employ the technique of a Reid diagram [Sei94]. This means that we will draw the degree of the leading coefficients (with respect to the chosen order of the Gröbner basis) in a grid. All points covered from the sector starting at this point do not need to be considered any more. So each free point just gives another degree of freedom.

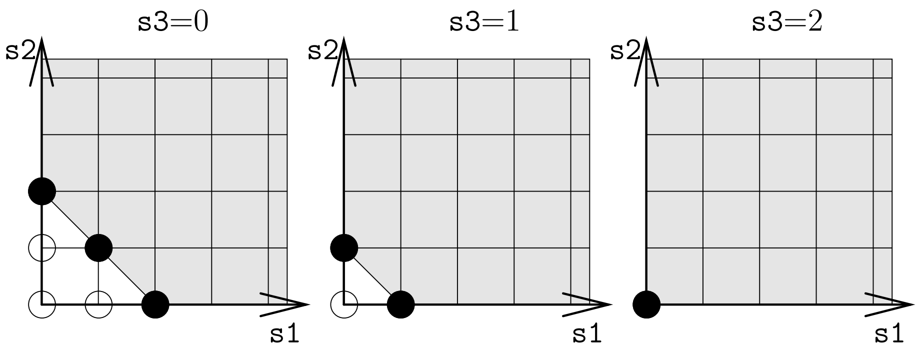
Lemma 2.11

Our system of partial differential equations possesses a 14 dimensional space of solutions. It can be parted in the following way.

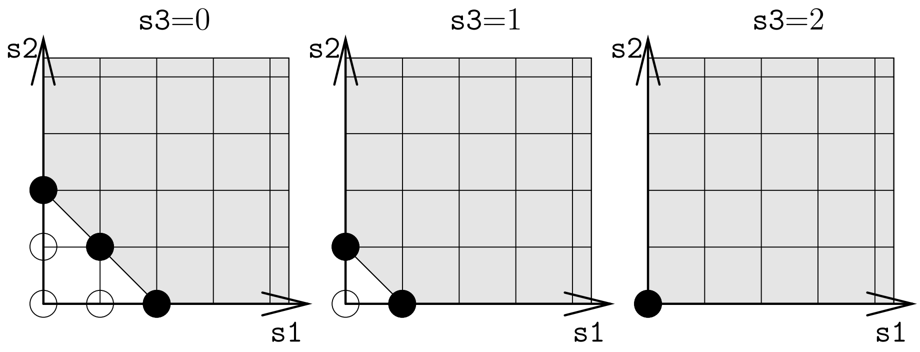
- *3 degrees of freedom for choosing the* $\overline{b}_i$.
- *4 degrees of freedom for choosing* D *for fixed* $\overline{b}_i$.
- *4 degrees of freedom for choosing* D_3 *for fixed* $\overline{b}_i$, D.
- *2 degrees of freedom for choosing* D_2 *for fixed* $\overline{b}_i$, D, D_3.
- *1 degree of freedom for choosing* D_1 *for fixed* $\overline{b}_i$, D, D_3, D_2.

Proof

The $\overline{b}_i$ are independent real variables, hence we are having three degrees of freedom for choosing them.
Now we consecutively show the relevant pictures for D, D_3, D_2 and D_1. In these pictures we denote the position of the leading monomial by a black dot, the area which is covered by the intersection of the sectors stretched by these points are shaded and the possible starting values (and hence degrees of freedom) are denoted as white dots. In order to get a better overview the picture is sliced into different layers with respect to the `s3` component. Now we just need to count the white dots.
Consider the first picture. For D we have `s3^2`, `s2 * s3`, `s1 * s3`, `s2^2`, `s1 * s2` and `s1^2` as leading polynomials. For `s3^2` we get the point $(0,0,2)$, for `s2 * s3` the point $(0,1,1)$, for `s2^2` the point $(0,2,0)$, for `s1 * s2` the point $(1,1,0)$ and for `s1^2` the point $(2,0,0)$
This results in the following Reid diagram.

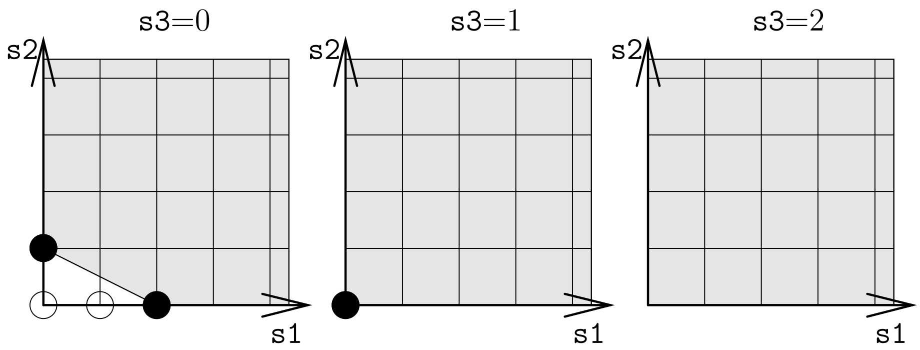


Counting the dots we get 4 possible degrees of freedom.
For D_3 we have `s3^2`, `s2*s3`, `s1*s3`, `s2^2`, `s1 * s2` and `s1^2` as leading polynomials and hence the following points: $(0,0,2)$, $(0,1,1)$, $(1,0,1)$, $(0,2,0)$, $(1,1,0)$ and finally $(2,0,0)$. As a result get the following Reid diagram.



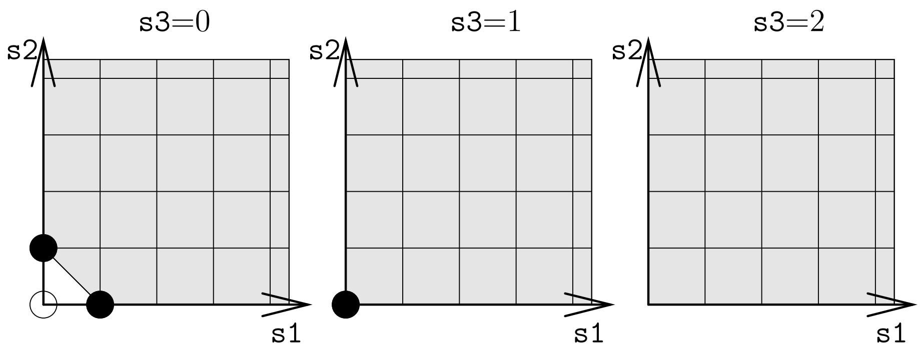
These are 4 possible degrees of freedom.

For D_2 we have `s3`, `s2` and `s1^2` as leading polynomials and thus $(0,0,1)$, $(0,1,0)$ and $(2,0,0)$ to cover. Hence we get the following Reid diagram.



These are 2 degrees of freedom.

For D_2 we have `s3`, `s2` and `s1` and hence the points $(0,0,1)$, $(0,1,0)$ and $(1,0,0)$. So we get the following Reid diagram.



So we are just having one degree of freedom for choosing the last solution.

This proves the proposition. q.e.d.

On the other hand *Maple* tells us the following 14 dimensional set of solutions. These computations were made possible in an early state of the work because we incorporated some more assumptions suggested by Marcus Hausdorf (University of Mannheim) [Hau02]. Combining this result with the last lemma we obtain that these are actually all solutions.

Theorem 2.12

When we set $B_i = 2\overline{b}_i$ with $\overline{b}_i$ constant, and assume that $b = \overline{b}$ is constant, then we get the following result:

$$\overline{b} = \overline{b}_1^2 + \overline{b}_2^2 + \overline{b}_3^2$$

and

$$\begin{aligned}
D =& \boldsymbol{e}^{-(\overline{b}_1 x_1 + \overline{b}_2 x_2 + \overline{b}_3 x_3)}(c_{q1}x_1 + c_{q2}x_2 + c_{q3}x_3 + c) \\
D_1 =& \boldsymbol{e}^{-(\overline{b}_1 x_1 + \overline{b}_2 x_2 + \overline{b}_3 x_3)}(c_1 + c_r x_1 + c_{\neg 3}x_2 + c_{\neg 2}x_3 \\
&\qquad + c_{q1}(x_1^2 - x_2^2 - x_3^2) + 2c_{q2}x_1x_2 + 2c_{q3}x_1x_3) \\
D_2 =& \boldsymbol{e}^{-(\overline{b}_1 x_1 + \overline{b}_2 x_2 + \overline{b}_3 x_3)}(c_2 - c_{\neg 3}x_1 + c_r x_2 + c_{\neg 1}x_3 \\
&\qquad + c_{q1}x_1x_2 + c_{q2}(-x_1^2 + x_2^2 - x_3^2) + 2c_{q3}x_2x_3) \\
D_3 =& \boldsymbol{e}^{-(\overline{b}_1 x_1 + \overline{b}_2 x_2 + \overline{b}_3 x_3)}(c_3 - c_{\neg 2}x_1 - c_{\neg 1}x_2 + c_r x_3 \\
&\qquad + c_{q1}x_1x_3 + 2c_{q2}x_2x_3 + c_{q3}(-x_1^2 - x_2^2 + x_3^2))
\end{aligned}$$

These are all *solutions of our problem under these conditions.*

Proof

The above functions constitute a 14 dimensional space. By simple calculations we can show that all of them are solutions. Hence, combined with the fact that the space of solutions cannot have more then 14 dimensions we have shown the proposition. q.e.d.

We see that the common prefactor $\boldsymbol{e}^{-(\overline{b}_1 x_1 + \overline{b}_2 x_2 + \overline{b}_3 x_3)}$ just changes the length, but not the direction of our differential operator. Therefore we will drop it from now on and assume furthermore $\overline{b}_1 = \overline{b}_2 = \overline{b}_3 = 0$. This implies $B = B_1 = B_2 = B_3 = 0$ and hence $\Delta_{\not d} = \Delta$. So we get the following 11 dimensional vector space of solutions:

Theorem 2.13

If we have $\Delta = \Delta_{\not d}$ and $\not d = \sum_i D_i \partial_i + D$ then the $D_\boxdot$ have to fulfill the following relations, where the $c_\boxdot$ are real valued constants.

$$\begin{aligned}
D =& c_{q1}x_1 + c_{q2}x_2 + c_{q3}x_3 + c \\
D_1 =& c_1 + c_r x_1 + c_{\neg 3}x_2 + c_{\neg 2}x_3 \\
&\qquad + c_{q1}(x_1^2 - x_2^2 - x_3^2) + 2c_{q2}x_1x_2 + 2c_{q3}x_1x_3 \\
D_2 =& c_2 - c_{\neg 3}x_1 + c_r x_2 + c_{\neg 1}x_3 \\
&\qquad + 2c_{q1}x_1x_2 + c_{q2}(-x_1^2 + x_2^2 - x_3^2) + 2c_{q3}x_2x_3 \\
D_3 =& c_3 - c_{\neg 2}x_1 - c_{\neg 1}x_2 + c_r x_3 \\
&\qquad + 2c_{q1}x_1x_3 + 2c_{q2}x_2x_3 + c_{q3}(-x_1^2 - x_2^2 + x_3^2)
\end{aligned}$$

2.2.8 Kernels

Now we want to take a closer look at the possible differential operators resulting from the preceding classification procedure. Therefore we will especially emphasize the following points which are important in the geoscientifical context:

- Shape of the differential operators (i.e., the underlying vector fields).
- Their interaction with harmonics.
- Their kernel spaces.

In order to analyze these operators we will consider the underlying vector fields which are constituted by $(D_1\ D_2\ D_3)^T : \mathbb{R}^3 \to \mathbb{R}^3$

First we want to consider some of them which are playing the role of the odd one out: Revolving vector fields. W.l.o.g. we just display the one with x_1 axis and neglect the non-differential part:

$\mathscr{d}_{rev} = (x_1^2 - x_2^2 - x_3^2)\partial_1 + 2x_1x_2\partial_2 + 2x_1x_3\partial_3 + x_1$

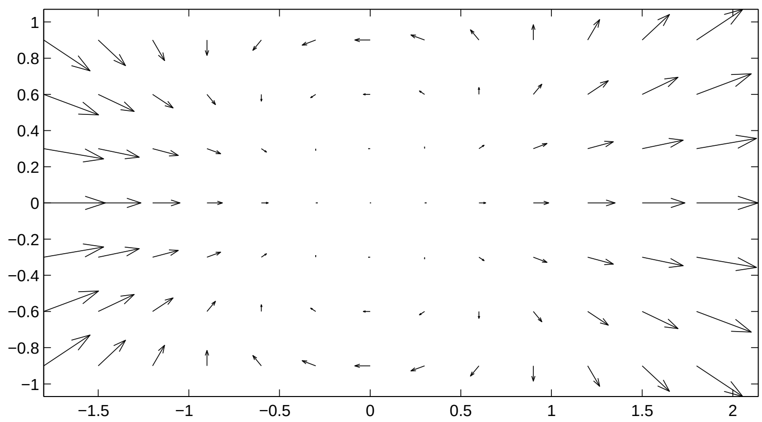


Figure 2.1: revolving vector field

We will not consider the revolving vector fields further because they have a severe disadvantage. For any practical application we will never exactly measure such a mixed differential operator, but pure ones, either the identity or pure first order differentials. Additionally for applications in geodesy we mostly cannot measure the identity. Therefore this differential is of no particular use for us in most applications in gravity determination. However, there may be other applications (e.g., magnetics), where such a field could prove suitable.

So from this point onwards we will concentrate on the left over 8 dimensional solution space:

$$
\begin{aligned}
D &= c \\
D_1 &= c_1 + c_r x_1 + c_{\neg 3} x_2 + c_{\neg 2} x_3 \\
D_2 &= c_2 - c_{\neg 3} x_1 + c_r x_2 + c_{\neg 1} x_3 \\
D_3 &= c_3 - c_{\neg 2} x_1 - c_{\neg 1} x_2 + c_r x_3
\end{aligned}
$$

More detailed considerations can be found in the chapter about integration.

If we turn our attention to the kernel spaces now, we observe using the above result that $\mathrm{sker}(\mathscr{d}) = \ker(\mathscr{d})$. This is a direct consequence of the well-known Min-Max principle for harmonic functions.

This yields in particular that we do not have to test, if a solution of the easier problem with the split operator is really a solution of the whole problem. The only thing which is still left are the kernels of our differential operators which circumvent an exact reconstruction.

Because it will be rather hard to consider the kernels of the composite operators we will first take a look at the separate components and their kernels.

- Identity operator $\mathscr{d}_{id} = 1$.

  The functionality of this operator is clear and does not need any further remark.

- Constant vector fields (w.l.o.g. just x_1 direction): $\mathscr{d}_{const} = \partial_1$.

  These differential operators may be used to shift the next two classes of differential operators around.

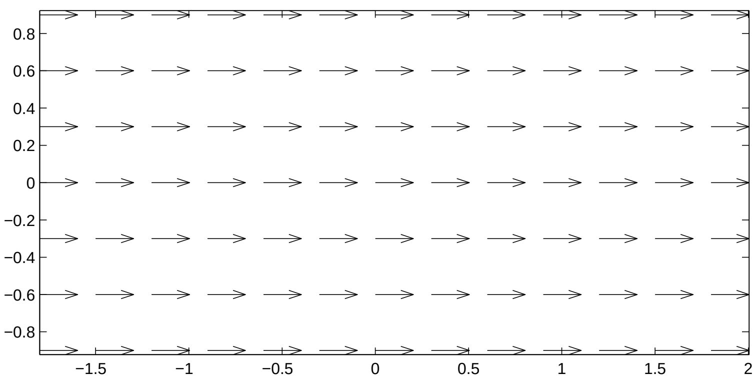


Figure 2.2: constant vector field

  In the kernel are all functions which are constant in the x_1 direction.

- Radial differential operators $\mathscr{d}_{rad} = x_1\partial_1 + x_2\partial_2 + x_3\partial_3$.

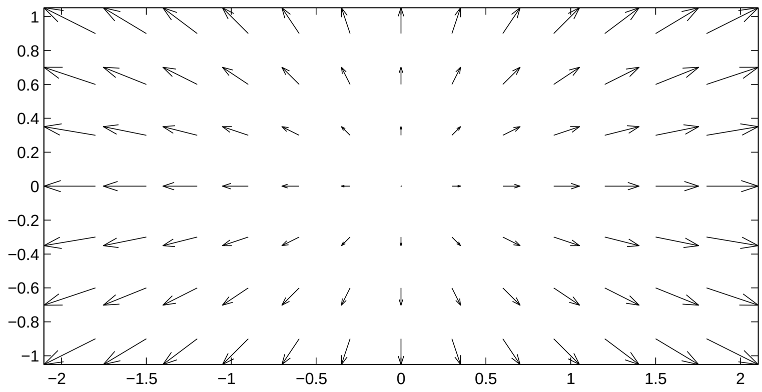


Figure 2.3: radial vector field

In the kernel are all functions which are constant on each ray originating from 0. We are dealing with smooth functions, hence these can just be the constant functions.

- Cylindrical differential operators (w.l.o.g. just x_3 axis): $\not{d}_{cyl} = x_2\partial_1 - x_1\partial_2$.

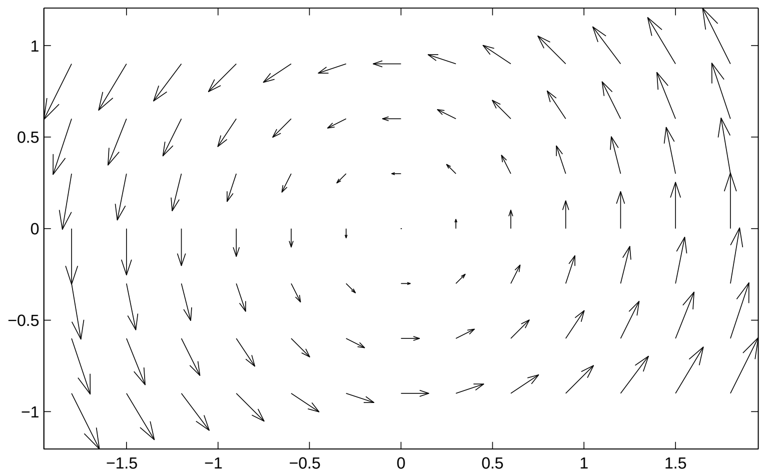


Figure 2.4: cylindrical vector field

In the kernel are all functions which are constant on each cylinder around the x_3 axis.

Now we will turn our attention to the kernel spaces. As the operators are invariant towards a rotation of the coordinate system we will pick just one of the three different prototypes. The next results will be proven in the next chapter.

Differential Operator $\not{d}_{const}$ The kernel just consists of the 0. (Again, Min-Max principle)

Differential Operator d_{rad} As there are no constant harmonics V which are defined in Σ_{ext} and fulfill $|V(x)| = O(||x||^{-1})$, the kernel just consists of the 0.

Differential Operator d_{cyl} For every degree of the spherical harmonics there is exactly one in the kernel. (In terms of spherical harmonics: The zonal spherical harmonics are in the kernel.)

In particular this result indicates that the size of the kernel space is comparably small. If we consider *any* two different differential operators the information obtained is sufficient to get a complete reconstruction of the original information when considering unbiased data.

2.2.9 Composition of Solutions for Pure Second Order Operators

Now we want to generate pure second order differential operators d out of first order differential operators which have the split operator $\Delta_{d} = \Delta$.

Of course, these are infinitely many, hence we need again a kind of classification procedure. In particular we will show, that we may rely on the following collection of prototypes which form a real vector space. For the sake of easier notation we introduce:

Definition 2.5

Define the following differential operators

$$\begin{aligned}
&\mathsf{d}_{id} = 1 \\
&\mathsf{d}_{x_1} = \partial_1 , \qquad \mathsf{d}_{x_2} = \partial_2 , \qquad \mathsf{d}_{x_3} = \partial_3 \\
&\mathsf{d}_{\neg x_1} = x_3\partial_2 - x_2\partial_3 , \qquad \mathsf{d}_{\neg x_2} = x_3\partial_1 - x_1\partial_3 , \qquad \mathsf{d}_{\neg x_3} = x_2\partial_1 - x_1\partial_2 \\
&\mathsf{d}_{r} = x_1\partial_1 + x_2\partial_2 + x_3\partial_3 , \qquad \mathsf{d}_{\overline{r}} = x_1\partial_1 + x_2\partial_2 + x_3\partial_3 - 1
\end{aligned}$$

Lemma 2.14

The differential operators shown below are pure second order operators which read the following way: ($\overline{i+k}$ *shall denote* $(i+k \mod 3)+1$)

$$\begin{aligned}
\mathsf{d}_{x_i}\mathsf{d}_{x_j} &= \partial_i\partial_j && \text{for all } i \leq j \\
\mathsf{d}_{\neg x_i}\mathsf{d}_{x_j} &= x_{\overline{i+2}}\partial_{\overline{i+1}}\partial_j - x_{\overline{i+1}}\partial_{\overline{i+2}}\partial_j && \text{for all } i, j
\end{aligned}$$

In both situations we do not allow $i = j = 3$.

$$\begin{aligned}
&\Big(\mathsf{d}_r\mathsf{d}_{x_i} = x_1\partial_1\partial_i + x_2\partial_2\partial_i + x_3\partial_3\partial_i \qquad \forall i\Big) \\
&\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_i} = (-x_{\overline{i+1}}^2 + x_{\overline{i+2}}^2)\partial_{\overline{i+1}}\partial_{\overline{i+2}} + x_{\overline{i+2}}x_i\partial_{\overline{i+1}}\partial_i - x_{\overline{i+1}}x_i\partial_{\overline{i+2}}\partial_i \\
&\qquad + x_{\overline{i+1}}x_{\overline{i+2}}\partial_{\overline{i+1}}\partial_{\overline{i+1}} - x_{\overline{i+1}}x_{\overline{i+2}}\partial_{\overline{i+2}}\partial_{\overline{i+2}} \qquad \forall i \\
&\mathsf{d}_{\overline{r}}\mathsf{d}_r = x_1^2\partial_1\partial_1 + x_2^2\partial_2\partial_2 + x_3^2\partial_3\partial_3 \\
&\qquad + 2x_1x_2\partial_1\partial_2 + 2x_1x_3\partial_1\partial_3 + 2x_2x_3\partial_2\partial_3
\end{aligned}$$

Remark

Note that the five solutions which are excluded in the $17+5$ solutions above can be obtained as a linear combination of the others and by using the fact that we are dealing with harmonic functions (i.e., $\partial_1\partial_1+\partial_2\partial_2+\partial_3\partial_3=\Delta=0$).

In order to show that these are all possibilities we will need the next section.

2.3 Split Operators with Respect to a Purely Second Order Operator Condition

Because of a huge number of complications arising we will not seek a split operator for a general second order operator but we will restrict ourselves to an operator $\overline{\Delta}$ whose second order part equals the normal Laplace operator $\Delta=\partial_1\partial_1+\partial_2\partial_2+\partial_3\partial_3$.

The restrictions which we have to impose on V, $\overline{\Delta}$ and đ are the same as in the last section.

Problem 2.6

Assume

$$\overline{\Delta}=\sum_i \partial_i\partial_i+\sum_i A_i\partial_i+A$$

where the $A_{\boxdot}\in C^\infty(\overline{\Sigma_{ext}})$ *denote smooth functions.*

Additionally $\overline{\Delta}$ *should fulfill the following* technical condition. *For all differential operators* $\{1,\partial_i,\partial_k\partial_l,\partial_j\partial_k\partial_l,\partial_i\partial_j\partial_k\partial_l\}$ *with* $1\le i\le j\le k\le l\le 3$ *and* $k\ne 3$ *there should exist an half order* $\blacktriangleright$ *on the multi-indices and functions* $H,H_i,H_{ij},H_{ijk},H_{ijkl}$ *which fulfill for all values* (ν, μ *are multi-indices):*

- $H_\mu\in C^4(\overline{\Sigma_{ext}})$ *for all* μ
- $\overline{\Delta}H_\mu=0$ *for all* μ
- $\partial_\nu H_\mu=0$ *for all* $\nu\blacktriangleright\mu$
- $\partial_\nu H_\nu=\overline{H}_\nu\ne 0$ *for all* ν

Assume furthermore

$$\text{đ}=\sum_{i\le j} D_{ij}\partial_i\partial_j$$

where the $D_{\boxdot}\in C^\infty(\overline{\Sigma_{ext}})$ *are smooth functions.*

Furthermore we demand that for a fixed α *at every point there is at least one of the* $D_{ij}-\alpha\delta_{ij}\ne 0$. *(Due to* $\overline{\Delta}V=0$ *we can replace* đ *by* $\text{đ}-\alpha\overline{\Delta}$ *without facing problems).*

Does there exist a sensible split operator $\overline{\Delta}_{\text{đ}}$ *for* $\overline{\Delta}$ *with respect to* đ*? How does it look like? Which conditions has* đ *to fulfill?*

Lemma 2.15

The Laplace operator Δ fulfills the above requirements.

Proof

This proof works exactly as the one for first order differential operators in the last section. Additionally we take the functions

$$
\begin{aligned}
{}^0H_4^0 &= x_1^4 - 6x_1^2x_3^2 + x_3^4 & {}^0H_4^1 &= x_1^3x_2 - 3x_1x_2x_3^2 \\
{}^0H_4^2 &= x_1^2x_2^2 - x_1^2x_3^2 - x_2^2x_3^2 + \frac{1}{3}x_3^4 & {}^0H_4^3 &= x_1x_2^3 - 3x_1x_2x_3^2 \\
{}^0H_4^4 &= x_2^4 - 6x_2^2x_3^2 + x_3^4 & & \\
{}^1H_4^0 &= x_1^3x_3 - x_1x_3^3 & {}^1H_4^1 &= x_1^2x_2x_3 - \frac{1}{3}x_2x_3^3 \\
{}^1H_4^2 &= x_1x_2^2x_3 - \frac{1}{3}x_1x_3^3 & {}^1H_4^3 &= x_2^3x_3 - x_2x_3^2
\end{aligned}
$$

in order to fulfill the technical condition. q.e.d.

Again, a first order split operator does not make too much sense, hence we will skip this step this time and directly continue with a second order split operator. For our convenience we assume that the proposed split operator $\overline{\Delta}_{\not d}$ is denoted by

$$\widetilde{\Delta} = \sum_{i\leq j} B_{ij}\partial_i\partial_j + \sum_i B_i\partial_i + B$$

In the sequel we will employ exactly the same strategy as in the part about the first order differential operator. Therefore we will considerably shorten the argumentation and just point out the major steps and essential parts.

2.3.1 First Computations

First we will remove all terms with $\partial_3\partial_3$ parts using the fact that we are working with split operators, i.e., we just need the case $\overline{\Delta}V = 0$ directly implying $\widetilde{\Delta}_{\not d}V = 0$. So we are dealing with the following revised operator:

$$
\begin{aligned}
\widetilde{\Delta}_{\not d} + \Big(&B_{11}D_{11}\partial_1\partial_1 \\
&+ (B_{12}D_{11} + B_{11}D_{12})\partial_1\partial_2 \\
&+ (B_{13}D_{11} + B_{11}D_{13})\partial_1\partial_3 \\
&+ (B_{22}D_{11} + B_{11}D_{22} - B_{11}D_{11} + B_{12}D_{12})\partial_2\partial_2 \\
&+ (B_{23}D_{11} + B_{11}D_{23} + B_{12}D_{13} + B_{13}D_{12})\partial_2\partial_3 \\
&+ (B_{33}D_{11} + B_{11}D_{33} - B_{11}D_{11} + B_{13}D_{13})\partial_3\partial_3 \\
&+ (B_1D_{11} + 2\partial_1D_{11})\partial_1 \\
&+ (B_1D_{12} + 2\partial_2D_{11} + 2\partial_1D_{12} + B_2D_{11})\partial_2 \\
&+ (B_1D_{13} + 2\partial_3D_{11} + 2\partial_1D_{13} + B_3D_{11})\partial_3 \\
&+ (\partial_1\partial_1D_{11} + \partial_2\partial_2D_{22} + \partial_3\partial_3D_{11} \\
&\qquad + B_1\partial_1D_{11} + B_2\partial_2D_{11} + B_3\partial_3D_{11} + bD_{11})\Big)\overline{\Delta}
\end{aligned}
$$

Because of its length we have not displayed this revised operator at this point but we will consider the different parts consecutively. The interested reader may contact the author to obtain the corresponding *Maple 7* script.

Like in the section beforehand, the application of the functions H_μ yields, that all factors in front of the ∂_μ are 0. We will use this information step by step in the following parts.

2.3.2 Second order terms

The equations obtained from the fourth order terms of the above formula read:

$$
\begin{aligned}
0 =&(B_{ii} - B_{jj})D_{ij} + (D_{ii} - D_{jj})B_{ij} && \text{for all } i < j \\
0 =&(B_{ii} - B_{jj})(D_{ii} - D_{jj}) - B_{ij}D_{ij} && \text{for all } i < j \\
0 =&(D_{11} - D_{33})B_{23} + (B_{11} - B_{33})D_{23} + B_{13}D_{12} + B_{12}D_{13} \\
0 =&(D_{22} - D_{11})B_{13} + (B_{22} - B_{11})D_{13} + B_{12}D_{23} + B_{23}D_{12} \\
0 =&(D_{33} - D_{22})B_{12} + (B_{33} - B_{22})D_{12} + B_{23}D_{13} + B_{13}D_{23}
\end{aligned}
$$

Lemma 2.16

If $\mathcal{d}$ is a non-trivial second order operator we get that $\widetilde{\Delta}$ is essentially the Laplace operator, i.e., the second order part equals $F\Delta$, where F is a smooth function

Proof

As last time all considerations are made pointwise. Rewriting the first two sets of equations we get:

$$
0 = \begin{pmatrix} D_{ij} & D_{ii} - D_{jj} \\ D_{ii} - D_{jj} & -D_{ij} \end{pmatrix} \begin{pmatrix} B_{ii} - B_{jj} \\ B_{ij} \end{pmatrix} \qquad \text{for all } i < j
$$

Obviously we have $\det \left(\begin{smallmatrix} D_{ij} & D_{ii}-D_{jj} \\ D_{ii}-D_{jj} & -D_{ij} \end{smallmatrix}\right) = -\left(D_{ij}^2 + (D_{ii} - D_{jj})^2\right)$.

Hence we get for each pair (i, j) that either $D_{ii} - D_{jj} = D_{ij} = 0$ or $B_{ii} - B_{jj} = B_{ij} = 0$.

So we have to consider 8 different cases. Because of symmetry reasons we can restrict ourselves to three of them.

Case 1: $B_{11} - B_{22} = B_{12} = B_{11} - B_{33} = B_{13} = B_{22} - B_{33} = B_{23} = 0$

Obviously we get $B_{11} = B_{22} = B_{33} \neq 0$ and $B_{12} = B_{13} = B_{23} = 0$ which means that $\widetilde{\Delta}$ is essentially the Laplace operator.

Case 2: $D_{11} - D_{22} = D_{12} = D_{11} - D_{33} = D_{13} = D_{22} - D_{33} = D_{23} = 0$

Again we would get $D_{11} = D_{22} = D_{33}$ and $D_{12} = D_{13} = D_{23} = 0$ which implies that $\mathcal{d}$ is essentially the Laplace operator. Hence choosing $\alpha = D_{11}$ we have $D_{ij} - \alpha\delta_{ij} = 0$ contradicting our conditions.

Case 3: $D_{11} - D_{22} = D_{12} = D_{11} - D_{33} = D_{13} = B_{22} - B_{33} = B_{23} = 0$.

Hence we additionally get $D_{22} - D_{33} = 0$. If we do not want to get case 2 we have to assume $D_{23} \neq 0$.
Using the set of the last three equations we get:

$$
\begin{aligned}
0 =& (B_{11} - B_{33})D_{23} \\
0 =& B_{12}D_{23} \\
0 =& B_{13}D_{23}
\end{aligned}
$$

Thus we arrive in case 1 and the claim is proved. q.e.d.

There is strong evidence that we could get the above result even if we did not claim that $\overline{\Delta}$ is essentially the Laplace operator.

2.3.3 Further equations

Using the result that $\widetilde{\Delta}$ is essentially the Laplace operator we can deduce without loss of generality that $D_{33} = 0$ everywhere.

For simplicity we will now assume that $\overline{\Delta} = \Delta = \widetilde{\Delta}$. Otherwise the equations we get will be very large and seem to be unsolvable with current methods. Hence we get the following set of twelve equations, where we already incorporated the knowledge of $D_{33} = 0$. Of course we associate D_{ij} with D_{ji} whenever $i > j$.

$$
\begin{aligned}
0 =& \Delta D_{ij} && \text{for all } i \leq j \\
0 =& \partial_j D_{ii} - \partial_j D_{jj} + \partial_i D_{ij} && \text{for all } i \neq j \\
0 =& \partial_1 D_{23} + \partial_2 D_{13} + \partial_3 D_{12}
\end{aligned}
$$

2.3.4 Number of Solutions

For determining the number of solutions of the above system of coupled linear partial differential equations we will translate the system into the language of commutative algebra and employ *Singular* [GPS01] again. The notation is exactly taken from the last section.

```
ring r=0,(s1,s2,s3),(c,dp(3));
vector v1= [s1^2+s2^2+s3^2,0,0,0,0];
vector v2= [0,s1^2+s2^2+s3^2,0,0,0];
vector v3= [0,0,s1^2+s2^2+s3^2,0,0];
vector v4= [0,0,0,s1^2+s2^2+s3^2,0];
vector v5= [0,0,0,0,s1^2+s2^2+s3^2];
vector v6= [0,0,s3,s2,s1];
vector v7= [s2,-s2,s1,0,0];
vector v8= [-s1,s1,s2,0,0];
vector v9= [s3,0,0,s1,0];
vector v10=[-s1,0,0,s3,0];
```

```
vector v11=[0,s3,0,0,s2];
vector v12=[0,-s2,0,0,s3];
module m = v1,v2,v3,v4,v5,v6,v7,v8,v9,v10,v11,v12;
std(m);
```

This results in the following output.

```
_[1]=[0,0,0,0,s2^2+s3^2]
_[2]=[0,0,0,0,s1^2]
_[3]=[0,0,0,0,s3^3]
_[4]=[0,0,0,0,s2*s3^2]
_[5]=[0,0,0,0,s1*s3^2]
_[6]=[0,0,0,0,s1*s2*s3]
_[7]=[0,0,0,s3^2,2*s1*s2]
_[8]=[0,0,0,s2*s3,s1*s3]
_[9]=[0,0,0,s1*s3,-s2*s3]
_[10]=[0,0,0,s2^2]
_[11]=[0,0,0,2*s1*s2,s3^2]
_[12]=[0,0,0,s1^2+s3^2]
_[13]=[0,0,s3,s2,s1]
_[14]=[0,0,s2^2,-s2*s3,s1*s3]
_[15]=[0,0,s1*s2,-s1*s3]
_[16]=[0,0,s1^2,s2*s3,-s1*s3]
_[17]=[0,s3,0,0,s2]
_[18]=[0,s2,0,0,-s3]
_[19]=[0,s1,s2,-s3]
_[20]=[s3,0,0,s1]
_[21]=[s2,0,s1,0,-s3]
_[22]=[s1,0,0,-s3]
```

Lemma 2.17

Our system of partial differential equations possesses a 17 dimensional space of solutions. It can be parted in the following way.

- *8 degrees of freedom for choosing D_{23}.*
- *4 degrees of freedom for choosing D_{13} for fixed D_{23}.*
- *3 degrees of freedom for choosing D_{12} for fixed D_{23}, D_{13}.*
- *1 degree of freedom for choosing D_{22} for fixed D_{23}, D_{13}, D_{12}.*
- *1 degree of freedom for choosing D_{11} for fixed D_{23}, D_{13}, D_{12}, D_{22}.*

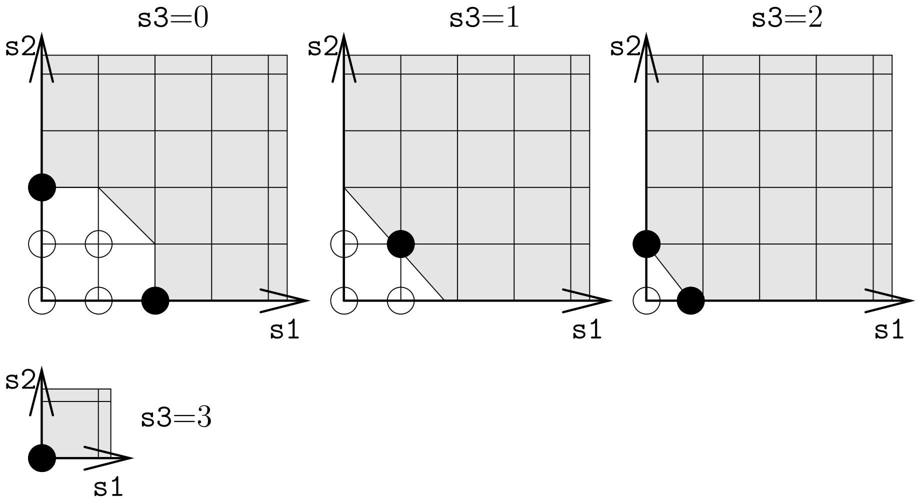
Proof

We consecutively show the relevant Reid diagrams for D_{23}, D_{13}, D_{12}, D_{22} and D_{11}. In these pictures we denote the position of the leading polynomial by a black dot in the grid, the area which is covered by the intersection of the sectors stretched by these points are shaded and the possible starting values (and hence degrees of freedom) are denoted as white dots. In order to get a better overview the picture is sliced into different layers with respect to the `s3` component.

In order to get the possible degrees of freedom we just need to count the white dots then and hence determine the cardinality of the Cauchy data set.

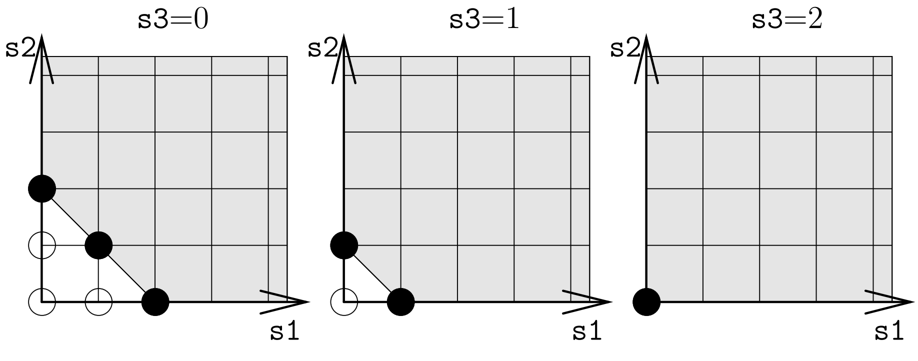
Let's consider the first picture. For D_{23} we have `s2^2`, `s1^2`, `s3^3`,`s2 * s3^2`, `s1 * s3^2`, `s1 * s2 * s3`, as leading polynomials. Hence we get the points $(0,2,0)$, $(2,0,0)$, $(0,0,3)$, $(0,1,2)$, $(1,0,2)$, $(1,1,1)$ to cover.

This results in the following Reid diagram.



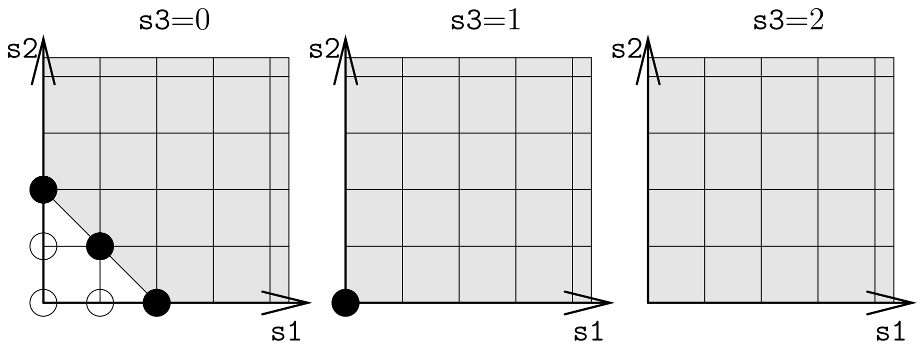
Counting the dots we get 8 possible degrees of freedom.

For D_{13} we have `s3^2`, `s2*s3`, `s1*s3`, `s2^2`, `s1*s2` and `s1^2` as leading polynomials and hence the following points: $(0,0,2)$, $(0,1,1)$, $(1,0,1)$, $(0,2,0)$, $(1,1,0)$ and finally $(2,0,0)$. As a result we get the following Reid diagram.



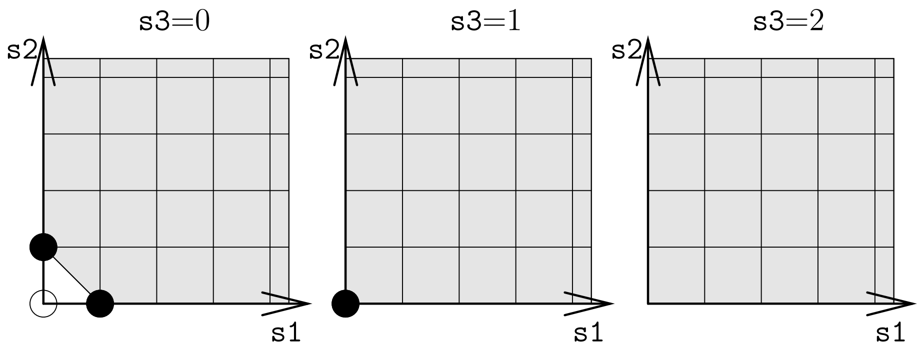
Counting the dots we get 4 different possible degrees of freedom.

For D_{12} we have `s3`, `s2^2`, `s1 * s2` and `s1^2` as leading polynomials and hence the following points: $(0,0,1)$, $(0,2,0)$, $(1,1,0)$ and $(2,0,0)$. As a result we get the following Reid diagram.



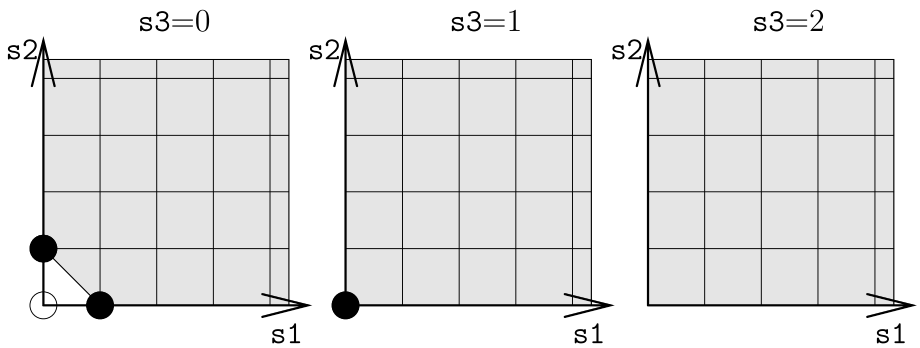
Counting the dots we observe 3 degrees of freedom.

For D_{22} we have `s3`, `s2` and `s1` and hence the points $(0, 0, 1)$, $(0, 1, 0)$ and $(1, 0, 0)$. So we get the following Reid diagram.



So we are just having one degree of freedom for choosing the solution.

For D_{11} we have again `s3`, `s2` and `s1` and hence the points $(0, 0, 1)$, $(0, 1, 0)$ and $(1, 0, 0)$. So we get the following Reid diagram.



So we are just having one degree of freedom for choosing the last solution.

This proves our claim. q.e.d.

On the other hand we already know the 17-dimensional space of solutions obtained by iterating the solutions for the first order derivative operator in the last section. Hence we get the following theorem:

Theorem 2.18

The above system of differential equations has the following solutions: (The names of the variables are chosen appropriately to the results beforehand.)

$$
\begin{aligned}
D_{11} =& c_{r,r}(x_1^2 - x_3^2) + c_{r,\neg 3}x_1x_2 - 2c_{r,\neg 2}x_1x_3 + c_{r,\neg 1}x_2x_3 \\
&+ c_{\neg 2,3}x_1 - c_{\neg 3,1}x_2 + c_{\neg 1,3}x_2 + c_{\neg 2,1}x_3 + c_{1,1} \\
D_{22} =& c_{r,r}(x_2^2 - x_3^2) - c_{r,\neg 3}x_1x_2 - c_{r,\neg 2}x_1x_3 + 2c_{r,\neg 1}x_2x_3 \\
&+ c_{\neg 2,3}x_1 - c_{\neg 3,2}x_1 + c_{\neg 1,3}x_2 - c_{\neg 1,2}x_3 + c_{2,2} \\
D_{12} =& c_{r,\neg 3}(x_2^2 - x_1^2) + 2c_{r,r}x_1x_2 + c_{r,\neg 1}x_1x_3 - c_{r,\neg 2}x_3x_2 \\
&+ c_{\neg 3,1}x_1 + c_{\neg 3,2}x_2 - c_{\neg 2,2}x_3 - c_{\neg 1,1}x_3 + c_{1,2} \\
D_{13} =& c_{r,\neg 2}(x_1^2 - x_3^2) - c_{r,\neg 1}x_1x_2 + 2c_{r,r}x_1x_3 + c_{r,\neg 3}x_3x_2 \\
&- c_{\neg 2,1}x_1 + c_{\neg 1,1}x_2 + c_{\neg 2,3}x_3 + c_{1,3} \\
D_{23} =& c_{r,\neg 1}(x_3^2 - x_2^2) + c_{r,\neg 2}x_1x_2 - c_{r,\neg 3}x_1x_3 + 2c_{r,r}x_2x_3 \\
&+ c_{\neg 2,2}x_1 + c_{\neg 1,2}x_2 + c_{\neg 1,3}x_3 + c_{2,3}
\end{aligned}
$$

Proof

Simple checking shows that these are solutions. On the other hand we know from the last lemma that we are dealing with a seventeen dimensional vector space, hence these are actually all solutions. q.e.d.

For simplicity we can include D_{33} again and hence get the following system:

Theorem 2.19

If we have $\Delta = \Delta_{\mathscr{d}}$ and $\mathscr{d} = \sum_{i\leq j} D_{ij}\partial_i\partial_j$ then the $D_{\boxdot}$ have to fulfill the following relations, where the $c_{\boxdot}$ are real valued constants.

$$
\begin{aligned}
D_{11} =& c_{r,r}x_1^2 + c_{r,\neg 3}x_1x_2 - c_{r,\neg 2}x_1x_3 - c_{\neg 3,1}x_2 + c_{\neg 2,1}x_3 + c_{1,1} \\
D_{22} =& c_{r,r}x_2^2 - c_{r,\neg 3}x_1x_2 + c_{r,\neg 1}x_2x_3 - c_{\neg 3,2}x_1 - c_{\neg 1,2}x_3 + c_{2,2} \\
D_{33} =& c_{r,r}x_3^2 + c_{r,\neg 2}x_1x_3 - c_{r,\neg 1}x_2x_3 - c_{\neg 2,3}x_1 - c_{\neg 1,3}x_2(+c_{3,3}) \\
D_{12} =& c_{r,\neg 3}(x_2^2 - x_1^2) + 2c_{r,r}x_1x_2 + c_{r,\neg 1}x_1x_3 - c_{r,\neg 2}x_3x_2 \\
&+ c_{\neg 3,1}x_1 + c_{\neg 3,2}x_2 - c_{\neg 2,2}x_3 - c_{\neg 1,1}x_3 + c_{1,2} \\
D_{13} =& c_{r,\neg 2}(x_1^2 - x_3^2) - c_{r,\neg 1}x_1x_2 + 2c_{r,r}x_1x_3 + c_{r,\neg 3}x_3x_2 \\
&- c_{\neg 2,1}x_1 + c_{\neg 1,1}x_2 + c_{\neg 2,3}x_3 + c_{1,3} \\
D_{23} =& c_{r,\neg 1}(x_3^2 - x_2^2) + c_{r,\neg 2}x_1x_2 - c_{r,\neg 3}x_1x_3 + 2c_{r,r}x_2x_3 \\
&+ c_{\neg 2,2}x_1 + c_{\neg 1,2}x_2 + c_{\neg 1,3}x_3 + c_{2,3}
\end{aligned}
$$

As the remarks concerning the behavior and kernel spaces of these operators are very similar to the ones we made beforehand for the split operator of the first order differential operators we will skip this right now. This similarity is not surprising because we are just dealing with a composition of our first order operators right now.

2.4 Conclusion

The initial question for this chapter was the following one:

> *How can one solve the oblique derivative problem occurring in the geoscientifical context?*

We could give one possible solution ansatz. Assume that $\mathscr{d}$ is our oblique derivative which constitutes the side condition and the Laplace operator Δ constitutes the underlying differential equation. We have shown that the only (geoscientifically interesting) second order operator $\Delta_{\mathscr{d}}$ which fulfills $\Delta_{\mathscr{d}}(\mathscr{d}V) = 0$ for all V which fulfill $\Delta V = 0$ is the Laplace operators, i.e., $\Delta_{\mathscr{d}} = \Delta$.

The possible $\mathscr{d}$ are now displayed, where the $c_{\boxdot}$ are real valued constants:

- First order differential operator $\mathscr{d} = \sum_{i=1}^{3} D_i \partial_i + D$.

$$\begin{pmatrix} D_1 \\ D_2 \\ D_3 \end{pmatrix} = \begin{pmatrix} c_r & c_{\neg 3} & c_{\neg 2} \\ -c_{\neg 3} & c_r & c_{\neg 1} \\ -c_{\neg 2} & -c_{\neg 1} & c_r \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} + \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix}$$

$$D = c$$

- Purely second order differential operator $\mathscr{d} = \sum_{i=1}^{3} \sum_{j=i}^{3} D_{ij} \partial_i \partial_j$.

$$\begin{aligned}
D_{11} =& c_{r,r} x_1^2 + c_{r,\neg 3} x_1 x_2 - c_{r,\neg 2} x_1 x_3 - c_{\neg 3,1} x_2 + c_{\neg 2,1} x_3 + c_{1,1} \\
D_{22} =& c_{r,r} x_2^2 - c_{r,\neg 3} x_1 x_2 + c_{r,\neg 1} x_2 x_3 - c_{\neg 3,2} x_1 - c_{\neg 1,2} x_3 + c_{2,2} \\
D_{33} =& c_{r,r} x_3^2 + c_{r,\neg 2} x_1 x_3 - c_{r,\neg 1} x_2 x_3 - c_{\neg 2,3} x_1 - c_{\neg 1,3} x_2 (+c_{3,3}) \\
D_{12} =& c_{r,\neg 3}(x_2^2 - x_1^2) + 2c_{r,r} x_1 x_2 + c_{r,\neg 1} x_1 x_3 - c_{r,\neg 2} x_3 x_2 \\
& + c_{\neg 3,1} x_1 + c_{\neg 3,2} x_2 - c_{\neg 2,2} x_3 - c_{\neg 1,1} x_3 + c_{1,2} \\
D_{13} =& c_{r,\neg 2}(x_1^2 - x_3^2) - c_{r,\neg 1} x_1 x_2 + 2c_{r,r} x_1 x_3 + c_{r,\neg 3} x_3 x_2 \\
& - c_{\neg 2,1} x_1 + c_{\neg 1,1} x_2 + c_{\neg 2,3} x_3 + c_{1,3} \\
D_{23} =& c_{r,\neg 1}(x_3^2 - x_2^2) + c_{r,\neg 2} x_1 x_2 - c_{r,\neg 3} x_1 x_3 + 2c_{r,r} x_2 x_3 \\
& + c_{\neg 2,2} x_1 + c_{\neg 1,2} x_2 + c_{\neg 1,3} x_3 + c_{2,3}
\end{aligned}$$

As important facts regarding these operators we observed:

- Any of the differential operators $\mathscr{d}$ have the Laplace operator $\Delta = \Delta_{\mathscr{d}}$ as split operator and hence the differentiated solution is also a potential, i.e., $\Delta V = 0 \Rightarrow \Delta \mathscr{d} V = 0$.

- We can use the same basis systems to solve the underlying boundary value type problem as for the radial derivatives or non-derived data.

- Solving an oblique derivative problem with purely second order side conditions specified above is as difficult as solving an oblique derivative problem with the first order side conditions given above (in the Laplace case!).

From the mathematical point of view one might add the following remark:

- If we restrict our attention to the Laplace operator as split operator we obtained a complete classification of possible first and pure second order differential operators. This means in particular that we do not have to search.
- The method is general enough to tackle other related problems with complicated side conditions.
- Many results also hold or can be easily extended to all dimensions ≥ 2.

The big advantage in comparison to other solution methods for the oblique derivative problem is that we can operate as if we actually would not have any oblique derivative. This means that we can rely on standard techniques for solving the oblique derivative problem which have been proven to be reliable in practice.

In particular we do not have any restrictions on our data location, every one which is suitable for the standard problem without derivatives as side conditions does the job. Especially for boundary value problems, where even a small quantity of derivatives which are sufficiently near to the tangent plane pose enormous problems this is really a leap forward. Additionally we can work with standard basis systems and do not have to switch to differentiated (anisotropic) ones.

However the most obvious advantage is that one has a particularly easy solution method for higher derivatives as side conditions. Even for derivatives higher than the second order ones we considered the approach transfers without major problems.

Chapter 3

Integration

How does the "integration" (i.e., inversion of the differential operator) look like with respect to the differential operators in the last chapter?

Do we have uniqueness in the reconstruction or do we have to take care of some kernel spaces? How do they look like?

As we know a precise answer to this question is just possible for a special basis of our underlying function space. Therefore we will restrict our attention to the $L^2(\Sigma)$-complete orthonormal system of spherical harmonics. Other possible basis systems which we have not discussed here can be found in [FM03b].

It does not matter if one has a description of the integration or of the differentiation because the two of them are inverse operators of each other. Therefore we will restrict ourselves to the differentiation part. However, the problem of finding the corresponding differentiation matrices is rather complicated. Therefore we will not launch a direct attack but we will first solve the problem for a basis system which allows easy differentiation. Afterwards we will do a basis change to the spherical harmonics.

3.1 Preliminaries

We will use the following results of potential theory taken from [ABR91, FGS98, Kel67, Néd01, Wal71] and therefore want to shortly cite them mostly without proof:

3.1.1 Kelvin Transform

First we want to introduce harmonics:

Definition 3.1 (Harmonics)

Take a smooth regular surface Σ in $\mathbb{R}^3 \cup \{\infty\}$ which divides $\mathbb{R}^3$ in a bounded part Σ_{int} and an unbounded part Σ_{ext}, i.e., $\infty \in \Sigma_{ext}$, where each part is assumed to be path connected. I.e., we have $\mathbb{R}^3 = \Sigma_{int} \cup^* \Sigma \cup^* \Sigma_{ext}$, where $\cup^*$ denotes the disjoint union. Without loss of generality assume $0 \in \Sigma_{int}$. Furthermore Σ should be a smooth surface.

All functions $V : \overline{\Sigma_{int}} \to \mathbb{R}$ *which fulfill*

$$V \in C^{(\infty)}(\Sigma_{int}) \cap C^{(0)}(\overline{\Sigma_{int}})$$
$$(\Delta V)|_{\Sigma_{int}} = 0$$

constitute the space $Pot(\overline{\Sigma_{int}})$.
All functions $V : \overline{\Sigma_{ext}} \to \mathbb{R}$ *which fulfill*

$$V \in C^{(\infty)}(\Sigma_{ext}) \cap C^{(0)}(\overline{\Sigma_{ext}})$$
$$|V(x)| = O(||x||^{-1})$$
$$(\Delta V)|_{\Sigma_{ext}} = 0$$

constitute the space $Pot(\overline{\Sigma_{ext}})$.

Remark

Any $V \in Pot(S)$ where S either $\overline{\Sigma_{int}}$ or $\overline{\Sigma_{ext}}$ is uniquely determined by the restriction $V|_{\Sigma}$.

There is an operation which transfers $Pot(\overline{\Sigma_{int}})$ to $Pot(\overline{\Sigma_{ext}})$ and vice versa, the Kelvin transform. Mathematically seen this is nothing but an inversion at the sphere.

Definition 3.2 (Kelvin Transform)

Let $\{0\} \subset S \subset \mathbb{R}^3 \cup \{\infty\}$. *Define* $\mathfrak{K}(S) = \left\{ x \in \mathbb{R}^3 \cup \{\infty\} \,\middle|\, \frac{x}{|x|^2} \in S \right\}$. *Furthermore, if* $V \in Pot(S)$ *define*

$$\breve{V} = \mathfrak{K}(V)\,(x) = \frac{1}{|x|}\, V\!\left(\frac{x}{|x|^2}\right)$$

The operator $\mathfrak{K}$ *is called Kelvin Transform.*

Lemma 3.1 (Kelvin Transform)

*We have the following two properties (*Id *is the identity operator):*

- $\mathfrak{K}(\mathfrak{K}(\cdot)) = \mathrm{Id}$
- $\mathfrak{K}(Pot(S)) = Pot(\mathfrak{K}(S))$

Please note that in the above lemma S and $\mathfrak{K}(S)$ have two different surfaces.

3.1.2 Homogeneous Harmonic Polynomials

Definition 3.3 (Homogeneous Harmonic Polynomials)

A polynomial H_n is called homogeneous of degree n if it fulfills

$$H_n(x) = ||x||^n H_n\left(\frac{x}{||x||}\right) \qquad \forall x \in \mathbb{R}^3 \setminus \{0\}$$

If furthermore $H_n \in Pot(\overline{\Sigma_{int}})$ it is called homogeneous harmonic polynomial of degree n, the corresponding space of all such polynomials is called $Pot_n(\overline{\Sigma_{int}})$.

Lemma 3.2

Any homogeneous harmonic polynomial H_n of degree n can be represented in the form

$$H_n(x) = H_n(x_1, x_2, x_3) = \sum_{j=0}^{n} A_{n-j}(x_1, x_2)\, x_3^j$$

where A_k denotes a homogeneous polynomial of degree k in the variables x_1 and x_2. Furthermore, the $A_\boxdot$ fulfill the following relation

$$A_{n-j-2}(x_1, x_2) = -\frac{1}{(j+1)\,(j+2)}\,(\partial_1\partial_1 + \partial_2\partial_2)\, A_{n-j}(x_1, x_2)$$

The dimension of the space of homogeneous harmonic polynomials of degree n is $2n + 1 = \dim(Pot_n(\overline{\Sigma_{int}}))$.
Any harmonic polynomial can be written in terms of convergent series of homogeneous harmonic polynomials.

Remark

Hence homogeneous harmonic polynomials are fully determined by their $x_1^k x_2^{n-k-i} x_3^i$ part, where $i \in \{0, 1\}$ and $0 \le k \le n$.

So the following basis of the space of harmonic functions is well-defined.

Definition 3.4

Define $H_n \in Pot_n(\overline{\Sigma_{int}})$ and $\breve{H}_n = \mathfrak{K}(H_n)$ as its Kelvin transformed counterpart.
Let furthermore ${}^iH_n^k$ denote the homogeneous harmonic polynomial with the leading term $x_1^k x_2^{n-k-i} x_3^i$, where $n \ge k \ge 0$ and $i \in \{0, 1\}$.
Again denote its Kelvin transformed counterpart by ${}^i\breve{H}_n^k = \mathfrak{K}\big({}^iH_n^k\big)$.
In order to keep our notation simple we will assume that ${}^i\breve{H}_n^k = {}^iH_n^k = 0$ if $k < 0$ or $k > n - i$.

Thus the ${}^iH_n^k$ constitute a $L^2(\Sigma)$-complete basis of $Pot(\overline{\Sigma_{int}})$ and the Kelvin transformed counterparts ${}^i\breve{H}_n^k$ constitute a $L^2(\Sigma)$-complete basis of $Pot(\overline{\Sigma_{ext}})$.

Remark

Neither the ${}^{i}H_n^k$ are an orthonormal basis for $Pot(\overline{\Sigma_{int}})$ nor the ${}^{i}\breve{H}_n^k$ for $Pot(\overline{\Sigma_{ext}})$ (with respect to the standard $L^2(\Sigma)$ inner product).

The homogeneous harmonic polynomials behave particularly nice under the Kelvin transform.

Lemma 3.3

Let H_n be a homogeneous harmonic polynomial of the degree n. The Kelvin transformed spherical harmonic $\mathfrak{K}(H_n) = \breve{H}_n$ is given by

$$\mathfrak{K}(H_n)\,(x) = \frac{1}{|x|^{2n+1}} H_n(x)$$

Proof

Straightforward using $\mathfrak{K}(H_n)\,(x) = \frac{1}{|x|}\ H_n\!\left(\frac{x}{|x|^2}\right)$ and the homogeneity. q.e.d.

3.1.3 Kelvin Transform and Derivatives

Now we want to give a transition formula which allows to convert relations we found for ordinary homogeneous harmonic polynomials H_n to their Kelvin transformed counterpart $\breve{H}_n$.

Lemma 3.4

We have

$$\partial_i \breve{H}_n(x) = \frac{(x_1^2 + x_2^2 + x_3^2)\,\partial_i H_n(x) - (2n+1)\,x_i H_n(x)}{|x|^{2n+3}}$$

Proof

Straightforward calculations yield

$$\begin{aligned}
\partial_i \breve{H}_n(x) &= \partial_i \frac{H_n(x)}{|x|^{2n+1}} \\
&= \frac{|x|^{2n+1}\partial_i H_n(x) - H_n(x)\,\partial_i |x|^{2n+1}}{|x|^{4n+2}} \\
&= \frac{|x|^{2n+1}\partial_i H_n(x) - (2n+1)\,|x|^{2n}\frac{x_i}{|x|} H_n(x)}{|x|^{4n+2}} \\
&= \frac{(x_1^2 + x_2^2 + x_3^2)\,\partial_i H_n(x) - (2n+1)\,x_i H_n(x)}{|x|^{2n+3}}
\end{aligned}$$

q.e.d.

3.2 Homogeneous Harmonic Polynomials

As we have seen above we may have two different kind of homogeneous harmonic polynomials in order to approximate functions. The one version could be used for inner Dirichlet problems, the Kelvin transformed version for outer Dirichlet problems.

We are mainly interested in harmonics in $Pot(\overline{\Sigma_{ext}})$, because this the case we observe when we are talking about the geopotential field. However, we need the ones in $Pot(\overline{\Sigma_{int}})$ to determine the derivatives of the ones in $Pot(\overline{\Sigma_{ext}})$. So, for the sake of completeness we will include a treatment of both versions in this text.

Because all second order differential operators we considered in the last section are an iteration of first order operators we just need to do our considerations for first order differential operators

$$\mathsf{d}_{id}\,, \quad \mathsf{d}_{x_i}\,, \quad \mathsf{d}_{\neg x_i}\,, \quad \mathsf{d}_r \qquad \forall i < j$$

which we will apply to our basis ${}^{i}H_n^k$ of homogeneous harmonic polynomials in $Pot(\overline{\Sigma_{int}})$ and afterwards rewrite this result in terms of homogeneous harmonic polynomials ${}^{i}\breve{H}_n^k$ in $Pot(\overline{\Sigma_{ext}})$.

We will strongly use two facts for our computations without pointing out every time when we apply them.

- Applying any of the above differential operators to a harmonic function leaves the function harmonic
- In order to categorize a harmonic polynomial we just need to consider the part consisting of $x_1^k x_2^{n-k-i} x_3^i$, where $n \geq k \geq 0$ and $i \in \{0, 1\}$.

3.2.1 Differential Operator d_{id}

Obviously we do not need to anything because we trivially have that every harmonic function and hence every harmonic polynomial stays the way it is.

3.2.2 Differential Operator d_{x_i}

3.2.2.1 Ordinary Homogeneous Harmonic Polynomials

Lemma 3.5

$$\begin{aligned}
\mathsf{d}_{x_1}\,{}^{i}H_n^k &= k\,{}^{i}H_{n-1}^{k-1}\\
\mathsf{d}_{x_2}\,{}^{i}H_n^k &= (n-k-i)\,{}^{i}H_{n-1}^{k}\\
\mathsf{d}_{x_3}\,{}^{1}H_n^k &= {}^{0}H_{n-1}^{k}\\
\mathsf{d}_{x_3}\,{}^{0}H_n^k &= -k\,(k-1)\,{}^{1}H_{n-1}^{k-2} - (n-k)\,(n-k-1)\,{}^{1}H_{n-1}^{k}
\end{aligned}$$

Proof

In the sequel we will use $P(x)$ and $Q(x)$ for arbitrary polynomials in x_1, x_2 and x_3. In particular, $P(x)$ and $Q(x)$ are different in every equation.
Furthermore we define $\partial_i x_i^0 = x_i^{-1} = 0 = x_i^{-2} = \partial_i \partial_i x_i^0$ for the sake of simpler notation. Hence we get

$$\begin{aligned}
\mathsf{d}_{x_1}\,{}^iH_n^k =&\partial_1\,{}^iH_n^k \\
=&\partial_1\left(x_1^k x_2^{n-k-i} x_3^i + x_3^2 P(x)\right) \\
=&k x_1^{k-1} x_2^{n-k-i} x_3^i + x_3^2 Q(x) \\
=&k\,{}^iH_{n-1}^{k-1}
\end{aligned}$$

$$\begin{aligned}
\mathsf{d}_{x_2}\,{}^iH_n^k =&\partial_2\,{}^iH_n^k \\
=&\partial_2\left(x_1^k x_2^{n-k-i} x_3^i + x_3^2 P(x)\right) \\
=&\left(n-k-i\right) x_1^k x_2^{n-k-i-1} x_3^i + x_3^2 Q(x) \\
=&\left(n-k-i\right)\,{}^iH_{n-1}^k
\end{aligned}$$

$$\begin{aligned}
\mathsf{d}_{x_3}\,{}^1H_n^k =&\partial_3\,{}^1H_n^k \\
=&\partial_3\left(x_1^k x_2^{n-k-1} x_3 + x_3^3 P(x)\right) \\
=&x_1^k x_2^{n-k-1} + x_3^2 Q(x) \\
=&{}^0H_{n-1}^k
\end{aligned}$$

The only difficult part is while regarding ${}^0H_n^k$. We have

$$\begin{aligned}
{}^0H_n^k =&x_1^k x_2^{n-k} - \frac{1}{2}\left(\partial_1^2 + \partial_2^2\right)\left(x_1^k x_2^{n-k}\right) x_3^2 + \left(P(x)\right) x_3^4 \\
=&x_1^k x_2^{n-k} + \left(P(x)\right) x_3^4 \\
&- \frac{1}{2}\left(k\left(k-1\right) x_1^{k-2} x_2^{n-k} + \left(n-k\right)\left(n-k-1\right) x_1^k x_2^{n-k-2}\right) x_3^2
\end{aligned}$$

Thus we have:

$$\begin{aligned}
\mathsf{d}_{x_3}\,{}^0H_n^k =&\partial_3\,{}^0H_n^k \\
=&Q(x)\, x_3^3 \\
&- \left(k\left(k-1\right) x_1^{k-2} x_2^{n-k} + \left(n-k\right)\left(n-k-1\right) x_1^k x_2^{n-k-2}\right) x_3 \\
=& -k\left(k-1\right)\,{}^1H_{n-1}^{k-2} - \left(n-k\right)\left(n-k-1\right)\,{}^1H_{n-1}^k
\end{aligned}$$

This proves our lemma. q.e.d.

Remark

The resulting systems of linear equations are underdetermined because we have

$$\begin{aligned}\mathsf{d}_{x_1}\,{}^iH_n^0 &= 0\\ \mathsf{d}_{x_2}\,{}^iH_n^{n-i} &= 0\end{aligned}$$

Of course this fact also holds for d_{x_3} and mixed derivatives of such kind. The most easy way to see that is using a standard basis transformation which maps our differential to d_{x_1}.

3.2.2.2 Kelvin Transformed Homogeneous Harmonic Polynomials

Lemma 3.6

$$\begin{aligned}\mathsf{d}_{x_1}\,{}^i\breve{H}_n^k =& k\,{}^i\breve{H}_{n+1}^{k-1} - (2n+1-k)\,{}^i\breve{H}_{n+1}^{k+1}\\ \mathsf{d}_{x_2}\,{}^i\breve{H}_n^k =& -(n+k+i+1)\,{}^i\breve{H}_{n+1}^{k} + (n-k-i)\,{}^i\breve{H}_{n+1}^{k+2}\\ \mathsf{d}_{x_3}\,{}^1\breve{H}_n^k =& {}^0\breve{H}_{n+1}^{k} + {}^0\breve{H}_{n+1}^{k+2}\\ \mathsf{d}_{x_3}\,{}^0\breve{H}_n^k =& -k\,(k-1)\,{}^1\breve{H}_{n+1}^{k-2} - (n-k)\,(n-k-1)\,{}^1\breve{H}_{n-1}^{k+2}\\ & -(k\,(k-1) + (n-k)\,(n-k-1) + (2n+1))\,{}^1\breve{H}_{n-1}^{k}\end{aligned}$$

Proof

As stated beforehand we have a formula which allows us to write the derivatives of the Kelvin transformed homogeneous polynomials in terms of the derivative of the original polynomial. Among others we will use this fact strongly.

Again we will denote polynomials we do not need with $P(x)$ and $Q(x)$ which are different in each equation.

First we will consider the case $k=0$ for the first equation. Then we get

$$\begin{aligned}\mathsf{d}_{x_1}\,{}^i\breve{H}_n^0 =& \partial_1\,{}^i\breve{H}_n^0\\ =& \frac{(x_1^2+x_2^2+x_3^2)\,\partial_1\,{}^iH_n^0 - (2n+1)\,x_1\,{}^iH_n^0}{|x|^{2n+3}}\\ =& \frac{-(2n+1)\,x_1\,{}^iH_n^0}{|x|^{2n+3}}\\ =& -(2n+1)\,\frac{\left(x_1x_2^{n-i}x_3^i + x_3^2P(x)\right)}{|x|^{2n+3}}\\ =& -(2n+1)\,\frac{{}^iH_{n+1}^1}{|x|^{2(n+1)+1}}\\ =& -(2n+1)\,{}^i\breve{H}_{n+1}^1\\ =& k\,{}^i\breve{H}_{n+1}^{k-1} - (2n+1-k)\,{}^i\breve{H}_{n+1}^{k+1}\end{aligned}$$

Now we will consider the first equation for $k > 0$. In particular we have $\partial_1 {}^i H_n^k \neq 0$

$$\begin{aligned}
\mathsf{d}_{x_1} {}^i\breve{H}_n^k =& \partial_1 {}^i\breve{H}_n^k \\
=& \frac{(x_1^2 + x_2^2 + x_3^2)\,\partial_1 {}^i H_n^k - (2n+1)\,x_1 {}^i H_n^k}{|x|^{2n+3}} \\
=& \frac{(x_1^2 + x_2^2 + x_3^2)\,k\,{}^i H_{n-1}^{k-1} - (2n+1)\,x_1 {}^i H_n^k}{|x|^{2n+3}} \\
=& \frac{k x_1^{k-1} x_2^{n-k+2-i} x_3^i - (2n+1-k)\,x_1^{k+1} x_2^{n-k-i} x_3^i + x_3^2 P(x)}{|x|^{2n+3}} \\
=& \frac{k\,{}^i H_{n+1}^{k-1} - (2n+1-k)\ {}^i H_{n+1}^{k+1}}{|x|^{2(n+1)+1}} \\
=& k\,{}^i\breve{H}_{n+1}^{k-1} - (2n+1-k)\ {}^i\breve{H}_{n+1}^{k+1}
\end{aligned}$$

Now we will prove the second equation. First consider the case $k = n - i$:

$$\begin{aligned}
\mathsf{d}_{x_2} {}^i\breve{H}_n^{n-i} =& \partial_2 {}^i\breve{H}_n^{n-i} \\
=& \frac{(x_1^2 + x_2^2 + x_3^2)\,\partial_2 {}^i H_n^{n-i} - (2n+1)\,x_2 {}^i H_n^{n-i}}{|x|^{2n+3}} \\
=& \frac{-(2n+1)\,x_2 {}^i H_n^{n-i}}{|x|^{2n+3}} \\
=& -(2n+1)\,\frac{x_1^{n-i} x_2^1 x_3^i + x_3^2 P(x)}{|x|^{2n+3}} \\
=& -(2n+1)\,\frac{{}^i H_{n+1}^{n-i}}{|x|^{2(n+1)+1}} \\
=& -(2n+1)\ {}^i\breve{H}_{n+1}^{n-i} \\
=& -(n+k+i+1)\ {}^i\breve{H}_{n+1}^{k} + (n-k-i)\ {}^i\breve{H}_{n+1}^{k+2}
\end{aligned}$$

Now we will assume $k < n - i$. Hence we get:

$$\begin{aligned}
\mathsf{d}_{x_2} {}^i\breve{H}_n^k =& \partial_2 {}^i\breve{H}_n^k \\
=& \frac{(x_1^2 + x_2^2 + x_3^2)\,\partial_2 {}^i H_n^k - (2n+1)\,x_2 {}^i H_n^k}{|x|^{2n+3}} \\
=& \frac{(x_1^2 + x_2^2 + x_3^2)\,(n-k-i)\ {}^i H_{n-1}^k - (2n+1)\,x_2 {}^i H_n^k}{|x|^{2n+3}} \\
=& \frac{(n-k-i)\,x_1^{k+2} x_2^{n-i-1-k} x_3^i}{|x|^{2n+3}} \\
&- \frac{(n+1+k+i)\,x_1^k x_2^{n+1-k-i} x_3^i + x_3^2 P(x)}{|x|^{2n+3}} \\
=& \frac{(n-k-i)\ {}^i H_{n+1}^{k+2} - (n+k+i+1)\ {}^i H_{n+1}^k}{|x|^{2(n+1)+1}} \\
=& -(n+k+i+1)\ {}^i\breve{H}_{n+1}^k + (n-k-i)\ {}^i\breve{H}_{n+1}^{k+2}
\end{aligned}$$

The next equation will be considered the same way.

$$
\begin{aligned}
\mathsf{d}_{x_3}\,{}^1\breve{H}_n^k =& \partial_3\,{}^1\breve{H}_n^k \\
=& \frac{(x_1^2+x_2^2+x_3^2)\,\partial_3\,{}^1H_n^k-(2n+1)\,x_3\,{}^1H_n^k}{|x|^{2n+3}} \\
=& \frac{(x_1^2+x_2^2+x_3^2)\,{}^0H_{n-1}^k-(2n+1)\,x_3\,{}^1H_n^k}{|x|^{2n+3}} \\
=& \frac{(x_1^2+x_2^2+x_3^2)\,x_1^k x_2^{n-k-1}-(2n+1)\,x_1^k x_2^{n-k-1}x_3^2+x_3^2P(x)}{|x|^{2n+3}} \\
=& \frac{x_1^{k+2}x_2^{n-k-1}+x_1^k x_2^{n-k+1}+x_3^2Q(x)}{|x|^{2n+3}} \\
=& \frac{{}^0H_{n+1}^{k+2}+{}^0H_{n+1}^k}{|x|^{2(n+1)+1}} \\
=& {}^0\breve{H}_{n+1}^k+{}^0\breve{H}_{n+1}^{k+2}
\end{aligned}
$$

The last equation is also the most complicated one. The special cases $k<2$ and $k>n-2$ should be treated separately. However, as it works the same way we will skip this step end immediately introduce the main case.

$$
\begin{aligned}
\mathsf{d}_{x_3}\,{}^0\breve{H}_n^k =& \partial_3\,{}^0\breve{H}_n^k \\
=& \frac{(x_1^2+x_2^2+x_3^2)\,\partial_3\,{}^0H_n^k-(2n+1)\,x_3\,{}^0H_n^k}{|x|^{2n+3}} \\
=& \frac{(x_1^2+x_2^2+x_3^2)\left(-k\,(k-1)\;{}^1H_{n-1}^{k-2}\right)}{|x|^{2n+3}} \\
& -\frac{(x_1^2+x_2^2+x_3^2)\left((n-k)\,(n-k-1)\;{}^1H_{n-1}^{k}\right)}{|x|^{2n+3}} \\
& \quad -\frac{(2n+1)\,x_3\,{}^0H_n^k}{|x|^{2n+3}} \\
=& \frac{-k\,(k-1)\,x_1^{k-2}x_2^{n-k+2}x_3}{|x|^{2n+3}} \\
& -\frac{(2n+1+k\,(k-1)+(n-k)\,(n-k-1))\,x_1^k x_2^{n-k}x_3}{|x|^{2n+3}} \\
& \quad +\frac{-(n-k)\,(n-k-1)\,x_1^{k+2}x_2^{n-k-2}x_3+x_3^2Q(x)}{|x|^{2n+3}} \\
=& \frac{-k\,(k-1)\;{}^1H_{n+1}^{k-2}}{|x|^{2(n+1)+1}} \\
& +\frac{-(2n+1+k\,(k-1)+(n-k)\,(n-k-1))\;{}^1H_{n+1}^{k}}{|x|^{2(n+1)+1}} \\
& \quad +\frac{-(n-k)\,(n-k-1)\;{}^1H_{n+1}^{k+2}}{|x|^{2(n+1)+1}}
\end{aligned}
$$

$$
\begin{aligned}
&= -k\,(k-1)\ {}^1\breve{H}_{n+1}^{k-2} - (n-k)\,(n-k-1)\ {}^1\breve{H}_{n-1}^{k+2} \\
&\quad - (k\,(k-1) + (n-k)\,(n-k-1) + (2n+1))\ {}^1\breve{H}_{n-1}^{k}
\end{aligned}
$$

This shows our proposition. q.e.d.

Remark

In contrast to the non-Kelvin transformed case we now map from a smaller to a bigger vector space. Obviously the kernel of this map is $\{0\}$ because otherwise we would have a harmonic in $Pot(\overline{\Sigma_{ext}})$ which is non-zero at infinity which would be a contradiction.

3.2.3 Differential Operator $\mathsf{d}_{\neg x_i}$

3.2.3.1 Ordinary Spherical Harmonics

Lemma 3.7

$$
\begin{aligned}
\mathsf{d}_{\neg x_1}\,{}^0H_n^k &= k\,(k-1)\ {}^1H_n^{k-2} + (n-k)^2\ {}^1H_n^k \\
\mathsf{d}_{\neg x_1}\,{}^1H_n^k &= -\ {}^0H_n^k \\
\mathsf{d}_{\neg x_2}\,{}^0H_n^k &= k^2\,{}^1H_n^{k-1} + (n-k)\,(n-k-1)\ {}^1H_n^{k+1} \\
\mathsf{d}_{\neg x_2}\,{}^1H_n^k &= -\ {}^0H_n^{k+1} \\
\mathsf{d}_{\neg x_3}\,{}^iH_n^k &= k\,{}^iH_n^{k-1} - (n-k-i)\ {}^iH_n^{k+1}
\end{aligned}
$$

Proof

For this task we may use the relations we got while differentiating with ∂_i. Hence we get:

$$
\begin{aligned}
\mathsf{d}_{\neg x_1}\,{}^0H_n^k &= (x_3\partial_2 - x_2\partial_3)\ {}^0H_n^k \\
&= (n-k)\,x_3\,{}^0H_{n-1}^k + k\,(k-1)\,x_2\,{}^1H_{n-1}^{k-2} \\
&\qquad + (n-k)\,(n-k-1)\,x_2\,{}^1H_{n-1}^k \\
&= (n-k)\ {}^1H_n^k + k\,(k-1)\ {}^1H_n^{k-2} \\
&\qquad + (n-k)\,(n-k-1)\ {}^1H_n^k \\
&= k\,(k-1)\ {}^1H_n^{k-2} + (n-k)^2\ {}^1H_n^k
\end{aligned}
$$

$$
\begin{aligned}
\mathsf{d}_{\neg x_1}\,{}^1H_n^k &= (x_3\partial_2 - x_2\partial_3)\ {}^1H_n^k \\
&= (n-k-1)\,x_3\,{}^1H_{n-1}^k - x_2\,{}^0H_{n-1}^k \\
&= 0 - {}^0H_n^k \\
&= -\ {}^0H_n^k
\end{aligned}
$$

$$\begin{aligned}
\mathsf{d}_{\neg x_2}\, {}^0H_n^k =& (x_3\partial_1 - x_1\partial_3)\ {}^0H_n^k \\
=& k\ x_3\, {}^0H_{n-1}^{k-1} + k\,(k-1)\, x_1\, {}^1H_{n-1}^{k-2} \\
& \quad + (n-k)\,(n-k-1)\, x_1\, {}^1H_{n-1}^{k} \\
=& k\, {}^1H_n^{k-1} + k\,(k-1)\ {}^1H_n^{k-1} \\
& \quad + (n-k)\,(n-k-1)\ {}^1H_n^{k+1} \\
=& k^2\, {}^1H_n^{k-1} + (n-k)\,(n-k-1)\ {}^1H_n^{k+1}
\end{aligned}$$

$$\begin{aligned}
\mathsf{d}_{\neg x_2}\, {}^1H_n^k =& (x_3\partial_1 - x_1\partial_3)\ {}^1H_n^k \\
=& k\ x_3\, {}^1H_{n-1}^{k-1} - x_1\, {}^0H_{n-1}^{k} \\
=& 0 -\ {}^0H_n^{k+1} \\
=& -\ {}^0H_n^{k+1}
\end{aligned}$$

$$\begin{aligned}
\mathsf{d}_{\neg x_3}\, {}^iH_n^k =& (x_2\partial_1 - x_1\partial_2)\ {}^iH_n^k \\
=& k\ x_2\, {}^iH_{n-1}^{k-1} - (n-k-i)\, x_1\, {}^iH_{n-1}^{k} \\
=& k\, {}^iH_n^{k-1} - (n-k-i)\ {}^iH_n^{k+1}
\end{aligned}$$

This proves our claim. q.e.d.

Remark

Again, the kernel of this map is obviously non-zero. We can see this particularly easy for the operators $\mathsf{d}_{\neg x_1}$ and $\mathsf{d}_{\neg x_2}$ because we cannot reach ${}^0H_n^n$ and ${}^0H_n^0$ respectively.

Again, a coordinate transformation transfers this result to $\mathsf{d}_{\neg x_3}$.

3.2.3.2 Kelvin Transformed Spherical Harmonics

Lemma 3.8

$$\begin{aligned}
\mathsf{d}_{\neg x_1}\, {}^0\breve{H}_n^k =& (n-k)^2\ {}^1\breve{H}_n^k + k\,(k-1)\ {}^1\breve{H}_n^{k-2} \\
\mathsf{d}_{\neg x_1}\, {}^1\breve{H}_n^k =& -\ {}^0\breve{H}_n^k \\
\mathsf{d}_{\neg x_2}\, {}^0\breve{H}_n^k =& k^2\, {}^1\breve{H}_n^{k-1} + (n-k)\,(n-k-1)\ {}^1\breve{H}_n^{k+1} \\
\mathsf{d}_{\neg x_2}\, {}^1\breve{H}_n^k =& -\ {}^0\breve{H}_n^{k+1} \\
\mathsf{d}_{\neg x_3}\, {}^i\breve{H}_n^k =& k\, {}^i\breve{H}_n^{k-1} - (n-k-i)\ {}^i\breve{H}_n^{k+1}
\end{aligned}$$

Proof

We have

$$x_j\partial_i\breve{H}_n(x) = \frac{(x_1^2+x_2^2+x_3^2)\,x_j\partial_i H_n - (2n+1)\,x_ix_jH_n}{|x|^{2n+3}}$$
$$= \frac{x_j\partial_i H_n(x)}{|x|^{2n+1}} - \frac{(2n+1)\,x_ix_jH_n(x)}{|x|^{2n+3}}$$

And thus

$$(x_j\partial_i - x_i\partial_j)\,\breve{H}_n(x) = \frac{(x_j\partial_i - x_i\partial_j)\,H_n(x)}{|x|^{2n+1}}$$

So, using the last lemma yields the above result. q.e.d.

Remark

In particular this means that we are having structurally seen the same kernel in the normal and in the Kelvin transformed case. The kernel of these operators are exactly the rotationally invariant harmonic functions.

3.2.4 Differential Operator d_r

3.2.4.1 Ordinary Spherical Harmonics

Lemma 3.9

$$\mathsf{d}_r\,{}^iH_n^k = n\,{}^iH_n^k$$

Proof

Again we may use the result of the previous subsections. For $n = 0$ we trivially get the above result. Hence we may assume that $n > 0$.

$$\begin{aligned}
\mathsf{d}_r\,{}^0H_n^k =& (x_1\partial_1 + x_2\partial_2 + x_3\partial_3)\,{}^0H_n^k\\
=& k\,x_1\,{}^0H_{n-1}^{k-1} + (n-k)\,x_2\,{}^0H_{n-1}^k\\
&\quad - x_3\left(k\,(k-1)\,{}^1H_{n-1}^{k-2} + (n-k)\,(n-k-1)\,{}^1H_{n-1}^k\right)\\
=& k\,{}^0H_n^k + (n-k)\,{}^0H_n^k + 0\\
=& n\,{}^0H_n^k
\end{aligned}$$

and

$$\begin{aligned}
\mathsf{d}_r\,{}^1H_n^k =& (x_1\partial_1 + x_2\partial_2 + x_3\partial_3)\,{}^1H_n^k\\
=& kx_1\,{}^1H_{n-1}^{k-1} + (n-k-1)\,x_2\,{}^1H_{n-1}^k + x_3\,{}^0H_{n-1}^k\\
=& k\,{}^1H_n^k + (n-k-1)\,{}^1H_n^k + {}^1H_n^k\\
=& n\,{}^1H_n^k
\end{aligned}$$

which proves the above proposition. q.e.d.

Remark

In this special case integration is just multiplication by n^{-1} and hence a fast and numerically stable task.

3.2.4.2 Kelvin Transformed Spherical Harmonics

We have the following lemma:

Lemma 3.10

$$\mathsf{d}_r\, {}^i\breve{H}_n^k = -\left(n+1\right) {}^i\breve{H}_n^k$$

Proof

Using the lemmas beforehand we get:

$$\begin{aligned}
\mathsf{d}_r\, {}^i\breve{H}_n^k &= \left(x_1\partial_1 + x_2\partial_2 + x_3\partial_3\right) {}^i\breve{H}_n^k \\
&= \sum_i \frac{x_i\partial_i\, {}^iH_n^k}{|x|^{2n+1}} - \left(2n+1\right)\sum_i \frac{x_i^2\, {}^iH_n^k}{|x|^{2n+3}} \\
&= n\frac{{}^iH_n^k}{|x|^{2n+1}} - \left(2n+1\right)\frac{{}^iH_n^k}{|x|^{2n+1}} \\
&= -\left(n+1\right)\frac{{}^iH_n^k}{|x|^{2n+1}} \\
&= -\left(n+1\right) {}^i\breve{H}_n^k
\end{aligned}$$

which yields the above result. q.e.d.

Remark

Again integration is just an easy to perform division. But this time all occurring kernels are 0 and hence we do not encounter any problems.

Note that this is the well known solution we already had for our radial derivative case.

3.3 Kernel Spaces and other Remarks

Concluding we observe the following three stunning facts (some of them are old, but the collection is still worthwhile to consider): Our operators (if considered purely)

- map harmonics to harmonics
- map $Pot(\overline{\Sigma_{int}})$ to $Pot(\overline{\Sigma_{int}})$ and $Pot(\overline{\Sigma_{ext}})$ to $Pot(\overline{\Sigma_{ext}})$.
- obey the degree of the harmonics, i.e., harmonics of the equal degree map to equal degree.

This enables us to consider differentiation and integration as a *finite* dimensional matrix operation.

However there is a drawback. If we want to stay finite dimensional we cannot combine the d_{x_i} derivatives with the other derivative operators because harmonics are not degree invariant under this operation.

This makes it particularly difficult to consider the occurring kernel spaces explicitly. However, we can observe that our linear combination of all the above vector fields incorporates not just the rotational vector fields we are dealing with a finite dimensional (in most cases one or zero dimensional) overall kernel. (E.g., $2{*}\mathsf{d}_{id}{+}\mathsf{d}_r$ has a one dimensional kernel!)

Just if we are dealing with purely rotational invariant vector fields we observe that we have a one dimensional kernel in every degree and hence an infinite dimensional kernel.

These remarks also hold for the next section because spherical harmonics are nothing but an orthonormal system of the harmonic polynomials.

3.4 Spherical Harmonics

The basis system for the harmonics $Pot(\overline{\Sigma_{ext}})$ we used beforehand is not the standardly used one. Therefore we will introduce the system of spherical harmonics [Hob55]:

Definition 3.5 (Spherical Harmonics)

Define the spherical harmonics Y_n^l in polar coordinates by:

$$\begin{aligned} Y_n^l &= C_n^l P_n^{|l|}(\sin\varphi) \begin{cases} \cos l\lambda & l \geq 0 \\ \sin |l|\lambda & l < 0 \end{cases} \\ &= \varepsilon_l \sqrt{2n+1} \sqrt{\frac{(n-|l|)!}{(n+|l|)!}} P_n^{|l|}(\sin\varphi) \begin{cases} \cos l\lambda & l \geq 0 \\ \sin |l|\lambda & l < 0 \end{cases} \end{aligned}$$

where

$$\varepsilon_l = \begin{cases} 1 & l = 0 \\ \sqrt{2} & \textit{otherwise} \end{cases}$$

and P_n^m is the associated Legendre function fulfilling

$$P_n^m(x) = \frac{(-1)^m}{2^n n!}(1-x^2)^{m/2}\frac{\partial^{n+m}}{\partial x^{n+m}}(x^2-1)^n$$

This particular system fulfills the following properties.

Lemma 3.11

The spherical harmonics Y_n^l constitute a complete orthonormal system under the standard L^2 inner product on the unit sphere.

Furthermore, when continued over the rim of the sphere by multiplication with new radius r^n (for harmonics in $Pot(\overline{\Sigma_{int}})$) and r^{-n-1} (for harmonics in $Pot(\overline{\Sigma_{ext}})$) respectively, these function constitute a basis of $Pot(\overline{\Sigma_{int}})$ and $Pot(\overline{\Sigma_{ext}})$ harmonics, respectively.

We will introduce the necessary conversion formulae between the two systems in use. Afterwards we will use these formulae to determine a direct way to integrate and differentiate the spherical harmonics.

3.4.1 Basis Change Matrices

The old basis of homogeneous harmonic polynomials was written in Cartesian coordinates which made differentiations more easy. Hence we need the transformation into polar coordinates (y_1, y_2, y_3) by now.

$$
\begin{aligned}
y_1 &= r \cos\varphi \cos\lambda \\
y_2 &= r \cos\varphi \sin\lambda \\
y_3 &= r \sin\varphi
\end{aligned}
$$

Note that we have not told right now which of the x_i of our original Cartesian coordinate system is assigned to which element of the triple (y_1, y_2, y_3).

For the following computations we will use the following formulae [AS68, BS79] ($l \geq 0$, $l > 0$ respectively).

$$
\begin{aligned}
\cos l\lambda &= \sum_{m=0}^{\left[\frac{l}{2}\right]} (-1)^m \binom{l}{2m} \sin^{2m}\lambda \cos^{l-2m}\lambda \\
\sin l\lambda &= \sum_{m=0}^{\left[\frac{l-1}{2}\right]} (-1)^m \binom{l}{2m+1} \sin^{2m+1}\lambda \cos^{l-2m-1}\lambda
\end{aligned}
$$

and

$$
\begin{aligned}
P_n(t) =& 2^{-n} \sum_{m=0}^{\left[\frac{n}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} t^{n-2m} \\
P_n^{|l|}(t) =& \left(1-t^2\right)^{l/2} \frac{\partial^l}{\partial t^l} P_n(t) \\
=& 2^{-n} \left(1-t^2\right)^{l/2} \sum_{m=0}^{\left[\frac{n-l}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \frac{(n-2m)!}{(n-2m-l)!} t^{n-2m-l} \\
=& \frac{l!}{2^n} \left(1-t^2\right)^{l/2} \sum_{m=0}^{\left[\frac{n-l}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{l} t^{n-2m-l}
\end{aligned}
$$

For the next computations we will strongly rely on the fact that we know that the Y_n^l are homogeneous harmonic polynomials of degree n. In order to get this degree we will use the property

$$1 = \cos^2 + \sin^2$$

which will enable us to additionally get higher dimensions.

For reasons of simplicity we will just drop the constant $C_n^l \frac{l!}{2^n}$ right now. (I.e: $\widetilde{Y}_n^l C_n^l \frac{|l|!}{2^n} = Y_n^l$). Thus we get:

$$\begin{aligned}
\widetilde{Y}_n^l =& \frac{1}{|l|!} P_n^{|l|}(\sin\varphi) \begin{cases} \cos l\lambda & l \geq 0 \\ \sin |l|\lambda & l < 0 \end{cases} \\
=& \cos^{|l|}\varphi \sum_{m=0}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} \sin^{n-2m-|l|}\varphi \\
& \begin{cases} \sum_{m=0}^{\left[\frac{l}{2}\right]} (-1)^m \binom{l}{2m} \sin^{2m}\lambda \cos^{l-2m}\lambda & l \geq 0 \\ \sum_{m=0}^{\left[\frac{|l|-1}{2}\right]} (-1)^m \binom{l}{2m+1} \sin^{2m+1}\lambda \cos^{l-2m-1}\lambda & l < 0 \end{cases} \\
=& \begin{cases} \sum_{m=0}^{\left[\frac{l}{2}\right]} (-1)^m \binom{l}{2m} y_2^{2m} y_1^{l-2m} & l \geq 0 \\ \sum_{m=0}^{\left[\frac{|l|-1}{2}\right]} (-1)^m \binom{|l|}{2m+1} y_2^{2m+1} y_1^{|l|-2m-1} & l < 0 \end{cases} \\
& \sum_{m=0}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} \\
& \qquad \sin^{n-2m-|l|}\varphi \left(\sin^2\varphi \cos^2\varphi\right)^m \\
=& \begin{cases} \sum_{m=0}^{\left[\frac{l}{2}\right]} (-1)^m \binom{l}{2m} y_2^{2m} y_1^{l-2m} & l \geq 0 \\ \sum_{m=0}^{\left[\frac{|l|-1}{2}\right]} (-1)^m \binom{|l|}{2m+1} y_2^{2m+1} y_1^{|l|-2m-1} & l < 0 \end{cases} \\
& \sum_{m=0}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} y_3^{n-2m-|l|} \\
& \qquad \left(y_1^2 + y_2^2 + y_3^2\right)^m
\end{aligned}$$

We just want to remind the reader that for the definition of the homogeneous harmonic polynomial basis the terms which had a term of x_3 in a power higher than 1 were not relevant. In order to minimize the complexity of the matrices we now choose

$$\begin{aligned}
y_1 &:= x_1 \\
y_2 &:= x_3 \\
y_3 &:= x_2
\end{aligned}$$

Hence we just need the polynomials which contain at most one y_2 in the previous formula. Writing $\widetilde{\widetilde{Y}}_n^l + y_2^2 P(y_1, y_2, y_3) = \widetilde{Y}_n^l$, where $\widetilde{\widetilde{Y}}_n^l$ does not contain any higher power of y_2

and doing the above substitution we get:

$$\begin{aligned}
\widetilde{\widetilde{Y}}{}^l_n =& \begin{cases} x_1^l & l \geq 0 \\ |l| x_1^{|l|-1} x_3 & l < 0 \end{cases} \\
& \sum_{m=0}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} x_2^{n-2m-|l|} \left(x_1^2 + x_2^2\right)^m \\
=& x_1^{|l|-1} \begin{cases} x_1 & l \geq 0 \\ |l| x_3 & l < 0 \end{cases} \\
& \sum_{m=0}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} \sum_{k=0}^{m} \binom{m}{k} x_2^{n-|l|-2k} x_1^{2k} \\
=& x_1^{|l|-1} \begin{cases} x_1 & l \geq 0 \\ |l| x_3 & l < 0 \end{cases} \\
& \sum_{m=0}^{\left[\frac{n-|l|}{2}\right]} \sum_{k=0}^{m} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} \binom{m}{k} x_2^{n-|l|-2k} x_1^{2k} \\
=& x_1^{|l|-1} \begin{cases} x_1 & l \geq 0 \\ |l| x_3 & l < 0 \end{cases} \\
& \sum_{k=0}^{\left[\frac{n-|l|}{2}\right]} x_1^{2k} x_2^{n-|l|-2k} \sum_{m=k}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} \binom{m}{k}
\end{aligned}$$

Hence we have

$$\begin{aligned}
\widetilde{Y}{}^l_n = & \sum_{k=0}^{\left[\frac{n-|l|}{2}\right]} \begin{cases} {}^0H_n^{|l|+2k} & l \geq 0 \\ |l| \, {}^1H_n^{|l|+2k-1} & l < 0 \end{cases} \\
& \sum_{m=k}^{\left[\frac{n-|l|}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{|l|} \binom{m}{k}
\end{aligned}$$

Thus we get for $l \geq 0$

$$\begin{aligned}
Y_n^l =& \varepsilon_l \sqrt{2n+1} \sqrt{\frac{(n-l)!}{(n+l)!}} \frac{l!}{2^n} \\
& \sum_{k=0}^{\left[\frac{n-l}{2}\right]} {}^0H_n^{l+2k} \sum_{m=k}^{\left[\frac{n-l}{2}\right]} (-1)^m \binom{n}{m} \binom{2n-2m}{n} \binom{n-2m}{l} \binom{m}{k} \\
=& \varepsilon_l \sqrt{2n+1} \sqrt{\frac{(n-l)!}{(n+l)!}} 2^{-n} \\
& \sum_{k=0}^{\left[\frac{n-l}{2}\right]} {}^0H_n^{l+2k} \sum_{m=k}^{\left[\frac{n-l}{2}\right]} (-1)^m \frac{(2n-2m)!}{(n-m)!\,(n-2m-l)!k!\,(m-k)!}
\end{aligned}$$

and for $l > 0$

$$
\begin{aligned}
Y_n^{-l} =& \sqrt{2}\sqrt{2n+1}\sqrt{\frac{(n-l)!}{(n+l)!}}\frac{l!}{2^n}l \\
& \sum_{k=0}^{\left[\frac{n-l}{2}\right]} {}^1H_n^{l-1+2k} \sum_{m=k}^{\left[\frac{n-l}{2}\right]} (-1)^m \binom{n}{m}\binom{2n-2m}{n}\binom{n-2m}{l}\binom{m}{k} \\
=& \sqrt{2}\sqrt{2n+1}\sqrt{\frac{(n-l)!}{(n+l)!}}2^{-n}l \\
& \sum_{k=0}^{\left[\frac{n-l}{2}\right]} {}^1H_n^{l-1+2k} \sum_{m=k}^{\left[\frac{n-l}{2}\right]} (-1)^m \frac{(2n-2m)!}{(n-m)!\,(n-2m-l)!k!\,(m-k)!}
\end{aligned}
$$

Taking a closer look on the structure of the corresponding basis change matrices we observe that they correspond to triangular matrices when we reorder the Y_n^l according to positive and negative and odd and even l. Correspondingly we need to reorder the ${}^iH_n^k$ according to the value of i and positive and negative k.

3.4.2 Direct Integration

Using the conversion formulae above and the results we obtained for the differentiation of the homogeneous harmonic polynomials we can determine the differentiation formulae for the spherical harmonics in $Pot(\overline{\Sigma_{ext}})$. The following differentials are an analogue to the old ones just with the new coordinate system (y_1, y_2, y_3), where again ∂_i differentiates in the y_i direction.

Conjecture

In order to make the formulae simpler we will denote (for $|l| > 1$):

$$
l_+ = \begin{cases} l+1 & \textit{if} \quad l > 1 \\ l-1 & \textit{if} \quad l < -1 \end{cases} \qquad\qquad l_- = \begin{cases} l-1 & \textit{if} \quad l > 1 \\ l+1 & \textit{if} \quad l < -1 \end{cases}
$$

i.e., the "+" shifts the l one away from 0, the "−" does the inverse operation. Furthermore denote the sign of $-l$ by l_s

Due to easier notation all spherical harmonics with impossible coefficients are assumed to be zero.

Sometimes the cases for $|l| \leq 1$ are displayed separately. The following formulae for general l is then just holding for $|l| \geq 2$, of course.

Differential Operator $\mathsf{d}_{id} = 1$

$$
\mathsf{d}_{id} Y_n^l = 1 \cdot Y_n^l
$$

Differential Operator $\mathsf{d}_r = y_1\partial_1 + y_2\partial_2 + y_3\partial_3$

$$
\mathsf{d}_r Y_n^l = -(n+1) \cdot Y_n^l
$$

Differential Operator $\mathsf{d}_{y_1} = \partial_1$

$$\mathsf{d}_{y_1} Y_n^0 = -\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+1)(n+2)}{2}} \cdot Y_{n+1}^1$$

$$\mathsf{d}_{y_1} Y_n^{-1} = -\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^{-2}$$

$$\begin{aligned}\mathsf{d}_{y_1} Y_n^1 &= +\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{n(n+1)}{2}} \cdot Y_{n+1}^0 \\ &\quad -\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^2\end{aligned}$$

$$\begin{aligned}\mathsf{d}_{y_1} Y_n^l &= +\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n-|l|+1)(n-|l|+2)}{4}} \cdot Y_{n+1}^{l_-} \\ &\quad -\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+|l|+1)(n+|l|+2)}{4}} \cdot Y_{n+1}^{l_+}\end{aligned}$$

Differential Operator $\mathsf{d}_{y_2} = \partial_2$

$$\mathsf{d}_{y_2} Y_n^0 = -\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+1)(n+2)}{2}} \cdot Y_{n+1}^{-1}$$

$$\mathsf{d}_{y_2} Y_n^1 = -\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^{-2}$$

$$\begin{aligned}\mathsf{d}_{y_2} Y_n^{-1} &= +\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{n(n+1)}{2}} \cdot Y_{n+1}^0 \\ &\quad +\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^2\end{aligned}$$

$$\begin{aligned}\mathsf{d}_{y_2} Y_n^l &= l_s\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n-|l|+1)(n-|l|+2)}{4}} \cdot Y_{n+1}^{-l_-} \quad + \\ &\quad l_s\sqrt{\frac{2n+1}{2n+3}}\sqrt{\frac{(n+|l|+1)(n+|l|+2)}{4}} \cdot Y_{n+1}^{-l_+}\end{aligned}$$

Differential Operator $\mathsf{d}_{y_3} = \partial_3$

$$\mathsf{d}_{y_3} Y_n^l = -\sqrt{\frac{2n+1}{2n+3}}\sqrt{(n+1-l)(n+1+l)} \cdot Y_n^l$$

Differential Operator $\mathsf{d}_{\neg y_1} = y_3\partial_2 - y_2\partial_3$

$$\mathsf{d}_{\neg y_1} Y_n^0 = -\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^{-1}$$

$$\mathsf{d}_{\neg y_1} Y_n^1 = -\sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^{-2}$$

$$\begin{aligned}\mathsf{d}_{\neg y_1} Y_n^{-1} &= +\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^0 \\ &\quad +\sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^2\end{aligned}$$

$$\mathsf{d}_{\neg y_1} Y_n^l = l_s \sqrt{\frac{(n-|l|+1)(n+|l|)}{4}} \cdot Y_n^{-l_-} + l_s \sqrt{\frac{(n-|l|)(n+|l|+1)}{4}} \cdot Y_{n+1}^{-l_+}$$

Differential Operator $\mathsf{d}_{\neg y_2} = y_3 \partial_1 - y_1 \partial_3$

$$\mathsf{d}_{\neg y_2} Y_n^0 = -\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^1$$

$$\mathsf{d}_{\neg y_2} Y_n^{-1} = -\sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^{-2}$$

$$\mathsf{d}_{\neg y_2} Y_n^1 = +\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^0 - \sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^2$$

$$\mathsf{d}_{\neg y_2} Y_n^l = +\sqrt{\frac{(n-|l|+1)(n+|l|)}{4}} \cdot Y_n^{l_-} - \sqrt{\frac{(n-|l|)(n+|l|+1)}{4}} \cdot Y_{n+1}^{l_+}$$

Differential Operator $\mathsf{d}_{\neg y_3} = y_2 \partial_1 - y_1 \partial_2$

$$\mathsf{d}_{\neg y_3} Y_n^l = l \cdot Y_n^{-l}$$

The proof consists of simple, but very lengthy calculations using the differentiation formulae for the homogeneous harmonic polynomials and the conversion formulae of the spherical harmonics to homogeneous harmonic polynomials we have obtained beforehand. This proof would just fill dozens of pages with incomprehensible formulae but would not really add to a deeper understanding of the matter and would give the whole topic a weight in this thesis which it does not have considering its mathematical impact. That's why we omitted it.

Furthermore, at least for the $\mathsf{d}_{\neg y_i}$ we can find these differentials in books about quantum mechanics [Edm64, Mes61], where $\mathsf{d}_{\neg y_i}$ can be interpreted as an angular momentum. Additionally the result for d_r is well known and can be found e.g., in [FGS98].

3.5 Other Basis Systems

As we have seen the calculations are getting very lengthy even for the most easy case of spherical harmonics.

Therefore we will not determine the corresponding derivatives of other widely used approximation functions or their kernels respectively. On the contrary we will rely on the fact that for most kernels we actually know an expansion into spherical harmonics, where we could let our operator act on.

This approach to general basis systems is not really elegant. However it is applicable and hence we may leave the derivatives of these more general basis functions as subject for future research. We want to emphasize that this is *not* a restriction to the method of old basis systems like spherical harmonics but just the first building block which could be used as foundation for the usage within modern approximation schemes.

3.6 Conclusion

The important facts which we can extract out of this chapter are the following:

- We can invert each of the differential operators we found in the last chapter and have an explicit representation of the corresponding operators.
- We obtained some insight in the kernel spaces.
- We know which kind of data are easily combinable.

Chapter 4

Geoscientifical Problems

Which mathematical tasks do we have to perform for the oblique boundary value problem and especially for the oblique satellite problem?

After having described what kind of oblique derivative problems we are able to tackle we want to turn our attention to the problems occurring in the determination of the gravitational field of the Earth.

Therefore we will first show the data situation. Afterwards we will give a brief mathematical description of the oblique boundary value and oblique satellite problem. We will see that there is just one major difference between the two problems, the downward-continuation. We will attack this severely ill-posed problem in the chapter "Noise and Regularization".

4.1 Data Situation and Open Problems

Now we want to give a rough overview on the raw data which are available for the gravitational potential V. Please note that we are just having data at discrete points. We will assume further that these data are free of non-gravitational effects and the exterior space of the earth has no gravitational sources.

Observable	Location	Observation method
$V(x)$	$x \in$ ocean	Satellite Altimetry
$\lvert\nabla V(x)\rvert$	$x \in$ continent	Gravimetry
$\frac{\nabla V(x)}{\lvert\nabla V(x)\rvert}$	$x \in$ continent	Geometric-Astronomical Levelling
$(\nabla \otimes \nabla)V(x)$	$x \in$ continent	Terrestrial Gradiometry
$\nabla V(x)$	$x \in$ satellite track	Satellite-to-Satellite Tracking (SST)
$(\nabla \otimes \nabla)V(x)$	$x \in$ satellite track	Satellite Gravity Gradiometry (SGG)

At least for satellite data we cannot easily choose the points, where the measurements should be taken. In particular the satellites are descending slowly in the direction of the Earth such that we only get measurements in a spherical shell and not on a surface. Therefore we cannot expect several measurements at the same point for error reduction.

As we have seen above the data are coming from various different sources. Usually their error level can just be estimated. Even within one satellite mission we observe different error levels, e.g., for GOCE the six directions of the Hesse tensor $(\nabla \otimes \nabla)$ are determined with different accuracy.

4.2 Mathematical Description

Now we will shortly present our problem in mathematical terms. Again, we assume all other sources of gravity outside the Earth (including the atmosphere) to be negligible. The following considerations are mostly taken from [FGS98, Fre99].

4.2.1 The Gravitational Field

The gravitational potential V is an harmonic in the outer space (i.e., $V \in Pot(\overline{\Sigma_{ext}})$) as defined in [Fre99]. The space $Pot(\overline{\Sigma_{ext}})$ is a separable Hilbert space with the standard $L^2(\Sigma)$ inner product.

4.2.2 Spectral Representation

We would like to have V in spectral representation, i.e., we have a $L^2(\Sigma)$-complete basis system of $Pot(\overline{\Sigma_{ext}})$ and a Fourier expansion of V in this basis system. As we know from potential theory (see e.g., [ABR91, Kel67]) it is sufficient to have a representation with a complete basis system $\{U_n\}_{n\in\mathbb{N}}$ on the boundary Σ. The corresponding Fourier coefficients are denoted by $\{V^\wedge(n)\}_{n\in\mathbb{N}}$.

$$V|_\Sigma = \sum_{n\in\mathbb{N}} V^\wedge(n) U_n$$

This Fourier expansion is meant in the $L^2(\Sigma)$ sense, where the harmonic continuation of the U_n provides a locally compact approximation in Σ_{ext} (i.e., in any compact subset we have uniform convergence).

Equivalently we can define a spectral representation at satellite height with respect to the satellite orbit Σ_S and at plane height Σ_F for airborne campaigns.

From now on we will restrict our attention to the case, where the underlying surface Σ, Σ_F or Σ_S is a sphere. In principle all (orthonormal) basis systems would suit our purposes. However, we chose the basis of spherical harmonics which allows a particularly easy numerical treatment in the end.

4.2.3 From Data to a Solution

Now we want to analyze mathematically the steps we have to perform in order to solve our problem out of one input data set with respect to the oblique derivative $\mathcal{d}$, one time when we are facing an oblique satellite problem, another time when we have a boundary value problem.

4.2.3.1 Oblique Satellite Problem

Input Data Our data are now given in the form $\{\mathcal{d}(V)(p_k)\}$ with $\{p_k\} = \Sigma_D$ is the set of points, where a measurement has been done. $\mathcal{d}$ can be either a first or second order differential, depending on the underlying measurement method.

In the sequel we will address this kind of information by *discrete (input) data.*

Approximation If we assume that $\mathcal{d}$ has Δ as split operator we can approximate V on the data location Σ_D which we assume to be a subset of a sphere. Hence we get a solution for V for the space outside of Σ_D

We need to approximate the data with a suitable basis system and hence get a differentiated version of the gravitational field in spectral representation which will now be called *differentiated data.*

Integration Out of the differentiated data $\mathcal{d}V$ we need to reconstruct V, both on Σ_D. We will demand that this reconstruction is also given in spectral representation on Σ_D. Depending on the differential operator $\mathcal{d}$ the function V does neither need to exist or to be unique.

The corresponding solution will be called *integrated data.*

Downward-Continuation Using the assumption that the way between Σ_D and Σ is source free we can extend the solution down to the Earth. In the standard topology this is a severely (exponentially) ill-posed problem [FGS98] i.e., small perturbations in the discrete input data result in a large error of our solution.

We are not just interested in a pure regularization but in an optimal regularization, i.e., we want to get as close as possible to the real solution. Assuming that we do not have further information on the error in the data and on the behavior of the solution this is an unsolved problem, yet. Important is the appropriate choice of a regularization parameter/stopping criterion.

The data after downward continuation will be called *regularized data.*

4.2.3.2 Oblique Boundary Value Problem

The only difference to the oblique satellite problem is the downward continuation which is unnecessary because we are already at the desired height. This rather small difference results in the fact that the oblique boundary value problem is well-posed.

4.2.3.3 Combination

We do not just have data for one differential operator $\mathcal{d}$ but for several different ones. Furthermore we can have data from different satellite missions and ground based campaigns. These solutions have to be combined in order to get a final solution.

4.2.3.4 Remarks

Please note that sometimes several or even all of the above steps are combined to realize gains both in speed and accuracy. Furthermore the order of the steps is not necessarily fixed but it can be changed according to the utilized algorithm.

4.3 Conclusion

In order to be able to solve an oblique satellite problem we have at least to show a possible regularization technique which will be part of the next chapter. After having accomplished this task the oblique satellite problem and the oblique derivative problem are rather similar in their treatment.

Chapter 5

Noise and Regularization

Does there exist a sensible stopping criterion for the inverse problem "downward continuation"?

We need to know an approximate error level of our solution after regularization.

When we consider satellite problem we do not want to know the solution at satellite height but down at the Earth. This problem is known as downward-continuation problem which is severely ill-posed [Fre99].

Please note that if we are dealing with satellite data we are facing another severe problem. Our data and hence also our data error are given in the space domain. However, there is no regularization method which does not require the knowledge of these in the frequency domain. In order to have a manageable base we will assume that our data are given on a (spherical) integration grid near the satellite orbit which allows an easy way to change from space to frequency domain and vice versa.

We know that the transfer of the data from the satellite track to such an integration grid is non-trivial and structurally seen ill-posed. One of the most elaborated procedures we know to obtain a solution on this problem is the one presented by [Fen02] which utilizes localizing spline techniques.

5.1 Data Error for the Satellite Problem

For the regularization process a profound knowledge of the behavior of the error we face is indispensable. Therefore we will first investigate how the error transfers from the space to the frequency domain.

Satellites measuring the gravitational field have to fly in a very low orbit which results in a short mission time. Hence, we can just expect that we have *one* measurement at each point which means in particular that we cannot rely on a time series which is the standard tool in statistics.

On the other hand we are having quite a variety of data at different points. The behavior of the noise in this case was estimated relying on personal communications with Dr. J-P. Stockis [Sto03].

5.1.1 Integration Grid

For approximation purposes we need to know a good integration grid on the sphere. The problem of most integration grids is that one does not know the weight coefficients. Therefore we mostly rely on the Driscoll-Healy grid [May01]:

Definition 5.1

The Driscoll-Healy Grid of dimension m is defined by the point system $\left(s\frac{\pi}{2m+1}, r\frac{2\pi}{2m+1}\right)$ and the integration weights

$$W_{s,r} = \frac{2\pi}{2m+1}\frac{4}{2m+1}\sin\left(\frac{s\pi}{2m+1}\right)\sum_{l=0}^{m-1}\frac{1}{2l+1}\sin\left(\frac{(2l+1)s\pi}{2m+1}\right)$$

Lemma 5.1

The Driscoll-Healy grid of dimension m allows exact integration for all spherical harmonics up to degree m by the formula:

$$\int_\Omega F(\omega)\,d\omega = \sum_{s=0}^{2m}\sum_{r=0}^{2m} W_{s,r}F\left(s\frac{\pi}{2m+1}, r\frac{2\pi}{2m+1}\right)$$

5.1.2 Stochastical Preliminaries

We just want to present some basic definitions and facts and notation concerning stochastics. A much more thorough treatment may be found in [BD96], e.g..

$\xi \in (\Omega, \Sigma, \mathbb{P})$ is called random variable of the space Ω with the underlying sigma algebra Σ and the probability measure $\mathbb{P}$.

The expectation of a random variable ξ is denoted by $\mathbb{E}(\xi)$ and the variance of a random variable ξ is denoted by $\mathbb{E}\big((\xi - \mathbb{E}(\xi))^2\big)$

A random variable ξ is chosen according to the Gaussian distribution (normal distribution) $\mathcal{N}(0, \sigma^2)$ with expectation $\mathbb{E}(\xi) = 0$ and variance $\mathbb{E}(\xi^2) = \sigma^2$ if

$$\mathcal{N}\left(0, \sigma^2\right)(x) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{x^2}{2\sigma^2}\right)$$

Expectation and variance fulfill the following particular useful lemma [Bos96]:

Lemma 5.2

Let ζ and ξ be random variables with zero expectation which are independent (i.e., $\mathbb{E}(\zeta\xi) = 0$). Then the random variable $\zeta + r\xi$ has the expectation $\mathbb{E}(\zeta + r\xi) = \mathbb{E}(\zeta) + r\mathbb{E}(\xi)$ and the variance $\mathbb{E}\big((\zeta + r\xi)^2\big) = \mathbb{E}(\zeta^2) + r^2\mathbb{E}(\xi^2)$, where $r \in \mathbb{R}$.

5.1.3 Uncorrelated Noise Case

Now we can reformulate our satellite problem mathematically.

Problem 5.1

Let $\mathbb{G}_N$ be an integration grid (incorporating N points) on the sphere Ω which allows exact integration of the orthonormal system $\{Y_n^k\}_{n\leq m,|k|\leq n}$ up to order $2m$.

On each point $x \in \mathbb{G}_N$ of the integration grid a random variable $F(x)$ with distribution $\mathcal{N}(0, \delta^2)$ is given.

Consider the truncated Fourier transform of this given random function F:

$$F \approx \sum_{n=0}^{m} \sum_{k=-n}^{n} F^\wedge(n,k) Y_n^k$$

where

$$\int_\Omega F Y_n^k d\omega \approx F^\wedge(n,k) = \sum_{p\in\mathbb{G}_N} W(p) Y_n^k(p) F(p)$$

The $F^\wedge(n,k)$ are random variables.

How are they distributed?

In order to keep notation simple we will write:

Definition 5.2

The grid constant $\mathbb{G}_N^\wedge(n,k)$ is defined by

$$\mathbb{G}_N^\wedge(n,k) = \sum_{p\in\mathbb{G}_N} W(p)^2 Y_n^k(p)^2$$

Using this notation we obtain:

Lemma 5.3

The Fourier coefficients $F^\wedge(n,k)$ are random variables with distribution

$$\mathcal{N}\left(0, \delta^2 \mathbb{G}_N^\wedge(n,k)\right)$$

Proof

We know about the expectation

$$\begin{aligned}
\mathbb{E}(F^\wedge(n,k)) =& \mathbb{E}\left(\sum_{p\in\mathbb{G}_N} W(p) Y_n^k(p) F(p)\right) \\
=& \sum_{x\in\mathbb{G}_N} W(p) Y_n^k(p) \mathbb{E}(F(p)) \\
=& \sum_{x\in\mathbb{G}_N} W(p) Y_n^k(p) 0 \\
=& 0
\end{aligned}$$

Furthermore we have for the variance

$$\begin{aligned}\mathbb{E}(F^\wedge(n,k))^2 &= \sum_{p\in\mathbb{G}_N} W(p)^2 Y_n^k(p)^2 \mathbb{E}(F(p)^2) \\ &= \sum_{p\in\mathbb{G}_N} W(p)^2 Y_n^k(p)^2 \delta^2 \\ &= \delta^2 \sum_{p\in\mathbb{G}_N} W(p)^2 Y_n^k(p)^2 \\ &= \delta^2 \mathbb{G}_N^\wedge(n,k)\end{aligned}$$

This yields the desired result because the sum of normally distributed random variables is normally distributed. q.e.d.

We see that the chosen integration grid influences heavily the result we get. On the other hand we did not use the fact that we are working on the sphere. Hence our result should in special cases be the same as the ones normally known in probability theory. This gives rise to the following remark:

Remark

If $\mathbb{G}_N$ is (almost) equally distributed we have

$$W(p) \approx N^{-1} \qquad \forall p \in \mathbb{G}_N$$

Substituting this result in the formula we derived in the last lemma, we get using the fact $||Y_n^k|| = 1$

$$\mathbb{E}(F^\wedge(n,k))^2 \approx N^{-1}\delta^2$$

This result is known from the general theory [BD96].

5.1.4 Correlated Noise Case

After having covered the easy case of uncorrelated noise we will include correlations in our model. These correlations are likely to enter because of outer interferences which are similar at points near to each other or mathematically imposed by the transfer from the satellite track to the integration grid.

Mathematically seen this corresponds to the following problem.

Problem 5.2

Let $\mathbb{G}_N$ be an integration grid on the sphere Ω which allows exact integration of the orthonormal system $\{Y_n^k\}_{n\le m,|k|\le n}$ up to order $2m$.

On each point $p \in \mathbb{G}_N$ of the integration grid a random variable $G(p)$ is given which is of the following form:

$$G(p) = \sum_{q\in\mathbb{G}} W(q)K(p,q)F(q)$$

where the $F(p)$ are distributed with $\mathcal{N}(0, \delta^2)$. Consider the truncated Fourier transform of this given random function G:

$$G \approx \sum_{n=0}^{m} \sum_{k=-n}^{n} G^{\wedge}(n,k) Y_n^k$$

where

$$\int_{\Omega} G Y_n^k d\omega \approx G^{\wedge}(n,k) = \sum_{p \in \mathbb{G}_N} W(p) Y_n^k(p) G(p)$$

The $G^{\wedge}(n,k)$ are random variables.

How are they distributed?

As we see the problem strongly depends on the choice of $K(\cdot,\cdot)$. We do not know how our error looks like in reality. But in order to have the possibility to draw further conclusions we may assume $K(\cdot,\cdot)$ is symmetric and translation invariant.

A good and easy to handle choice seems to be the Abel-Poisson kernel [FGS98]

$$\begin{aligned} K_h(p,q) =& \frac{1}{4\pi} \frac{1-h^2}{(1+h^2-2hp\cdot q)^{3/2}} \\ =& \sum_{n=0}^{\infty} \frac{2n+1}{4\pi} h^n P_n(p\cdot q) \\ =& \sum_{n=0}^{\infty} \sum_{k=-n}^{n} h^n Y_n^k(p) Y_n^k(q) \end{aligned}$$

The particular advantage of the above kernel is that it is self reproducing [FGS98], i.e.,

$$\begin{aligned} < K_h(p,\cdot), Y_n^k(\cdot) >=& h^n Y_n^k(p) \\ & \Big(= \sum_{q \in \mathbb{G}_N} W(q) K_h(p,q) Y_n^k(q) \Big) \end{aligned}$$

We will do our next considerations just for this special kernel. However, we could do them with any one which has a self-reproducing structure as above, the Abel-Poisson kernel is just a (physically motivated) example.

Lemma 5.4

The Fourier coefficients $G^{\wedge}(n,k)$ are random variables and have the distribution

$$\mathcal{N}\left(0, \delta^2 h^{2n} \mathbb{G}_N^{\wedge}(n,k)\right)$$

if we choose the Abel-Poisson Kernel K_h as correlation.

Proof

First we will rewrite $G^\wedge(n,k)$ in terms of $F(x)$.

$$\begin{aligned} G^\wedge(n,k) &= \sum_{p\in\mathbb{G}_N} W(p)Y_n^k(p)G(p) \\ &= \sum_{p\in\mathbb{G}_N} W(p)Y_n^k(p) \sum_{q\in\mathbb{G}_N} W(q)K_h(p,q)F(q) \\ &= \sum_{p,q\in\mathbb{G}_N} W(p)W(q)K_h(p,q)Y_n^k(p)F(q) \\ &= \sum_{q\in\mathbb{G}_N} W(q)F(q) \sum_{p\in\mathbb{G}_N} W(p)K_h(p,q)Y_n^k(p) \\ &= \sum_{q\in\mathbb{G}_N} h^n W(q)F(q)Y_n^k(q) \\ &= h^n \sum_{x\in\mathbb{G}_N} W(p)F(p)Y_n^k(p) \end{aligned}$$

The proposition now directly follows from the uncorrelated case. q.e.d.

5.1.5 Combinations

Of course it is not reasonable to assume that we have pure correlated or pure uncorrelated noise in our data.

So we will consider a combination of the two noise types above. Assuming that the noise level for the uncorrelated case is $c_u\delta$ and for the uncorrelated one $c_c\delta$ we get noise with distribution

$$\mathcal{N}(0, \delta^2(c_u^2 + c_c^2 h^{2n})\mathbb{G}_N^\wedge(n,k))$$

for the coefficient of Y_n^k.

Note that for low coefficients we have a domination of the correlated noise and for high Fourier coefficients a domination of the uncorrelated noise.

5.1.6 Noise Estimation

In order to get an idea what kind of noise we are having on our satellite data we may employ the following strategy.

First we will simulate noisy satellite data on the real track. These can be fitted with the three parameter function $c_u^2 + c_c^2 h^{2n}$.

Lemma 5.5

Assume that the constants c_u, c_c and h are given. Assume furthermore that we have random variables $F^\wedge(n,k)$ for the Fourier coefficients of Y_n^k which are

$$\mathcal{N}(0, \delta^2(c_u^2 + c_c^2 h^{2n})\mathbb{G}_N^\wedge(n,k))$$

distributed up to degree m.

Then the best possible estimate for the noise level δ is given by

$$\frac{1}{n+1}\sqrt{\sum_{n=0}^{l}\sum_{k=-n}^{n}\frac{(F^\wedge(n,k))^2}{(c_u^2+c_c^2h^{2n})\mathbb{G}_N^\wedge(n,k)}}$$

The proof just consists out of standard methods from stochastics [BD96]. Note that this approach is rather rough and just constitutes one possibility. However, we may draw two important conclusions out of these calculations.

- It is reasonable to assume that our Fourier coefficients are biased with Gaussian white noise depending on the degree of the Fourier coefficients. Comparing two different coefficients this noise can be assumed as uncorrelated. Because any other basis like wavelets or splines has a representation in that particular standard basis this results again in uncorrelated white noise for the coefficients of the new basis.
- It is likely that the variance in the Fourier coefficients is bounded and asymptotically a constant.

Both of these observations indicate that the method of choice should not be a regularization method for deterministic but for stochastic noise.

5.2 Auto-Regularization

Now we will strongly rely on some results which we will present in a very condensed form in the next few pages (without proofs). Please note that a lot of the subsequent inverse problem results are based on the recent work of Prof. S. Pereverzev [Per03a, Per03b], whereas the theorems using stochastical methods were mostly obtained in cooperation with Dr. J-P. Stockis [Sto03]. Some information on stochastical noise and wavelets can be found in [FP01].

For the sake of readability we indexed the occurring probabilities and expectations with the random variable it originally refers to. Please observe that in this section we are requiring a large number of different constants which are not important in itself. Therefore, if not stated otherwise all of them just have a scope of the particular theorem or lemma, where they were introduced and no further.

5.2.1 Functional Analysis Preliminaries

In this part we want to introduce the necessary results to be capable to regularize our problem including some notation.

When we have a solution X_α^δ of the equation

$$\mathfrak{A}X = Z$$

with respect to the noisy data Z^δ our error has the two components regularization error $\psi(\alpha)$ which mainly depends on the smoothness of our function X and the data error which is $\frac{\delta}{2\sqrt{\alpha}}$ when we use Tikhonov-Phillips regularization, for example, i.e.

$$||X - X_\alpha^\delta|| \leq \psi(\alpha) + \frac{\delta}{2\sqrt{\alpha}}$$

Although the common theory is dealing with deterministic noise we observe in practice mainly stochastic noise. Therefore we will introduce the necessary notions to handle stochastic noise as well. The next few pages are purely working along the lines given by [Per03b]. Further background information can be obtained from [GP00, MP03]. In order to keep the introduction short we will just present the major results.

From now on let $\mathcal{X}$ and $\mathcal{Z}$ be separable Hilbert spaces with inner products $< \cdot, \cdot >_{\mathcal{X}}$ and $< \cdot, \cdot >_{\mathcal{Z}}$ with basis $\{U_k\}_{k\in\mathbb{N}}$ and $\{V_k\}_{k\in\mathbb{N}}$ respectively. If no confusion is likely to arise we will denote the inner product just by $< \cdot, \cdot >$. Additionally assume $X \in \mathcal{X}$ and $Z \in \mathcal{Z}$ if not stated otherwise.

Furthermore assume $\mathfrak{A}$ is a map $\mathfrak{A} : \mathcal{X} \to \mathcal{Z}$ which is a continuous linear compact operator with infinite rank. $\mathfrak{A}$ shall admit a singular value decomposition

$$\mathfrak{A}X = \sum_{k=1}^{\infty} s_k V_k \langle U_k, X \rangle$$

where $s_k \geq s_{k+1} > 0$ for all $k \in \mathbb{N}$. Hence the adjoint operator has the representation

$$\mathfrak{A}^* Z = \sum_{k=1}^{\infty} s_k U_k \langle V_k, Z \rangle$$

The inverse operator has the formal representation

$$\mathfrak{A}^{-1} Z = \sum_{k=1}^{\infty} s_k^{-1} U_k \langle V_k, Z \rangle$$

Definition 5.3

The Moore Penrose inverse is defined as: $\mathfrak{A}^+ = (\mathfrak{A}^*\mathfrak{A})^{-1} \mathfrak{A}^*$

Lemma 5.6 (Picard Criterion)

$\mathfrak{A}^*\mathfrak{A}X = \mathfrak{A}^*Z$ *is solvable in* $\mathcal{X}$ *iff* $\sum_{k=1}^{\infty} s_k^{-2} \langle V_k, Z \rangle^2 < \infty$

Now we will introduce an approach to regularization which is rather general. Therefore we need the following

Definition 5.4

Let $\mathfrak{A} : \mathcal{X} \to \mathcal{X}$ *be self-adjoint and* F *a real valued continuous function. Then* $F(\mathfrak{A})$ *is defined by*

$$F(\mathfrak{A}) = \sum_{k=1}^{\infty} F(s_k)\, U_k \langle U_k, \cdot \rangle$$

Remark

Inversion of an operator can be written in this notation as well. We simply have $\mathfrak{A}^{-1} = F(\mathfrak{A})$ using $F : \lambda \mapsto \lambda^{-1}$

Furthermore

Definition 5.5

The family of bounded real valued functions $\{G_\alpha\}_{\alpha\in\mathbb{R}^+}$ *is called regularization family for* $\mathfrak{A}$ *if for all* $\alpha > 0$

- $\exists c: \, |\lambda G_\alpha(\lambda)| \leq c$
- $\forall\lambda \in]0, ||\mathfrak{A}||^2] : \, \lim_{\alpha\to 0} G_\alpha(\lambda) = \lambda^{-1}$

This yields the following result:

Lemma 5.7

Let Z fulfill the Picard criterion. Then

$$\lim_{\alpha\to 0} \left|\left|\mathfrak{A}^{-1}Z - G_\alpha(\mathfrak{A}^*\mathfrak{A})\,\mathfrak{A}^*Z\right|\right| = 0$$

Remark

Examples for regularization families are

- Cut-Off scheme

$$G_\alpha(\lambda) = \begin{cases} \lambda^{-1} & \lambda \geq \alpha \\ 0 & 0 < \lambda < \alpha \end{cases}$$

- Tikhonov - Phillips

$$G_\alpha(\lambda) = (\alpha + \lambda)^{-1}$$

In order to compare the different methods we can introduce the following definitions:

Definition 5.6

Define the constants γ_0, $\gamma_{-\frac{1}{2}}$ *and* γ_{-1} *by*

- $\sup_{\lambda\in[0,||\mathfrak{A}||^2[} |1 - G_\alpha(\lambda)\lambda| \leq \gamma_0$
- $\sup_{\lambda\in[0,||\mathfrak{A}||^2[} \left|G_\alpha(\lambda)\lambda^{\frac{1}{2}}\right| \leq \frac{\gamma_{-\frac{1}{2}}}{\alpha^{\frac{1}{2}}}$
- $\sup_{\lambda\in[0,||\mathfrak{A}||^2[} |G_\alpha(\lambda)| \leq \frac{\gamma_{-1}}{\alpha}$

Definition 5.7 (Qualification)

The qualification *of a regularization family* $\{G_\alpha\}$ *is the maximal p such that there is a* γ_q*:*

$$\sup_{\lambda\in[0,||\mathfrak{A}||^2[} |1 - G_\alpha(\lambda)\lambda|\, \lambda^p \leq \gamma_q \alpha^p$$

Remark

Simplifying one may say that the bigger the qualification, the better the performance of the particular regularization scheme.

This is due to the fact that for all $p \geq q > 1$ even for the much stronger norm $||g||_{\lambda^q} = \sup_{\lambda \in [0, ||\mathfrak{A}||^2[} \lambda^q |g(\lambda)\,|$ the term $||\lambda^{-1} - G_\alpha(\lambda)\,||_{\lambda^q}$ converges. If the qualification is ∞ and if we are having uniform convergence it even follows pointwise convergence. This means in particular that the function λ^{-1} gets approximated in an optimal way.

If the qualification is not high enough we cannot guarantee to reach the best possible order of approximation. In particular we will have some results requiring a minimum qualification. For the two regularization methods proposed above the constants adopt the following values:

Remark

The qualification of the spectral cut-off scheme is ∞, whereas Tikhonov-Phillips just has qualification 1. However, the advantage of the Tikhonov-Phillips regularization is that we do not require the knowledge of the singular value decomposition. Both spectral cut-off scheme as well as Tikhonov-Phillips regularization fulfill the above definition with constants $\gamma_0 = \gamma_{-\frac{1}{2}} = \gamma_1 = 1$ and $\gamma_0 = \gamma_1 = 1$ and $\gamma_{-\frac{1}{2}} = \sqrt{2}$ respectively.

In the sequel we will consider two mutually different noise models:

Definition 5.8 (Deterministic Noise)

The data Z^δ are biased with deterministic noise (in comparison to Z) if $||Z - Z^\delta|| \leq \delta$, i.e., there exists a (random) vector ξ with $||\xi|| \leq 1$ such that $Z^\delta = Z + \delta\xi$.

Definition 5.9 (Stochastic Noise)

Let $(\Omega, \Sigma, \mathbb{P})$ be the ordinary probability space. Furthermore $Z^\delta = Z + \delta\xi$, where ξ is a random vector fulfilling

- *For all $Z \in \mathcal{Z}$ we have that $\xi_Z(\omega) = \langle Z, \xi \rangle$, where $\xi_Z(\omega) : \Omega \to \mathbb{R}$ is a random variable. Assume furthermore $\forall t : \{\omega \,|\, \omega \in \Omega, \xi_Z(\omega) \leq t\} \in \Sigma$*
- $\mathbb{E}_\xi \langle Z, \xi \rangle = 0$
- $\mathbb{E}_\xi \langle Z, \xi \rangle^2 = ||Z||_{\mathcal{Z}}$
- *ξ_Z is normally distributed around 0.*

Then Z^δ is called to be biased with stochastic noise.

Remark

For most results the condition ξ_Z Gaussian is not necessary. In order to be more accurate we could introduce different variances for each basis vector V_i. However, the general results presented in the sequel transfer without a problem to this more general situation.

After having introduced the error we need to consider the smoothness separately:

Definition 5.10

Let $\psi : [0, ||\mathfrak{A}||^2] \to \mathbb{R}^+$ be non-decreasing with $\psi(0) = 0$. $Z = \mathfrak{A}X$ has the smoothness ψ if

$$\sum_{k=1}^{\infty} \frac{\langle U_k, Z\rangle^2}{s_k^2 \psi^2(s_k^2)} < \infty$$

Furthermore the generalized smoothness assumption is defined as

$$\big(\mathfrak{A}^+ Z =\big)\, X^+ \in \mathfrak{A}_\psi(r) = \{z \in \mathcal{X} | z = \psi(\mathfrak{A}^*\mathfrak{A})\, \tilde{z}, \quad ||\tilde{z}|| \le r\}$$

Definition 5.11

Let ψ defined as above. Then define $\theta(\lambda) = \sqrt{\lambda}\psi(\lambda)$.

Definition 5.12

ψ is called to fulfill the Δ_2 condition if:

$$\exists \varpi > 1 \forall \lambda \in \left[0, ||\mathfrak{A}||^2\right] : \psi\,(2\lambda) \le \varpi \psi(\lambda)$$

This means that the smoothness should not decrease faster than an exponential function. Now we consider the accuracy of our methods:

Definition 5.13

The best order of accuracy with respect to $\mathfrak{A}$ and δ is defined by:

$$\sup_{X \in \mathfrak{A}_{\psi(R)}} \inf_{G_\alpha} \sup_{\substack{Z^\delta, Z \\ ||Z - Z^\delta|| \le \delta}} ||X - G_\alpha(\mathfrak{A}^*\mathfrak{A})\, \mathfrak{A}^* Z^\delta||$$

If we assume deterministic noise this order can be obtained by the cut-off scheme as well as by Tikhonov-Phillips regularization as long as the qualification covers the smoothness (i.e. $\frac{\lambda^p}{\psi(\lambda)} \to_{\lambda\to\infty} \infty$ for qualification p).

Lemma 5.8

Let ψ be s.t. θ is strictly increasing and $\psi\left(\left((\theta^2)^{-1}\right)(\lambda)\right)$ concave. Furthermore let ψ fulfill the Δ_2 condition.

Under the above conditions we have for the deterministic noise model the best possible order of accuracy is $\psi(\theta^{-1}(\delta))$ which can be reached by either the cut-off scheme or Tikhonov Phillips regularization if the qualification covers the smoothness.

Remark

For the standard smoothness $\psi(\lambda) = \lambda^\mu$ we have the well known best order of accuracy $\delta^{\frac{\mu}{\mu+\frac{1}{2}}}$.

If we work along a Hilbert scale [EHN96] (which we do not want to define in this text) with $d||u||_{\mathcal{X}_{\nu-a}} \leq ||\mathfrak{A}u||_{\mathcal{Z}_\nu} \leq D||u||_{\mathcal{X}_{\nu-a}}$ we have the best possible order of accuracy $\delta^{\frac{\mu}{\mu+a}}$.

Now we will consider the case of stochastic instead of deterministic noise where we use the obvious adaptation of the best order of accuracy, namely

$\sup_{X\in\mathfrak{A}_{\psi(R)}} \inf_{G_\alpha} \mathbb{E}_\xi ||X - G_\alpha(\mathfrak{A}^*\mathfrak{A})\, \mathfrak{A}^* \left(\mathfrak{A}X + \delta\xi\right)||^2$

Definition 5.14

Define $\theta_s(\lambda) = \lambda^{\frac{2s+1}{4s}}\psi(\lambda)$, where we have for the singular values s_k of $\mathfrak{A}$: $\exists c1, c2 :$ $c_1, c_2 : c_1 k^{-s} \leq s_k \leq c_2 k^{-s}$.

Lemma 5.9

Assume that θ_s is increasing and that ψ fulfills the Δ_2 condition. Furthermore there should exist a p s.t. $\frac{\lambda^p}{\psi(\lambda)}$ is increasing.

Then for the stochastic noise model the best order of accuracy is $\psi(\theta_s^{-1}(\delta))$ which can be reached by either the cut-off scheme or Tikhonov Phillips regularization if the qualification covers the smoothness.

Remark

For the standard smoothness $\psi(\lambda) = \lambda^\mu$ we have $\delta^{\frac{\mu}{\mu+\frac{1}{2}+\frac{1}{4s}}}$ as best order of accuracy which is slightly worse than for the deterministic noise case.

This difference vanishes for the exponentially ill-posed problem.

For all these regularization methods we need quite a lot of a priori knowledge in order to use them successfully. In particular there is the following remarkable result, which will be presented with proof (taken from [Per03b]):

Lemma 5.10 (Bakushinskii, 1984)

If the regularization operator $\mathfrak{R}$ does not depend explicitly on the noise level δ, then for any (infinite rank) compact operator $\mathfrak{A}$ there is an $Z \in \mathrm{Dom}(\mathfrak{A}^+)$ for which

$$\lim_{\delta\to 0} \sup_{\substack{Z_\delta \\ ||Z-Z_\delta||\leq\delta}} ||\mathfrak{R}Z_\delta - \mathfrak{A}^+ Z|| > 0$$

Proof

Suppose there exists such an operator $\mathfrak{A}$ s.t. for all $Z \in \mathrm{Dom}(\mathfrak{A}^+)$ fulfilling

$$\lim_{\delta\to 0} \sup_{\substack{Z_\delta \\ ||Z-Z_\delta||\le\delta}} ||\mathfrak{R}Z_\delta - \mathfrak{A}^+ Z|| = 0$$

$\mathrm{Dom}(\mathfrak{A}^+)$ is a closed subspace of $\mathcal{Z}$. $\mathfrak{A}^+$ is a linear but *not* a continuous operator mapping $\mathrm{Dom}\,\mathfrak{A}^+ \to \mathcal{X}$ because $\mathfrak{A}$ is an infinite rank compact operator.

Now, we will show that under the above assumption $\mathfrak{A}^+$ has to be continuous.

Assume $Z_1 \in \mathrm{Dom}(\mathfrak{A}^+)$. Then our assumption yields that for any $\varepsilon > 0$ there exists $\delta > 0$ s.t.

$$\sup_{\substack{Z_\delta \\ ||Z_1-Z_\delta||\le\delta}} ||\mathfrak{R}Z_\delta - \mathfrak{A}^+ Z_1|| < \frac{\varepsilon}{2}$$

Then for all $Z_2 \in \mathrm{Dom}(\mathfrak{A}^+)$ with $||Z_1 - Z_2|| \le \delta$ we have

$$||\mathfrak{R}Z_2 - \mathfrak{A}^+ Z_1|| < \frac{\varepsilon}{2}$$

Using our assumption again we have a δ_2 fulfilling

$$\sup_{\substack{Z_{\delta_2} \\ ||Z_2-Z_{\delta_2}||\le\delta_2}} ||\mathfrak{R}Z_\delta - \mathfrak{A}^+ Z_2|| < \frac{\varepsilon}{2}$$

which directly implies

$$||\mathfrak{R}Z_2 - \mathfrak{A}^+ Z_2|| < \frac{\varepsilon}{2}$$

Applying the triangle inequality we finally get

$$||\mathfrak{A}^+ Z_2 - \mathfrak{A}^+ Z_1|| \le ||\mathfrak{R}Z_2 - \mathfrak{A}^+ Z_1|| + ||\mathfrak{R}Z_2 - \mathfrak{A}^+ Z_2|| < \varepsilon$$

which is just another formulation for $\mathfrak{A}^+$ being continuous. This is a contradiction.

q.e.d.

Remark

Note that one does not really need the noise level δ. E.g., if we know the smoothness of the solution we can get enough information to get a sufficiently good estimate for the noise level.

However, if we know neither smoothness nor noise level we have no possibility to regularize our solution. We cannot guarantee that we get near to the real solution.

5.2.2 The Situation

Assume the sequence of operators $\{\mathfrak{A}_n\}$ converging to $\mathfrak{A}$. We will consider the following noisy solutions of our operator equation (noise element $\delta\xi$ with the standard formulation for a stochastical noise element ξ):

$$X_n^\delta = \mathfrak{A}_n^+(\mathfrak{A}X + \delta\xi) = (\mathfrak{A}_n^*\mathfrak{A}_n)^{-1}\mathfrak{A}_n^*(\mathfrak{A}X + \delta\xi) = X_n^0 + \delta\eta_n^\xi$$

where

$$\eta_n^\xi = \mathfrak{A}_n^+\xi = (\mathfrak{A}_n^*\mathfrak{A}_n)^{-1}\mathfrak{A}_n^*\xi$$

where η_n^ξ is a Gaussian random element. (The spectral cut-off scheme fulfills this property, e.g.). From now on we assume that there exist functions ρ and ψ fulfilling:

Definition 5.15

Define $\rho : [1,\infty[\to [0,a]$ to be a decreasing function which fulfills

- $\rho(n+1) \geq c\rho(n)$ *for a constant c*
- $\mathbb{E}_\xi||\eta_n^\xi||^2 \leq \frac{1}{\rho^2(n)}$

Furthermore define the decreasing function $\psi : [1,\infty[\to [0,a]$ to be such that $||X - X_n^0|| \leq \psi(n)$.

Remark

The function ρ may be associated with a kind of error spread by the operator $\mathfrak{A}$ over the various frequencies, whereas the function ψ denotes the smoothness of the solution.

If we assume that X is in the Sobolev space $\mathcal{H}^r$ we can set $\psi(n) = c_X n^{-r}$, where $c_X \in \mathbb{R}$.

Before starting with the main results we need the following supporting lemma:

Lemma 5.11

The following probability estimate holds:

$$\mathbb{P}_\xi\left\{||\eta_n^\xi||\rho(n) > \tau\right\} \leq 4\exp\left(-\frac{\tau^2}{8}\right)$$

Proof

We have using $\mathbb{E}_\xi||\eta_n^\xi||^2 \leq \frac{1}{\rho^2(n)}$ and the probability estimate for Gaussian random vectors [LT91]:

$$\begin{aligned}\mathbb{P}_\xi\left\{||\eta_n^\xi||\rho(n) > \tau\right\} =& \mathbb{P}_\xi\left\{||\eta_n^\xi|| > \frac{\tau}{\rho(n)}\right\} \\ \leq& 4\exp\left(-\frac{\tau^2}{8\rho(n)^2\mathbb{E}_\xi||\eta_n^\xi||^2}\right) \\ \leq& 4\exp\left(-\frac{\tau^2}{8}\right)\end{aligned}$$

q.e.d.

5.2.3 Regularization with Known Smoothness

Now we can determine the optimal regularization parameter via the following result which still needs the input of smoothness and error level but works for the stochastical noise case:

Lemma 5.12

When choosing

$$n_{opt} = \min\left\{n:\ \psi(n) \leq \frac{\delta}{\rho(n)}\right\}$$

we have

$$\sqrt{\mathbb{E}_\xi||X - X^\delta_{n_{opt}}||^2} \leq \frac{\sqrt{2}}{c}\psi\left((\psi\rho)^{-1}(\delta)\right)$$

The proof is taken from [Per03b]:

Proof

We have:

$$\begin{aligned}
\mathbb{E}_\xi||X - X^\delta_n||^2 =& \mathbb{E}_\xi\left\langle X - X^0_n - \delta\eta^\xi_n, X - X^0_n - \delta\eta^\xi_n\right\rangle \\
=& \mathbb{E}_\xi\left\langle X - X^0_n, X - X^0_n\right\rangle - 2\delta\mathbb{E}_\xi\left\langle X - X^0_n, \eta^\xi_n\right\rangle \\
& + \delta^2\mathbb{E}_\xi\left\langle \eta^\xi_n, \eta^\xi_n\right\rangle \\
=& ||X - X^0_n||^2 - 2\delta\mathbb{E}_\xi\left\langle X - X^0_n, (\mathfrak{A}^*_n\mathfrak{A}_n)^{-1}\mathfrak{A}^*_n\xi\right\rangle \\
& + \delta^2\mathbb{E}_\xi||\eta^\xi_n||^2 \\
=& ||X - X^0_n||^2 - 2\delta\mathbb{E}_\xi\left\langle \mathfrak{A}_n(\mathfrak{A}^*_n\mathfrak{A}_n)^{-1}(X - X^0_n), \xi\right\rangle \\
& + \delta^2\mathbb{E}_\xi||\eta^\xi_n||^2 \\
=& ||X - X^0_n||^2 + \delta^2\mathbb{E}_\xi||\eta^\xi_n||^2 \\
\leq& \psi^2(n) + \frac{\delta^2}{\rho^2(n)}
\end{aligned}$$

The only non-obvious point in the above equation is

$$\mathbb{E}_\xi\left\langle \mathfrak{A}_n(\mathfrak{A}^*_n\mathfrak{A}_n)^{-1}(X - X^0_n), \xi\right\rangle = 0$$

which holds because for every set M we have $\mathbb{P}_\xi(\xi \in M) = \mathbb{P}_\xi(-\xi \in M)$
Balancing for the best possible order of accuracy yields that we need a n_0 fulfilling $\psi(n_0)\rho(n_0) = \delta$. On the one hand we have:

$$\psi(n_{opt})\rho(n_{opt}) \leq \delta = \psi(n_0)\rho(n_0)$$

On the other hand

$$\psi(n_{opt} - 1)\rho(n_{opt} - 1) > \delta = \psi(n_0)\rho(n_0)$$

Hence n_{opt} is optimal. This yields

$$\begin{aligned}
\mathbb{E}_\xi ||X - X^\delta_{n_{opt}}||^2 \leq & \psi^2(n_{opt}) + \frac{\delta^2}{\rho^2(n_{opt})} \\
\leq & \frac{2\delta^2}{\rho^2(n_{opt})} \\
\leq & \frac{\psi^2(n_0)\rho^2(n_0)}{\rho^2(n_0+1)} \\
\leq & \frac{2}{c^2}\psi^2(n_0) \\
= & \frac{2}{c^2}\psi^2\left((\psi\rho)^{-1}(\delta)\right)
\end{aligned}$$

q.e.d.

Remark

This can be formulated for deterministic noise as well.

If we have $\psi(n) = n^{-r}$ and $\rho(n) = n^{-a}$ then we would get

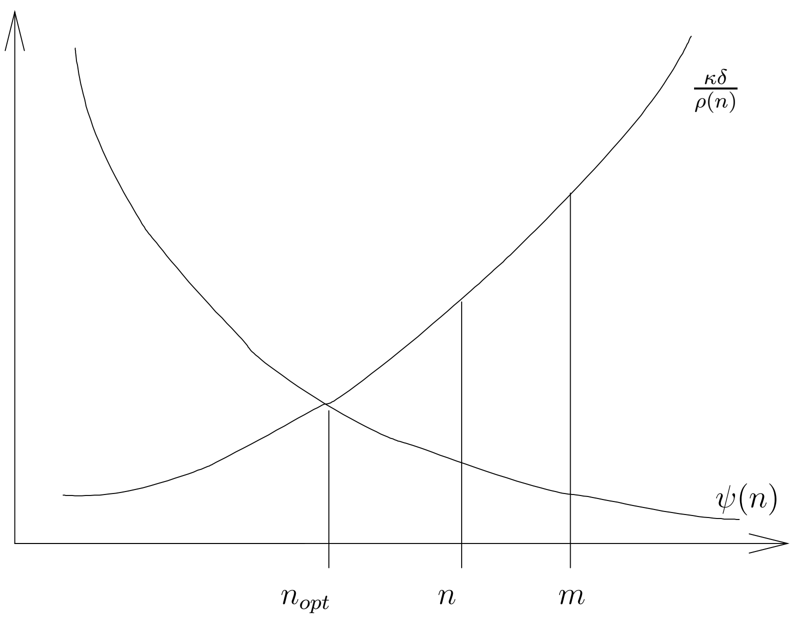
$$\psi\left((\psi\rho)^{-1}(\delta)\right) = \delta^{\frac{r}{r+a}}$$

which coincides which is the best possible order of accuracy for this kind of problem.

A similar result obviously holds for severely ill-posed problems.

5.2.4 Regularization with Unknown Smoothness

The above result has an obvious problem. Normally we do not know the smoothness of our solution. Therefore consider for $n < m$ and $n, m \in \{k : \ \psi(k) \leq \frac{\kappa\delta}{\rho(k)}\}$ the following picture:



Then we have

$$\begin{aligned} ||X_n^\delta - X_m^\delta|| \leq & ||X - X_n^\delta|| + ||X - X_m^\delta|| \\ \leq & \psi(n) + \delta||\eta_n^\xi|| + \psi(m) + \delta||\eta_m^\xi|| \\ \leq & \frac{2\kappa\delta}{\rho(n)} + \frac{2\kappa\delta}{\rho(m)} \\ \leq & \frac{4\kappa\delta}{\rho(m)} \end{aligned}$$

Now we use an idea by Lepskij [Lep90] and take

$$n_* = \min\left\{ n : \ ||X_n^\delta - X_m^\delta|| \leq \frac{4\kappa\delta}{\rho(m)}, \ N = \rho^{-1}(\delta) > m > n \right\}$$

Remark

In real applications it might be better to choose

$$n_* = \min\left\{ n : \ ||X_n^\delta - X_m^\delta|| \leq \frac{2\kappa\delta}{\rho(n)} + \frac{2\kappa\delta}{\rho(m)}, \ N = \rho^{-1}(\delta) > m > n \right\}$$

However, for the subsequent proofs we will use the simpler version.

This yields the following remarkable result which is an enhanced and re-engineered version of a similar theorem presented in [Per03b]. The major difference is another treatment of the important constant κ which now enables us to consider a larger variety of different cases and problem types.

Theorem 5.13

Let n_* be chosen as above with $\kappa \geq 1$. Then we have:

$$\mathbb{E}_\xi||X - X_{n_*}^\delta||^2 \leq C_1\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right) + C_2\kappa^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

where $C_1 = 36 \cdot 2^{11/2}$ and $C_2 = \frac{36}{c^2}$ in the stochastical noise case.
In the deterministic noise case we have $C_1 = 0$ from a certain δ onward.

Proof

First consider another notation for the expectation when we have the normal probability space $(\Omega, \Sigma, \mathbb{P})$:

$$\mathbb{E}_\xi||X - X_n^\delta||^2 = \int_\Omega ||X - X_n^\delta||^2 d\mathbb{P}_\xi(\omega)$$

Now define

$$\Xi_\rho(\omega) = \max_{1\leq n\leq N} ||\eta_n^\xi||\rho(n)$$

We divide the probability space in two subspaces:

$$\Omega_\kappa = \{\omega : \Xi_\rho(\omega) \leq \kappa\} \quad \text{and} \quad \overline{\Omega_\kappa} = \Omega \setminus \Omega_\kappa$$

The proof is mainly consisting of two different parts. The first one estimates the behavior for all "nice" cases Ω_κ. The second one deals with the "bad" cases, where the stochastic noise property produces results far away from the average Ω_κ . Therefore the second part has a strong emphasis on the probability when this case actually occurs.

Note that the second part has probability 0 as long as we are dealing with deterministic noise and δ is small enough.

Part 1: ("good" event $\omega \in \Omega_\kappa$)

Consider

$$n_{opt} = \min\left\{n : \ \psi(n) \leq \frac{\delta}{\rho(n)}\right\}$$

We want to show that $n_{opt} \geq n_*$. For all $n \geq n_{opt}$ we have (using $\frac{\kappa\delta}{\rho(n)} \geq \psi(n)$ and $\rho(n) < \rho(n_{opt})$ because $n \geq n_{opt}$):

$$\begin{aligned}
||X_n^\delta - X_{n_{opt}}^\delta|| \leq & ||X - X_n^\delta|| + ||X - X_{n_{opt}}^\delta|| \\
\leq & \psi(n) + \delta||\eta_n^\xi|| + \psi(n_{opt}) + \delta||\eta_{n_{opt}}^\xi|| \\
\leq & \psi(n) + \frac{\kappa\delta}{\rho(n)} + \psi(n_{opt}) + \frac{\delta}{\rho(n_{opt})} \\
\leq & \psi(n) + \frac{\kappa\delta}{\rho(n)} + \psi(n_{opt}) + \frac{\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{2\kappa\delta}{\rho(n)} + \frac{2\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{4\kappa\delta}{\rho(n)}
\end{aligned}$$

which tells that

$$n_* = \min\left\{n : ||X_n^\delta - X_m^\delta|| \leq \frac{4\kappa\delta}{\rho(n)}, \ N = \rho^{-1}(\delta) > m > n\right\} \leq n_{opt}$$

Then we have for all $\omega \in \Omega_\kappa$ using $n_{opt} \geq n_*$ and the last lemma

$$
\begin{aligned}
||X - X^\delta_{n_*}|| \leq & ||X - X^\delta_{n_{opt}}|| + ||X^\delta_{n_{opt}} - X^\delta_{n_*}|| \\
\leq & \psi(n_{opt}) + \frac{\delta}{\rho(n_{opt})} + \frac{4\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{2\delta}{\rho(n_{opt})} + \frac{4\kappa\delta}{\rho(n_{opt})} \\
\leq & \frac{2\kappa\delta}{\rho(n_{opt})} + \frac{4\kappa\delta}{\rho(n_{opt})} \\
\leq & 6\frac{\kappa}{c}\left(c\frac{\delta}{\rho(n_{opt})}\right) \\
\leq & 6\frac{\kappa}{c}\psi\left((\psi\rho)^{-1}(\delta)\right)
\end{aligned}
$$

Hence we get

$$
\int_{\Omega_\kappa} ||X - X^\delta_{n_*}||^2 d\mathbb{P}_\xi(\omega) \leq |\Omega_\kappa| \; ||X - X^\delta_{n_*}||^2 \leq 36\frac{\kappa^2}{c^2}\psi^2\left((\psi\rho)^{-1}(\delta)\right)
$$

Part 2: ("bad" event $\omega \in \overline{\Omega_\kappa}$)
Remember that we defined $n_{opt} \leq N = \rho^{-1}(\delta)$. Hence we get $\frac{\delta}{\rho(N)} = 1$ and $\psi(N) \leq \delta||\eta^\xi_N||$ and thus

$$
\begin{aligned}
||X - X^\delta_{n_*}|| \leq & ||X - X^\delta_N|| + ||X^\delta_N - X^\delta_{n_*}|| \\
\leq & \psi(N) + \delta||\eta^\xi_N|| + \frac{4\kappa\delta}{\rho(N)} \\
\leq & 2\delta||\eta^\xi_N|| + \frac{4\kappa\delta}{\rho(N)} \\
\leq & 2\frac{\delta||\eta^\xi_N||\rho(N)}{\rho(N)} + 4\kappa \\
\leq & 2\Xi_\rho + 4\Xi_\rho = 6\Xi_\rho
\end{aligned}
$$

Using this result we obtain:

$$
\begin{aligned}
\int_{\overline{\Omega_\kappa}} ||X - X^\delta_{n_*}||^2 d\mathbb{P}_\xi(\omega) \leq & 36\int_{\overline{\Omega_\kappa}} \Xi^2_\rho(\omega) d\mathbb{P}_\xi(\omega) \\
\leq & 36\sqrt{\int_{\overline{\Omega_\kappa}} \Xi^4_\rho(\omega) d\mathbb{P}_\xi(\omega)}\sqrt{\int_{\overline{\Omega_\kappa}} 1 d\mathbb{P}_\xi(\omega)}
\end{aligned}
$$

Now we estimate the two parts separately:
Consider $F(\tau) = \mathbb{P}_\xi\{\Xi_\rho(\omega) \leq \tau\}$ for $\tau > \kappa$. Then

$$
\begin{aligned}
G(\tau) = 1 - F(\tau) =& \mathbb{P}_\xi \left\{ \Xi_\rho(\omega) > \tau \right\} \\
\leq& \sum_{n=1}^{N} \mathbb{P}_\xi \left\{ ||\eta_n^\xi|| \rho(n) > \tau \right\} \\
\leq& 4N \exp\left(-\frac{\tau^2}{8} \right)
\end{aligned}
$$

So we get:

$$
\begin{aligned}
\int_{\overline{\Omega_\kappa}} \Xi_\rho^4 d\mathbb{P}_\xi(\omega) =& - \int_\kappa^\infty \tau^4 d(1 - F(\tau)) \\
\leq& - \int_0^\infty \tau^4 dG(\tau) \\
=& - \tau^4 G(\tau)|_0^\infty + 4 \int_0^\infty \tau^3 G(\tau) d\tau \\
=& 4 \int_0^\infty \tau^3 G(\tau) d\tau \\
\leq& 4N \int_0^\infty \tau^3 \exp\left(-\frac{\tau^2}{8} \right) d\tau \\
=& 2^9 N \int_0^\infty u \exp(-u) du \\
=& 2^9 N
\end{aligned}
$$

The other part gets:

$$
\int_{\overline{\Omega_\kappa}} 1 d\mathbb{P}_\xi(\omega) \leq 4 \exp\left(-\frac{\kappa^2}{8} \right)
$$

Hence we get

$$
\begin{aligned}
\int_{\overline{\Omega_\kappa}} \Xi_\rho^2 d\mathbb{P}_\xi(\omega) \leq& 2^{11/2} N \exp\left(-\frac{\kappa^2}{16} \right) \\
\leq& 2^{11/2} \rho^{-1}(\delta) \exp\left(-\frac{\kappa^2}{16} \right)
\end{aligned}
$$

This yields

$$
\mathbb{E}_\xi ||X - X_{n_*}^\xi||^2 \leq 36 \cdot 2^{11/2} \rho^{-1}(\delta) \exp\left(-\frac{\kappa^2}{16} \right) + 36 \frac{\kappa^2}{c^2} \psi^2 \left((\psi\rho)^{-1} (\delta) \right)
$$

This is exactly the proposition. q.e.d.

Now the main task will be choosing an appropriate κ for different possible scenarios.

5.2.4.1 Remarks on Smoothness and Error Spread

As we have seen above the bound for the square of the total error consists of two parts. The second part $\psi^2((\psi\rho)^{-1}(\delta))$ is just the best order of accuracy we can reach in a various number of cases. So we want that the first part $\rho^{-1}(\delta)\exp(-\frac{\kappa^2}{16})$ is negligible in comparison to the second one. It entered the equation when we considered the "bad" case $\omega \in \overline{\Omega_\kappa}$.

As remarked in the proof this part cancels automatically for deterministic noise:

Corollary 5.14

Assume that we are in the deterministic noise case. Then we have for $\kappa = 1$ in the above theorem the following estimate:

$$\sqrt{\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2} \leq \frac{6}{c}\psi\left((\psi\rho)^{-1}(\delta)\right)$$

Remark

This is the optimal order of convergence in this case.

Under weak restrictions we can do a straightforward balancing process for the stochastical noise case which yields the following result:

Lemma 5.15

Assume that we are in the stochastic noise case. Further assume that we know

$$F(\delta)\ln\rho^{-1}(\delta) \leq \ln\left(\psi\left((\psi\rho)^{-1}(\delta)\right)\right)$$

for all $\delta < \delta_0$.

Now choose in the κ in the above theorem

$$\kappa = 4\sqrt{\ln\rho^{-1}(\delta)}\sqrt{-2F(\delta)+1}$$

Then we have for an appropriate constant C for $\delta < \delta_0$:

$$\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2 \leq C\left(1 - 2F(\delta)\right)\ln\left(\rho^{-1}(\delta)\right)\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

Proof

We just need to show that the term imposed by the stochastical noise condition $\rho^{-1}(\delta)\exp(-\frac{\kappa^2}{16})$ is decreasing at least as strong as the general regularization term $\psi^2((\psi\rho)^{-1}(\delta))$.

We have for $\delta < \delta_0$:

$$\begin{aligned}\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right) &= \rho^{-1}(\delta)\exp\left(-\left(\ln\rho^{-1}(\delta)\right)\left(-2F(\delta)+1\right)\right)\\ &= \rho^{-1}(\delta)\left(\rho^{-1}(\delta)\right)^{2F(\delta)-1}\\ &= \left(\rho^{-1}(\delta)\right)^{2F(\delta)}\\ &\leq \psi^2\left((\psi\rho)^{-1}(\delta)\right)\end{aligned}$$

q.e.d.

Now we want to give some short remarks what the terms ρ^{-1} and $\psi((\rho\psi)^{-1})$ actually mean in practice. Assume that we have $\psi(n) = n^{-r}$ which means in particular that our solution is rather smooth, namely in the Sobolev space $X \in \mathcal{H}^r$.

Then we can distinguish the following two cases. Note that in both cases we do not need to consider a separate pre-factor because in an application we could not distinguish this one from δ.

Ordinarily Ill-Posed Problem For an ordinarily ill-posed problem we have $\rho(n)$ is a function fulfilling $\ln \rho(n) \asymp \ln n^{-1}$ (i.e., there exist c_1 and c_2 such that $c_1 \ln n^{-1} \leq \ln \rho(n) \leq c_2 \ln n^{-1}$).

In order to simplify our considerations we just assume that $\rho(n) = n^{-a}$. Then we have the following two properties:

$$\rho^{-1}(\delta) = \delta^{-\frac{1}{a}}$$

$$\psi\left((\psi\rho)^{-1}(\delta)\right) = \delta^{\frac{r}{r+a}}$$

Severely Ill-Posed Problem For a severely ill-posed problem we have $\rho(n) = p(n)\exp(an^{\beta})$, where $\ln p(n) \asymp \ln n^{-1}$. Again for reasons of simplicity we will assume $\rho(n) = n^{-\mu}\exp(an^{\beta})$. Then we have:

$$\rho^{-1}(\delta) \approx \left(\frac{\ln \delta^{-1}}{a}\right)^{\frac{1}{\beta}}$$

$$\psi\left((\psi\rho)^{-1}(\delta)\right) \approx \left(\frac{\ln \delta^{-1}}{a}\right)^{-\frac{r}{\beta}}$$

The approximate sign is due to the fact that the functions above are not algebraically invertible, but on the other hand for big n the term $\ln n$ becomes negligible in comparison to n.

5.2.4.2 Further implications

For these specific cases we may choose κ now according to our needs.

Corollary 5.16

Assume we have stochastic noise and furthermore our problem is ordinarily ill-posed, i.e., we have $\ln \frac{1}{u} \asymp \ln \rho^{-1}(u)$. (i.e., there exist constants μ_1 and μ_2 such that $\mu_1 \ln \frac{1}{u} \leq \ln \rho^{-1}(u) \leq \mu_2 \ln \frac{1}{u}$).

If δ is small enough one can choose the κ defined in the above theorem as $\kappa = \chi\hat{\kappa}$, where $\hat{\kappa} = 4\sqrt{p \ln \rho^{-1}(\delta)} \asymp \ln^{\frac{1}{2}} \frac{1}{\delta}$ and p such that $2^{\frac{11}{2}}(\rho^{-1}(\delta))^{-p+1} = \delta^2$.

Writing $\pi_1 = 1 + \frac{2}{\mu_2}$ and $\pi_2 = 1 + \frac{2}{\mu_1}$ we get

$$\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2 \leq C\delta^2 \delta^{-\mu_2 \frac{\pi_2}{\pi_1}\left(1-\chi^2\right)} + C\chi^2\left(\ln \delta^{-1}\right)\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

Proof

First we want to turn our attention to the constant p. We have

$$\left(\rho^{-1}(\delta)\right)^{-p+1} = 2^{-\frac{11}{2}}\delta^2$$

and hence

$$(-p+1)\ln\rho^{-1}(\delta) = -\frac{11}{2}\ln 2 + 2\ln\delta$$

which can be solved for p:

$$\begin{aligned} p-1 =& \frac{\frac{11}{2}\ln 2 - 2\ln\delta}{\ln\rho^{-1}(\delta))} \\ \asymp& \frac{\frac{11}{2}\ln 2 - 2\ln\delta}{\ln\delta^{-1}} \\ =& \frac{-\frac{11}{2}\ln 2}{-\ln\delta} + 2 \xrightarrow[\delta\to 0]{} 2 \end{aligned}$$

This means in particular that p is bounded by constants $\pi_1 \le p \le \pi_2$ independent of the error level δ. (The constants just depend on μ_1 and μ_2, where $\pi_1 = 1 + \frac{2}{\mu_2}$ and $\pi_2 = 1 + \frac{2}{\mu_1}$ for the case δ small enough.)
This implies in particular $4\sqrt{\frac{\pi_1}{\pi_2}} \le \frac{\kappa}{\ln\rho^{-1}(\delta)} \le 4\sqrt{\frac{\pi_2}{\pi_1}}$, i.e., for μ_1 near to μ_2 and δ not too small we have $\kappa = 4$ as a good solution.
Hence using the choice of κ we get

$$\begin{aligned} 2^{11/2}\rho^{-1}(\delta)\exp\left(-\frac{\kappa^2}{16}\right) =& 2^{11/2}\rho^{-1}(\delta)\exp\left(-\frac{\chi^2\hat{\kappa}^2}{16}\right) \\ \le& 2^{11/2}\rho^{-1}(\delta)\exp\left(-\frac{16\chi^2 p\ln\rho^{-1}(\delta)}{16}\right) \\ =& 2^{11/2}\left(\rho^{-1}(\delta)\right)^{1-p\chi^2} \\ \le& \delta^2\left(\rho^{-1}(\delta)\right)^{p(1-\chi^2)} \\ \le& \delta^2\left(\rho^{-1}(\delta)\right)^{\frac{\pi_2}{\pi_1}(1-\chi^2)} \end{aligned}$$

Using $\ln\rho^{-1}(\delta) \asymp \ln\delta^{-1}$ we can deduce that $\rho^{-1}(\delta) \le \delta^{-\mu_2}$ which immediately yields the proposition. q.e.d.

This additional factor χ will enable us to neglect the first term if $\chi \to_{\delta\to 0} 1$ fast enough. However this will be part of later discussion and we will just consider the case $\chi = 1$ right now:

Corollary 5.17

Assume that we have stochastic noise and furthermore that our problem is not severely ill-posed, i.e., we have $\ln\frac{1}{u} \asymp \ln\rho^{-1}(u)$. (i.e., there exist constants μ_1 and μ_2 such that $\mu_1\ln\frac{1}{u} \le \ln\rho^{-1}(u) \le \mu_2\ln\frac{1}{u}$).

If δ is small enough one can choose the κ defined in the above theorem as $\kappa = 4\sqrt{p \ln \rho^{-1}(\delta)} \asymp \ln^{\frac{1}{2}} \frac{1}{\delta}$ and p such that $2^{\frac{11}{2}}(\rho^{-1}(\delta))^{-p+1} = \delta^2$ which yields

$$\sqrt{\mathbb{E}_\xi ||X - X_{n_*}^\delta||^2} \leq C\sqrt{\ln \delta^{-1}} \psi\left((\psi\rho)^{-1}(\delta)\right) + o(\delta)$$

For the severely ill-posed case we will do again some balancing process:

Corollary 5.18

Assume that our problem is severely ill-posed with stochastical noise and polynomial smoothness of the solution ψ. Now choose $\kappa = \chi 4 \ln \ln \delta^{-1}$.
Then we have

$$\begin{aligned}\mathbb{E}_\xi ||X - X_{n_*}^\delta||^2 \leq\ & C\left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta} - \chi^2 \ln \ln \delta^{-1}} \\ & + C\chi^2 \left(\ln \ln \delta^{-1}\right)^2 \psi^2\left((\psi\rho)^{-1}(\delta)\right)\end{aligned}$$

Proof

Inserting κ we obtain

$$\begin{aligned} & C_1 \rho^{-1}(\delta) \exp\left(-\frac{\kappa^2}{16}\right) + C_2 \kappa^2 \psi^2\left((\psi\rho)^{-1}(\delta)\right) \\ & \asymp \left(\ln \delta^{-1}\right)^{\frac{1}{\beta}} \left(\ln \delta^{-1}\right)^{-\chi^2 \ln \ln \delta^{-1}} + \kappa^2 \psi^2\left((\psi\rho)^{-1}(\delta)\right) \\ & = \left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta} - \chi^2 \ln \ln \delta^{-1}} + \chi^2 \left(\ln \ln \delta^{-1}\right)^2 \psi^2\left((\psi\rho)^{-1}(\delta)\right)\end{aligned}$$

which yields the assertion. q.e.d.

Corollary 5.19

Assume that our problem is severely ill-posed with stochastical noise and polynomial smoothness of the solution ψ. Now choose $\kappa = 4 \ln \ln \delta^{-1}$.
Then we have if δ small enough

$$\sqrt{\mathbb{E}_\xi ||X - X_{n_*}^\delta||^2} \leq C\left(\ln \ln \delta^{-1}\right) \psi\left((\psi\rho)^{-1}(\delta)\right)$$

Proof

For a severely ill-posed problem with polynomial smoothness ψ we have as seen above

$$\rho^{-1}(\delta) \asymp \left(\frac{\ln \delta^{-1}}{a}\right)^{\frac{1}{\beta}}$$

and

$$\psi\left((\psi\rho)^{-1}(\delta)\right) \asymp \left(\frac{\ln\delta^{-1}}{a}\right)^{-\frac{r}{\beta}}$$

Hence using the fact that from some point onward

$$\ln\ln\delta^{-1} - \frac{1}{\beta} \geq 2\frac{r}{\beta}$$

we get (using $\chi = 1$):

$$\begin{aligned}
\left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta}-\ln\ln\delta^{-1}} &+ \left(\ln\ln\delta^{-1}\right)^2 \psi^2\left((\psi\rho)^{-1}(\delta)\right) \\
&\asymp \left(\ln\left(\delta^{-1}\right)\right)^{\frac{1}{\beta}-\ln\ln\delta^{-1}} + \left(\ln\ln\delta^{-1}\right)^2 \left(\ln\left(\delta^{-1}\right)\right)^{-2\frac{r}{\beta}} \\
&\asymp \left(\ln\ln\delta^{-1}\right)^2 \left(\ln\left(\delta^{-1}\right)\right)^{-2\frac{r}{\beta}} \\
&\asymp \left(\ln\ln\delta^{-1}\right)^2 \psi^2\left((\psi\rho)^{-1}(\delta)\right) \qquad \text{q.e.d.}
\end{aligned}$$

Remark

Note that κ is just increasing very slowly with decreasing δ and hence for practical applications could just be set to 4.

Furthermore, if we actually know (or have an idea) about the smoothness of the solution we can easily incorporate this knowledge in κ in order to get the above estimate already for much bigger δ.

This theorem and its corollaries are a really remarkable result. It tells, under certain conditions we just need the error (and error spread) and can obtain an (sometimes even order optimal) regularization procedure. This tells us further that the knowledge of δ is not just necessary as proposed in the lemma of Bakushinskii but also sufficient.

Another fact one could observe from the corollaries is that for big δ (and this is the case we are normally facing in practice) a good choice of κ seems to be near to 4 although such a fixed κ would, of course, not yield an order optimal solution procedure for δ tending to 0.

5.2.5 Estimations

As we have seen the above results still hold even if we introduce an additional parameter χ. Of course, in practice no-one would like to obstruct our optimal κ by purpose. However, when we work with estimated constants, for example δ, we automatically get different values for $\frac{4\kappa\delta}{\rho(m)}$ which are just due to the estimation process for ρ, κ, δ and the other underlying constants and functions.

Now we may consider the (multiplicative) difference between the actual and the estimated value exactly as the χ we have artificially introduced in the above corollaries.

If we write the estimated version of the various constants and functions with a tilde we have:

$$\frac{4\chi(m)\kappa\delta}{\rho(m)} = \frac{4\tilde{\kappa}\tilde{\delta}}{\tilde{\rho}(m)}$$

which yields

$$\chi(m) = \frac{\frac{4\tilde{\kappa}\tilde{\delta}}{\tilde{\rho}(m)}}{\frac{4\kappa\delta}{\rho(m)}} = \frac{\tilde{\kappa}\tilde{\delta}}{\kappa\delta}\frac{\rho(m)}{\tilde{\rho}(m)}$$

Now define

$$\chi = \max_{\substack{\chi(m) \\ m\in\{1\ldots\max\{N,\tilde{N}\}\}}} \left\{\chi(m),\, \chi(m)^{-1}\right\}$$

i.e., we are interested in the χ which has multiplicatively seen the biggest distance from 1.

As we have seen this parameter χ does not pose too many problems as long it is close enough to 1. Now we want to analyze if we can actually guarantee this if we have control over the differences between the original and the estimated version of the values.

Because we have different properties for the ordinary and severely ill-posed case we will also distinguish between these two cases in the sequel.

5.2.5.1 Ordinary Ill-Posed Problems

For technical reasons we will further assume that $\mu_1 \approx \mu \approx \mu_2$, i.e., we have the slightly harder restriction $\rho^{-1}(\delta) \approx \delta^{-\mu}$ in the above theorem.

Lemma 5.20

Assume that we estimated $\tilde{\mu}$ and $\tilde{\delta}$ by some method and δ small enough. Define

$$\mu_{max} = \max\{\tilde{\mu}, \mu\} \quad \textit{and} \quad \mu_{min} = \min\{\tilde{\mu}, \mu\}$$

and

$$\delta_{max} = \max\{\tilde{\delta}, \delta\} \quad \textit{and} \quad \delta_{min} = \min\{\tilde{\delta}, \delta\}$$

and furthermore $\delta_{diff} = \delta_{max} - \delta_{min}$ and $\mu_{diff} = \mu_{max} - \mu_{min}$. Then we can estimate χ for the original μ and δ by

$$\left(\frac{\delta_{min}}{\delta_{max}}\right)^{1+\varepsilon} \left(\delta_{min}^{-\mu_{max}}\right)^{-\mu_{diff}} \leq \chi \leq \left(\frac{\delta_{max}}{\delta_{min}}\right)^{1+\varepsilon} \left(\delta_{min}^{-\mu_{max}}\right)^{\mu_{diff}}$$

Furthermore there exist constants $\lambda_{\boxdot}^{\boxdot}$ which are at most linearly dependent on μ and δ^{-1} such that:

$$\left(1 - \lambda_1^1\delta_{diff}\right)^2 \left(1 - \lambda_1^2\mu_{diff}\right) \leq \chi \leq \left(1 + \lambda_2^1\delta_{diff}\right)^2 \left(1 + \lambda_2^2\mu_{diff}\right)$$

Proof

In order to distinguish between the original and the estimated version we will use a tilde for each variable which depends on estimated values.
In order to get χ we need to calculate the ratio between $\frac{4\tilde{\kappa}\tilde{\delta}}{\tilde{\rho}(m)}$ (the estimated κ) and $\frac{4\kappa\delta}{\rho(m)}$ (the optimal κ). Using the calculations of p done beforehand we get:

$$\chi(m) = \frac{\frac{4\tilde{\kappa}\tilde{\delta}}{\tilde{\rho}(m)}}{\frac{4\kappa\delta}{\rho(m)}} = \frac{\tilde{\kappa}\tilde{\delta}\rho(m)}{\kappa\delta\tilde{\rho}(m)} = \frac{\sqrt{\tilde{p}\ln\tilde{\rho}^{-1}(\tilde{\delta})}\tilde{\delta}\rho(m)}{\sqrt{p\ln\rho^{-1}(\delta)}\delta\tilde{\rho}(m)} = \left(\frac{\tilde{\delta}}{\delta}\right)^{1+\varepsilon} m^{\mu-\tilde{\mu}}$$

ε compensates the $\ln\delta$ terms which occur when expanding p. It can be either positive or negative but is rather small and fulfills $\varepsilon \rightarrow_{\delta\rightarrow 0} 0$.
Considering the above equation we observe that the best case is $m = 1$, whereas the worst case is

$$m = \max\left\{N, \tilde{N}\right\} = \max\left\{\rho^{-1}(\delta), \tilde{\rho}^{-1}(\tilde{\delta})\right\} \leq \delta_{min}^{-\mu_{max}}$$

Inserting this estimate yields

$$\left(\frac{\delta_{min}}{\delta_{max}}\right)^{1+\varepsilon} \left(\delta_{min}^{-\mu_{max}}\right)^{-\mu_{diff}} \leq \chi \leq \left(\frac{\delta_{max}}{\delta_{min}}\right)^{1+\varepsilon} \left(\delta_{min}^{-\mu_{max}}\right)^{\mu_{diff}}$$

Using for $0 \leq \varsigma \leq \frac{1}{2}$

$$\exp(\varsigma) = \sum_{n=0}^{\infty} \frac{\varsigma^n}{n!} \leq 1 + \varsigma \sum_{n=0}^{\infty} \varsigma^n = 1 + 2\varsigma$$

(The same holds for $-\frac{1}{2} \leq \varsigma \leq 0$). Hence for $\frac{1}{2}(\mu_{max} - \mu_{min})$ small enough the above formula can be relaxed to :

$$\begin{aligned} \left(\frac{\delta_{min}}{\delta_{max}}\right)^{1+\varepsilon} & \left(1 - \mu_{max}\ln(\delta_{min}^{-1})(\mu_{max} - \mu_{min})\right) \leq \chi \\ & \leq \left(\frac{\delta_{max}}{\delta_{min}}\right)^{1+\varepsilon} \left(1 + \mu_{max}\ln(\delta_{min}^{-1})(\mu_{max} - \mu_{min})\right) \end{aligned}$$

or using $\boxdot_{diff}$ and some constants $\lambda_{\boxdot}^{\boxdot}$ at most linearly depending on μ and δ^{-1} (again for δ and μ_{diff} small enough) and choosing $|\varepsilon| = \frac{1}{2}$

$$\left(1 - \lambda_1^1\delta_{diff}\right)^2 \left(1 - \lambda_1^2\mu_{diff}\right) \leq \chi \leq \left(1 + \lambda_2^1\delta_{diff}\right)^2 \left(1 + \lambda_2^2\mu_{diff}\right)$$

which is the desired result. q.e.d.

Remark

Hence we just need that our estimates are getting close enough. Then χ tends to 1 and hence $-\mu_2\frac{\pi_2}{\pi_1}(1-\chi^2)$ gets bigger than -1. This immediately implies that we get the same rate of convergence as in the case when $\chi = 1$.

5.2.5.2 Severely Ill-Posed Problems

Now we will do some similar estimates in the severely ill-posed case. For technical reasons we will assume that the same restrictions hold as described in the remarks beforehand.

Lemma 5.21

Let for μ, δ, a and β the versions $\tilde{\boxdot}$, $\boxdot_{min}$, $\boxdot_{max}$ and $\boxdot_{diff}$ be defined analogously to the lemma above. Then we have

$$\begin{aligned}
&\left(\frac{\delta_{min}}{\delta_{max}}\right)^{1+\varepsilon}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{-\mu_{diff}}{\beta_{min}}}\left(\delta_{min}^{-1}\right)^{\left(\frac{a_{min}}{a_{max}}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{min}}{\beta_{max}}-1}-1\right)} \leq \chi \\
&\quad\leq \left(\frac{\delta_{max}}{\delta_{min}}\right)^{1+\varepsilon}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\mu_{diff}}{\beta_{min}}}\left(\delta_{min}^{-1}\right)^{\left(\frac{a_{max}}{a_{min}}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{max}}{\beta_{min}}-1}-1\right)}
\end{aligned}$$

and

$$\begin{aligned}
&\left(1-\lambda_1^1\delta_{diff}\right)^2\left(1-\lambda_2^1\mu_{diff}\right)\left(1-\lambda_3^1\beta_{diff}\right)\left(1-\lambda_4^1 a_{diff}\right) \leq \chi \\
&\quad\leq \left(1+\lambda_1^2\delta_{diff}\right)^2\left(1+\lambda_2^2\mu_{diff}\right)\left(1+\lambda_3^2\beta_{diff}\right)\left(1+\lambda_4^2 a_{diff}\right)
\end{aligned}$$

for appropriate constants $\lambda_{\boxdot}^{\boxdot}$ which are just linearly dependent on the parameters μ, δ, a and β.

Proof

In order to distinguish between the original and the estimated version we will use a tilde for each variable which is dependent on estimated values.
In order to get χ we need to calculate the ratio between $\frac{4\tilde{\kappa}\tilde{\delta}}{\tilde{\rho}(m)}$ (the estimated κ) and $\frac{4\kappa\delta}{\rho(m)}$ (the optimal κ). Using the calculations of p done beforehand we get:

$$\begin{aligned}
\chi(m) &= \frac{\frac{4\tilde{\kappa}\tilde{\delta}}{\tilde{\rho}(m)}}{\frac{4\kappa\delta}{\rho(m)}} = \frac{\tilde{\kappa}\tilde{\delta}\rho(m)}{\kappa\delta\tilde{\rho}(m)} = \frac{(\ln\ln\tilde{\delta}^{-1})\tilde{\delta}\rho(m)}{(\ln\ln\delta^{-1})\delta\tilde{\rho}(m)} \\
&= \left(\frac{\tilde{\delta}}{\delta}\right)^{1+\varepsilon}\frac{p(m)\exp\left(-am^{\beta}\right)}{\tilde{p}(m)\exp\left(-\tilde{a}m^{\tilde{\beta}}\right)} \\
&= \left(\frac{\tilde{\delta}}{\delta}\right)^{1+\varepsilon} m^{\tilde{\mu}-\mu}\exp\left(\tilde{a}m^{\tilde{\beta}}-am^{\beta}\right)
\end{aligned}$$

holding for a very small (not necessarily positive) ε (depending on δ) which should compensate for neglecting the logarithms.

Again, like in the last lemma, the worst case which could happen (in terms of big χ) is

$$\begin{aligned}
m =& \max\left\{N, \tilde{N}\right\} = \max\left\{\rho^{-1}(\delta), \tilde{\rho}^{-1}(\tilde{\delta})\right\} \\
=& \max\left\{\left(\frac{\ln\delta^{-1}}{a}\right)^{\frac{1}{\beta}}, \left(\frac{\ln\tilde{\delta}^{-1}}{\tilde{a}}\right)^{\frac{1}{\tilde{\beta}}}\right\} \leq \left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{1}{\beta_{min}}}
\end{aligned}$$

Hence using that all of the differences $\boxdot_{diff}$ are relatively small and ε is small (so we can apply $\exp(\varsigma) \leq 1 + 2\varsigma$) we get:

$$\begin{aligned}
\chi \leq& \left(\frac{\tilde{\delta}}{\delta}\right)^{1+\varepsilon} \left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\tilde{\mu}-\mu}{\beta_{min}}} \\
& \qquad \exp\left(a_{max}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{max}}{\beta_{min}}} - a_{min}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{min}}{\beta_{min}}}\right) \\
=& \left(\frac{\tilde{\delta}}{\delta}\right)^{1+\varepsilon} \left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\tilde{\mu}-\mu}{\beta_{min}}} \\
& \qquad \exp\left((\ln\delta_{min}^{-1})\left(\frac{a_{max}}{a_{min}}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{max}}{\beta_{min}}-1} - 1\right)\right) \\
=& \left(\frac{\delta_{max}}{\delta_{min}}\right)^{1+\varepsilon} \left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\tilde{\mu}-\mu}{\beta_{min}}} (\delta_{min}^{-1})^{\left(\frac{a_{max}}{a_{min}}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{max}}{\beta_{min}}-1}-1\right)} \\
\leq& (1+\lambda_1^2\delta_{diff})^2(1+\lambda_2^2\mu_{diff})\left(1+\lambda^*\left(\frac{a_{max}}{a_{min}}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{max}}{\beta_{min}}-1} - 1\right)\right) \\
\leq& (1+\lambda_1^2\delta_{diff})^2(1+\lambda_2^2\mu_{diff}) \\
& \qquad \left(1+\lambda^*\left(\left(1+\overline{\lambda}a_{diff}\right)\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\beta_{max}}{\beta_{min}}-1} - 1\right)\right) \\
\leq& (1+\lambda_1^2\delta_{diff})^2(1+\lambda_2^2\mu_{diff}) \\
& \qquad \left(1+\lambda^*\left(\left(1+\overline{\lambda}a_{diff}\right)\left(1+\tilde{\lambda}\beta_{diff}\right) - 1\right)\right) \\
\leq& (1+\lambda_1^2\delta_{diff})^2(1+\lambda_2^2\mu_{diff})(1+\lambda_3^2\beta_{diff})(1+\lambda_4^2a_{diff})
\end{aligned}$$

The various constants $\lambda_{\boxdot}^{\boxdot}$ are at most linearly dependent on δ, μ, a and β.
The other part of the inequality follows easily, which yields the proposition. q.e.d.

In the situation $\beta = \tilde{\beta}$ we get:

Corollary 5.22

Let for μ, δ and a the versions $\tilde{\boxdot}$, $\boxdot_{min}$, $\boxdot_{max}$ and $\boxdot_{diff}$ be defined analogously to the lemma and the remark above. Then we have

$$\left(\frac{\delta_{min}}{\delta_{max}}\right)^{1+\varepsilon}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{-\mu_{diff}}{\beta_{min}}}(\delta_{min}^{-1})^{-\frac{a_{diff}}{a_{max}}}\leq\chi$$
$$\leq\left(\frac{\delta_{max}}{\delta_{min}}\right)^{1+\varepsilon}\left(\frac{\ln\delta_{min}^{-1}}{a_{min}}\right)^{\frac{\mu_{diff}}{\beta_{min}}}(\delta_{min}^{-1})^{\frac{a_{diff}}{a_{min}}}$$

and

$$\left(1-\lambda_1^1\delta_{diff}\right)^2\left(1-\lambda_2^1\mu_{diff}\right)\left(1-\lambda_3^1 a_{diff}\right)\leq\chi$$
$$\leq\left(1+\lambda_1^2\delta_{diff}\right)^2\left(1+\lambda_2^2\mu_{diff}\right)\left(1+\lambda_3^2 a_{diff}\right)$$

for appropriate constants $\lambda_{\boxdot}^{\boxdot}$ which are just linearly dependent on the parameters μ, δ, a and β.

Remark

Note that the corollary of the last section indicates that we just need to bound χ for the severely ill-posed problems.

The two last lemmas guarantee that we can reach the proposed level of convergence (which is not optimal, but really close to this) if we can estimate the relevant constants sufficiently good.

Remark

Note that in all of our above inequalities we can substitute $\left(\frac{\delta_{max}}{\delta_{min}}\right)^{\pm1}$ by $(1\pm\lambda\delta_{diff})$ for a constant just depends on δ^{-1}.

5.3 Noise Estimation out of Two Start Values

In practice we neither know the error level δ nor the error spread ρ. Now we will turn our attention on how one can obtain such information. Note that the lemma of Bakushinskii just tells that if we have *one* function as input data we cannot do anything. But in practice it is often possible to do get three sets of spectral data. (In particular the satellite missions generate enough data to justify such an idea).

So we will try the following ansatz. For reasons of simplicity we will restrict ourselves to the spectral cut-off scheme as regularization procedure.

- Invert the first two data sets, we get the sequences of regularized solutions $(X_{1,n})_{n\in\mathbb{N}}$ and $(X_{2,n})_{n\in\mathbb{N}}$ depending on the input data sets Z_1 and Z_2.
- Subtract pairwise the two sequences $(X_{1,n}-X_{2,n})_{n\in\mathbb{N}}=(X_{diff,n})_{n\in\mathbb{N}}$. This is now consisting of *pure* error $\delta\mathfrak{A}_n^+(\xi_1-\xi_2)=\delta\left(\eta_n^{\xi_1}-\eta_n^{\xi_2}\right)$.

- As we assumed the error is behaving like $\frac{\delta}{\rho(n)}$ for every $X_n^{diff} = ||X_{diff,n}||$.
- Under some further assumptions on ρ we can estimate the parameters which describe this function. In particular we will show that we can estimate every of these parameters with arbitrary precision.
- We choose the highest possible precision and regularize the third data set Z with our resulting estimate for $\frac{\delta}{\rho}$.

It is equivalent if we determine the behavior of either $\frac{\delta}{\rho(n)}$ or $\frac{\delta^2}{\rho(n)^2}$ or $\delta^2\widehat{\rho}(n)^2 := \frac{\delta^2}{\rho(n)^2} - \frac{\delta^2}{\rho(n-1)^2}$ because $\frac{\delta}{\rho(n)} = \sqrt{\sum_{i=1}^n \delta^2\widehat{\rho}(n)^2}$.

The particular advantage of the last method is that for the spectral cut-off scheme the errors of $(\widehat{X}_n^{diff})^2 := (X_n^{diff})^2 - (X_{n-1}^{diff})^2$ for each n are independent of each other and so do not impose practical difficulties for estimating $\delta\widehat{\rho}(n)$.

When we assume that $\frac{\delta}{\rho}$ is behaving like $\delta k^{\mu}\exp(ak^{\beta})F(k)$ for the severely ill-posed case and like $\delta k^{\mu}F(k)$ for the ordinarily ill-posed case (where F is assumed to be known) we get that $\delta\widehat{\rho}$ is behaving like $\widehat{\delta}k^{\widehat{\mu}}\exp(ak^{\beta})\widehat{F}(k)$ respectively like $\widehat{\delta}k^{\widehat{\mu}}\widehat{F}(k)$. As we know F we can calculate $\widehat{F}$ and so can assume to know it. Furthermore we can easily determine δ, μ (and a) out of $\widehat{\delta}$, $\widehat{\mu}$ (and a). Because we are having a smooth function between these it is sufficient to estimate $\widehat{\delta}$, $\widehat{\mu}$ (and a) with arbitrary precision in order to get δ, μ (and a) with arbitrary precision, as we will see later on.

Please note that although the estimation results will now be obtained for the simplified case a similar procedure would work in order to get an estimation of $\frac{\delta}{\rho}$ directly. However the independence of the random variables will simplify the proofs considerably.

First we will do the estimation part which was generated in cooperation with Dr. J-P. Stockis [Sto03]. Therefore we will introduce some further notation [BD96]:

Definition 5.16

A sequence $\{x_n\}$ of random variables is called asymptotically normally distributed with mean $\overline{x}_n$ and "standard deviation" σ_n if n sufficiently large and $\sigma_n^{-1}(x_n - \overline{x}_n)$ converges (in the sense of distributions) to $\mathcal{N}(0,1)$.
This property is denoted by $\{x_n\}$ is $\mathcal{AN}(\overline{x}_n, \sigma_n^2)$.

Definition 5.17

The sequence $\{x_n\}$ of random k-vectors is called asymptotically normal with "mean vector" $\overline{x}_n$ and "covariance matrix" Σ_n if

- *Σ_n has no zero diagonal elements*
- *For all $\lambda^T \in \mathbb{R}^k$ we have λx_n is asymptotically normal*
- *Σ_n is positive definite*

for all sufficiently large n.
This property is denoted by $\{x_n\}$ is $\mathcal{AN}(\overline{x}_n, \Sigma_n)$.

Lemma 5.23

Assume

$$\widehat{X}_k^{diff} = \widehat{\delta} k^{\widehat{\mu}} \exp(ak^{\beta}) F(k)$$

where $\beta \neq 0$ and $\widehat{F}(k) \neq 0$ are assumed to be known and a, $\widehat{\mu}$ and $\widehat{\delta}$ need to be estimated.
Assume that $(\widehat{\delta}_n, \widehat{\mu}_n, a_n)$ is the best estimation obtained using the first n values of $(X_k^{diff})_{k \in \mathbb{N}}$. Then the sequence $(\ln \widehat{\delta}_k, \widehat{\mu}_k, a_k)_{k \in \mathbb{N}}$ is asymptotically normally distributed. Furthermore one can estimate these parameters with arbitrary precision out of the $(X_k^{diff})_{k \in \mathbb{N}}$ if one chooses n big enough.

Proof

Reformulated we may say that the $\widehat{X}_k^{diff}$ are described by

$$\widehat{X}_k^{diff} = \left(\widehat{\delta} k^{\widehat{\mu}} \exp\left(ak^{\beta}\right) \widehat{F}(k)\right) |\varepsilon_k|$$

where ε_k is independently $\mathcal{N}(1, \sigma^2)$ distributed for some $\sigma > 0$. This yields

$$\ln\left(\frac{\widehat{X}_k^{diff}}{\widehat{F}(k)}\right) = \ln(\widehat{\delta}) + \widehat{\mu}\ln(k) + ak^{\beta} + \ln|\varepsilon_k|$$

Note that the expectation of $\ln|\varepsilon_k|$ is finite, because we have:

$$\begin{aligned}
0 < \mathbb{E}\ln|\varepsilon_k| &= \int_{-\infty}^{\infty} \ln|x| \left(\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-1)^2}{2\sigma^2}\right)\right) dx \\
&\leq -\int_{-\infty}^{-1} x \left(\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-1)^2}{2\sigma^2}\right)\right) dx \\
&\quad + \int_{-1}^{1} \ln|x| \frac{1}{\sigma\sqrt{2\pi}} dx \\
&\quad + \int_{1}^{\infty} x \left(\frac{1}{\sigma\sqrt{2\pi}} \exp\left(-\frac{(x-1)^2}{2\sigma^2}\right)\right) dx \\
&< \infty
\end{aligned}$$

Equivalently one can show that all other moments are finite as well. (The same and also the following considerations would hold for many other possible distributions, as long as for each moments there is a bound independent of k).
Now set $\overline{X}_k^{diff} = \ln\left(\frac{\widehat{X}_k^{diff}}{\widehat{F}(k)}\right)$, $\overline{\delta} = \ln\widehat{\delta} + \mathbb{E}\ln|\varepsilon_k|$ and $\overline{\varepsilon}_k = \ln|\varepsilon_k| - \mathbb{E}\ln|\varepsilon_k|$ which is independently identically distributed around 0 with finite variance σ_{ε}. Hence we get

$$\overline{X}_k^{diff} = \overline{\delta} + \widehat{\mu}\ln(k) + ak^{\beta} + \overline{\varepsilon}_k$$

This defines a three dimensional system of n linear equations, namely

$$x_n = \mathbf{w}_n \begin{pmatrix} \overline{\delta}_n \\ \widehat{\mu}_n \\ a_n \end{pmatrix}$$

where

$$\mathbf{w}_n = \begin{pmatrix} 1 & \ln 1 & 1^\beta \\ 2 & \ln 2 & 2^\beta \\ \vdots & \vdots & \vdots \\ i & \ln i & i^\beta \\ \vdots & \vdots & \vdots \\ n & \ln n & n^\beta \end{pmatrix} \qquad \text{and} \qquad x_n = \begin{pmatrix} \overline{X}_1^{diff} \\ \overline{X}_2^{diff} \\ \vdots \\ \overline{X}_i^{diff} \\ \vdots \\ \overline{X}_n^{diff} \end{pmatrix}$$

Now we have the following two properties [DS81]:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\begin{pmatrix} \overline{\delta}_n & \widehat{\mu}_n & a_n \end{pmatrix}^T\right) = \left(\mathbf{w}_n^T \mathbf{w}_n\right)^{-1} \mathbf{w}_n^T x_n$$

and

$$\mathbb{E}_{\xi_1-\xi_2}\left(\begin{pmatrix} \overline{\delta}_n & \widehat{\mu}_n & a_n \end{pmatrix}^T \begin{pmatrix} \overline{\delta}_n & \widehat{\mu}_n & a_n \end{pmatrix}\right) = \sigma_\varepsilon^2 \left(\mathbf{w}_n^T \mathbf{w}_n\right)^{-1}$$

Define:

$$\begin{aligned}
C_{n^3} &= \sum_{k=1}^{n} k^2 && \asymp n^3 \\
C_{n^2 \ln n} &= \sum_{k=1}^{n} k \ln k && \asymp n^2 \ln n \\
C_{n^{\beta+2}} &= \sum_{k=1}^{n} k^{\beta+1} && \asymp n^{\beta+2} \\
C_{n \ln^2 n} &= \sum_{k=1}^{n} (\ln k)^2 && \asymp n \ln^2 n \\
C_{n^{\beta+1} \ln n} &= \sum_{k=1}^{n} k^\beta \ln k && \asymp n^{\beta+1} \ln n \\
C_{n^{2\beta+1}} &= \sum_{k=1}^{n} k^{2\beta} && \asymp n^{2\beta+1}
\end{aligned}$$

Then we have

$$\mathbf{w}_n^T \mathbf{w}_n = \begin{pmatrix} C_{n^3} & C_{n^2 \ln n} & C_{n^{\beta+2}} \\ C_{n^2 \ln n} & C_{n \ln^2 n} & C_{n^{\beta+1} \ln n} \\ C_{n^{\beta+2}} & C_{n^{\beta+1} \ln n} & C_{n^{2\beta+1}} \end{pmatrix}$$

Using *Maple* we get:

$$(\mathbf{w}_n^T\mathbf{w}_n)^{-1} = \frac{1}{\overline{C}_{n^{5+2\beta}\ln^2 n}} \begin{pmatrix} \overline{C}_{n^{2+2\beta}\ln^2 n} & \overline{C}_{n^{3+2\beta}\ln n} & \overline{C}_{n^{3+\beta}\ln^2 n} \\ \overline{C}_{n^{3+2\beta}\ln n} & \overline{C}_{n^{4+2\beta}} & \overline{C}_{n^{4+\beta}\ln n} \\ \overline{C}_{n^{3+\beta}\ln^2 n} & \overline{C}_{n^{4+\beta}\ln n} & \overline{C}_{n^4\ln^2} \end{pmatrix}$$

where the $\overline{C}_{G(n)}$ denote functions which behave asymptotically as $G(n)$, respectively. Furthermore using *Maple* we obtain that $(\mathbf{w}_n^T\mathbf{w}_n)^{-1}$ is positive definite. Hence $\mathbb{E}_{\xi_1-\xi_2}\left(\left(\overline{\delta}_n \;\; \widehat{\mu}_n \;\; a_n\right)^T \left(\overline{\delta}_n \;\; \widehat{\mu}_n \;\; a_n\right)\right)$ is decreasing with at least $\frac{\ln^2 n}{n}$ for an increasing number n of observables and the sequence of estimations for $\left(\overline{\delta}_n, \widehat{\mu}_n, a_n\right)$ is asymptotically normally distributed [BD96, DS81].
This yields the proposition. q.e.d.

Remark

Note that there is an obvious adaptation to the non-severely ill-posed case. There we can set $a = 0$ right from the beginning and get a slightly simpler version of the above lemma.

Lemma 5.24

Assume

$$\widehat{X}_k^{diff} = \widehat{\delta} k^{\widehat{\mu}} \widehat{F}(k)$$

where $\widehat{F}(k) \neq 0$ *is assumed to be known and* $\widehat{\mu}$ *and* $\widehat{\delta}$ *need to be estimated.*
Assume that $(\widehat{\delta}_n, \widehat{\mu}_n)$ *is the best estimation obtained using the first* n *values of* $(X_k^{diff})_{k\in\mathbb{N}}$. *Then the sequence* $(\ln \widehat{\delta}_k, \widehat{\mu}_k)_{k\in\mathbb{N}}$ *is asymptotically normally distributed. Furthermore one can estimate these parameters with arbitrary precision out of the* $(X_k^{diff})_{k\in\mathbb{N}}$ *if one chooses* n *big enough.*

Proof

Reformulated we may say that the $\widehat{X}_k^{diff}$ are described by

$$\widehat{X}_k^{diff} = \left(\widehat{\delta} k^{\widehat{\mu}} \widehat{F}(k)\right) |\varepsilon_n|$$

where ε_k is independently $\mathcal{N}(1, \sigma^2)$ distributed for some $\sigma > 0$. This yields

$$\ln\left(\frac{\widehat{X}_k^{diff}}{\widehat{F}(k)}\right) = \ln(\widehat{\delta}) + \widehat{\mu}\ln(k) + \ln|\varepsilon_k|$$

Again we may set $\overline{X}_k^{diff} = \ln\left(\frac{\widehat{X}_k^{diff}}{\widehat{F}(k)}\right)$, $\overline{\delta} = \ln\widehat{\delta} + \mathbb{E}\ln|\varepsilon_k|$ and $\overline{\varepsilon}_k = \ln|\varepsilon_k| - \mathbb{E}\ln|\varepsilon_k|$ which is independently identically distributed around 0 with finite variance σ_ε. Hence we get

$$\overline{X}_k^{diff} = \overline{\delta} + \widehat{\mu}\ln(k) + \overline{\varepsilon}_k$$

This defines a two dimensional system of n linear equations, namely

$$x_n = \mathbf{w}_n \begin{pmatrix} \overline{\delta} \\ \widehat{\mu}_n \end{pmatrix}$$

where

$$\mathbf{w}_n = \begin{pmatrix} 1 & \ln 1 \\ 2 & \ln 2 \\ \vdots & \vdots \\ i & \ln i \\ \vdots & \vdots \\ n & \ln n \end{pmatrix} \qquad \text{and} \qquad x_n = \begin{pmatrix} \overline{X}_1^{diff} \\ \overline{X}_2^{diff} \\ \vdots \\ \overline{X}_i^{diff} \\ \vdots \\ \overline{X}_n^{diff} \end{pmatrix}$$

Again we have the following two properties [DS81]:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\begin{pmatrix}\overline{\delta}_n & \widehat{\mu}_n\end{pmatrix}^T\right) = \left(\mathbf{w}_n^T\mathbf{w}_n\right)^{-1}\mathbf{w}_n^T x_n$$

and

$$\mathbb{E}_{\xi_1-\xi_2}\left(\begin{pmatrix}\overline{\delta}_n & \widehat{\mu}_n\end{pmatrix}^T\begin{pmatrix}\overline{\delta}_n & \widehat{\mu}_n\end{pmatrix}\right) = \sigma_\varepsilon^2\left(\mathbf{w}_n^T\mathbf{w}_n\right)^{-1}$$

Defining the $C_{G(n)}$ as beforehand we get:

$$\mathbf{w}_n^T\mathbf{w}_n = \begin{pmatrix} C_{n^3} & C_{n^2\ln n} \\ C_{n^2\ln n} & C_{n\ln^2 n} \end{pmatrix}$$

Using *Maple* we get:

$$\left(\mathbf{w}_n^T\mathbf{w}_n\right)^{-1} = \frac{1}{\overline{C}_{n^4\ln^2}}\begin{pmatrix} \overline{C}_{n\ln^2 n} & \overline{C}_{n^2\ln n} \\ \overline{C}_{n^2\ln n} & \overline{C}_{n^3} \end{pmatrix}$$

where the $\overline{C}_{G(n)}$ denote functions which behaves asymptotically as $G(n)$, respectively. Furthermore using *Maple* we obtain that $(\mathbf{w}_n^T\mathbf{w}_n)^{-1}$ is positive definite. Hence $\mathbb{E}_{\xi_1-\xi_2}\left(\begin{pmatrix}\overline{\delta}_n & \widehat{\mu}_n\end{pmatrix}^T\begin{pmatrix}\overline{\delta}_n & \widehat{\mu}_n\end{pmatrix}\right)$ is decreasing with at least $\frac{\ln^2 n}{n}$ for an increasing number n of observables and the sequence of estimations for $\left(\overline{\delta}_n, \widehat{\mu}_n\right)$ is asymptotically normally distributed [BD96, DS81].

This yields the proposition. q.e.d.

Remark

As we have seen in both theorems we can estimate the values we need as exactly as we want. In particular the variance of our approximation is tending to zero.

Using the above remark the following lemmas gets especially interesting:

Lemma 5.25

Let the k-vector x_n be asymptotically normally distributed $\mathcal{AN}(\overline{x}, c_n^2\Sigma_n)$, where

- Σ_n *is symmetric and positive definite.*
- $||\Sigma_n||_2 = 1$ *and* $\lim_{n\to\infty}\Sigma_n = \Sigma$ *which is also symmetric and positive definite.*
- $\lim_{n\to\infty} c_n = 0$

Let furthermore $G : \mathbb{R}^k \to \mathbb{R}$ be a smooth function around $\overline{x}$ with derivative $\mathbf{d} = (\frac{\partial g}{\partial_i})_{i=1\ldots k}(\overline{x})$. If $\mathbf{d}^T\Sigma\mathbf{d}$ is non-zero, then we have:
$G(x_n)$ is $\mathcal{AN}(G(\overline{x}), c_n^2\mathbf{d}^T\Sigma_n\mathbf{d})$.

This is a slightly modified version of a theorem which can be found in [BD96].

When we denote the estimates for δ, μ (and a) which we get out of the first n of the $(X_k^{diff})_{k\in\mathbb{N}}$ by δ_n, μ_n (and a_n) this yields the following corollary.

Corollary 5.26

(δ_n, μ_n, a_n) (respectively (δ_n, μ_n) for the ordinarily ill-posed case) are asymptotically normal distributed with variances tending to 0.

For every of the estimates δ_n, μ_n (and a_n which we just have in the severely ill-posed case) we get a specific χ, namely χ_n. Using the inequalities we have obtained beforehand for χ we now get the following bounds which are again depending of the level of approximation n:

Corollary 5.27

In the case, where

$$\begin{aligned}\left(1-\lambda_1^1\delta_{diff,n}\right)^2\left(1-\lambda_2^1\mu_{diff,n}\right)\left(1-\lambda_3^1 a_{diff,n}\right) &\leq \chi_n \\ \leq \left(1+\lambda_1^2\delta_{diff,n}\right)^2\left(1+\lambda_2^2\mu_{diff,n}\right)\left(1+\lambda_3^2 a_{diff,n}\right)&\end{aligned}$$

the bounds for χ_n and χ_n^{-1} are asymptotically normally distributed where the variances are tending to 0. This also holds when a is assumed to be known (e.g., normally ill-posed case) and hence $a_{diff,n} = a_{diff} = 0$.

This gets especially useful because of the following lemma:

Lemma 5.28

For every constant $c_2 > 0$ there exists an n_0 such that for all $n > n_0$ every member χ_n of the sequence $(\chi_n)_{n\in\mathbb{N}}$ fulfills for $\tau > 1$:

$$\mathbb{P}_{\xi_1-\xi_2}\{\chi_n > \tau\} \leq c_1 \exp\left(-c_2\left(\tau - 1\right)\right)$$

and

$$\mathbb{P}_{\xi_1-\xi_2}\{\chi_n^{-1} > \tau\} \leq c_1 \exp\left(-c_2\left(\tau - 1\right)\right)$$

Furthermore c_1 is globally bounded from above.

Proof

The bounds of χ_n are asymptotically normal distributed with variances tending to 0. The result is now a straightforward consequence of Bernstein's inequality [Bos96] which holds because of the behavior of the moments for an (asymptotically) normal distribution [JK77]. q.e.d.

Remark

The result is quite natural because variances tending to 0 means that the distributions tend to the Dirac distribution, the property asymptotically normal implies that the higher moments are behaving not too bad, i.e. the function is falling fast enough.

From now on we choose a $\chi = \chi_n$ such that the constant c_2 is high enough for the subsequent theorems.

This yields the following remarkable theorem combining the results of the regularization theorems, the estimation of χ and the last results.

Please note that the variable χ in these theorems was introduced as completely independent from all other quantities. This holds in particular for the error in the input data.

5.3.1 Ordinary Ill-Posed Case

Theorem 5.29

Assume that we are in the stochastic noise case and furthermore that our problem is not severely ill-posed, i.e., we have $\ln\frac{1}{u} \asymp \ln\rho^{-1}(u)$. (i.e., there exist constants μ_1 and μ_2 such that $\mu_1\ln\frac{1}{u} \leq \ln\rho^{-1}(u) \leq \mu_2\ln\frac{1}{u}$).

We assume three non-regularized input data sets Z, Z_1 and Z_2 as given, which are biased in the same way. Assume furthermore that Z_1 is uncorrelated to Z_2 and $Z_1 - Z_2$ is uncorrelated to Z which is the input we want to regularize.

Assume for our convenience that $\rho(n) = n^{-\mu}$, at least asymptotically.

Then denote the estimates we got from the last theorems for δ as $\tilde{\delta}$ and for μ as $\tilde{\mu}$; there exists an approximation level which is sufficiently high to guarantee the later result (see proof of this theorem). Using $\tilde{\mu}$ we get an estimated version $\tilde{\rho}(n)$.
If δ is small enough one can choose $\kappa = 4\sqrt{p \ln \tilde{\rho}^{-1}(\tilde{\delta})}$ and p such that we have $2^{\frac{11}{2}}(\tilde{\rho}^{-1}(\tilde{\delta}))^{-p+1} = \tilde{\delta}^2$.
Now choose the cutting point as :

$$n_* = \min\left\{ n: \; ||X_n - X_m|| \leq \frac{4\kappa\tilde{\delta}}{\tilde{\rho}(m)}, \; N = \tilde{\rho}^{-1}(\tilde{\delta}) > m > n \right\}$$

Then we have for δ small enough:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2\right) \leq \overline{C} \ln \delta^{-1} \psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

for an appropriate constant $\overline{C}$.

Proof

The noise on Z is uncorrelated to the one on $Z_1 - Z_2$ and hence the noise on $X_{1,m} - X_{2,m}$ is uncorrelated to the one on X_n which implies that the noise on X_n, i.e. η^ξ_n is *uncorrelated* to χ holding for all pairs (n, m).
χ was just considered as an arbitrary variable in the theorems estimating $\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2$. Hence using the uncorrelatedness to ξ we can consider the following term which is an expectation in $\xi_1 - \xi_2$ and so in χ:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2\right) \leq \mathbb{E}_{\xi_1-\xi_2}\left(\Pi(\chi)\right)$$

where the function $\Pi(\chi)$ is defined as

$$\Pi(\chi) = C\delta^2\delta^{-c\left(1-\chi^2\right)} + C\chi^2\left(\ln\delta^{-1}\right)\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

as in the theorem estimating $\mathbb{E}_\xi ||X - X^\delta_{n_*}||^2$ in the ordinarily ill-posed case where $c = \mu_2 \frac{1+\frac{2}{\mu_1}}{1+\frac{2}{\mu_2}} > 0$.
In order to have an easier access to the separate parts of $\Pi(\chi)$ we define:

$$\Pi_1(\chi) = \delta^{-c\left(1-\chi^2\right)}$$
$$\Pi_2(\chi) = \chi^2$$

and hence

$$\Pi(\chi) = C\delta^2\,\Pi_1(\chi) + C\left(\ln\delta^{-1}\right)\psi^2\left((\psi\rho)^{-1}(\delta)\right)\Pi_2(\chi)$$

For technical reasons we choose an $\varepsilon > 0$, such that $\psi((\psi\rho)^{-1}(\delta))$ is decreasing at least as fast as $\delta^{1-\varepsilon/2}$ which we will use later on.

Now we want to get an estimate for

$$
\begin{aligned}
&\mathbb{E}_{\xi_1-\xi_2}\left(\Pi(\chi)\right)\\
&\quad=\int_0^\infty \Pi\left(\tau\right) d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}\\
&\quad=C\delta^2\int_0^\infty \Pi_1(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}\\
&\qquad+C\left(\ln\delta^{-1}\right)\psi^2\left(\left(\psi\rho\right)^{-1}(\delta)\right)\int_0^\infty \Pi_2(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}
\end{aligned}
$$

So it suffices to estimate the parts $\int_0^\infty \Pi_\boxdot(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}$ separately ($\delta<1$ is assumed to hold!). We furthermore require the parameter $\alpha=\left(\sqrt{1-\frac{\varepsilon}{c}}\right)^{-1}>1$ which is chosen such that $\Pi_1(\alpha^{-1})=\delta^{-\varepsilon}$

$$
\begin{aligned}
&\int_0^\infty \Pi_1(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}\\
&\qquad=\int_\infty^0 \Pi_1(\tau^{-1})d\mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\\
&\qquad=\Pi_1\left(\tau^{-1}\right)\mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\Big|_\infty^0\\
&\qquad\quad-\int_\infty^0 \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}d\Pi_1(\tau^{-1})\\
&\qquad=0-0+\int_0^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}d\Pi_1(\tau^{-1})\\
&\qquad=\int_0^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\frac{\partial}{\partial\tau}\Pi_1(\tau^{-1})d\tau\\
&\qquad\le\int_0^\alpha \frac{\partial}{\partial\tau}\Pi_1(\tau^{-1})d\tau\\
&\qquad\quad+\int_\alpha^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}2c\left(\ln\delta^{-1}\right)\tau^{-3}\delta^{-c\left(1-\tau^{-2}\right)}d\tau\\
&\qquad=\Pi_1(\alpha^{-1})-0\\
&\qquad\quad+2c\left(\ln\delta^{-1}\right)\int_\alpha^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\tau^{-3}\delta^{-c\left(1-\tau^{-2}\right)}d\tau\\
&\qquad\le\delta^{-\varepsilon}+2c\left(\ln\delta^{-1}\right)\int_\alpha^\infty c_1\exp\left(-c_2\left(\tau-1\right)\right)\tau^{-3}\delta^{-c\left(1-\tau^{-2}\right)}d\tau\\
&\qquad\le\delta^{-\varepsilon}+2c\,c_1\left(\ln\delta^{-1}\right)\delta^{-c(1-0)}\int_\alpha^\infty \exp\left(-c_2\left(\tau-1\right)\right)d\tau\\
&\qquad=\delta^{-\varepsilon}+2c\,c_1\left(\ln\delta^{-1}\right)\delta^{-c}c_2^{-1}\exp\left(-c_2\left(\alpha-1\right)\right)\\
&\qquad\le\delta^{-\varepsilon}+\widehat{C}\\
&\qquad\le\widetilde{C}\delta^{-\varepsilon}
\end{aligned}
$$

where $\widehat{C}$ and hence $\widetilde{C}$ are constants which can be bounded intendant of δ because we are free to choose c_2 as high as we want, like remarked beforehand.

The second term can be evaluated in a similar way:

$$
\begin{aligned}
&\int_0^\infty \Pi_2(\tau) d\mathbb{P}_{\xi_1-\xi_2}\{\chi < \tau\} \\
&\qquad = \int_0^\infty \tau^2 d\left(1 - \mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\}\right) \\
&\qquad = -\int_0^\infty \tau^2 d\mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\} \\
&\qquad = -\tau^2 \mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\}\big|_0^\infty + \int_0^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\} d\tau^2 \\
&\qquad =0 - 0 + \int_0^\infty 2\tau \mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\} d\tau \\
&\qquad = \int_0^2 2\tau \mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\} d\tau + \int_2^\infty 2\tau \mathbb{P}_{\xi_1-\xi_2}\{\chi > \tau\} d\tau \\
&\qquad \leq \int_0^2 2\tau d\tau + \int_2^\infty 2\tau c_1 \exp\left(-c_2\left(\tau - 1\right)\right) d\tau \\
&\qquad =4 + 2c_1 c_2^{-2}(1 + 2c_2)\exp\left(-c_2\right) \\
&\qquad \leq \widetilde{C}
\end{aligned}
$$

which can be assured when c_2 is chosen big enough.
Hence we get using these results:

$$
\begin{aligned}
&\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_\xi ||X - X_{n_*}^\delta||^2\right) \\
&\quad =C\delta^2 \int_0^\infty \Pi_1(\tau) d\mathbb{P}_{\xi_1-\xi_2}\{\chi < \tau\} \\
&\qquad + C\left(\ln \delta^{-1}\right) \psi^2\left(\left(\psi\rho\right)^{-1}\left(\delta\right)\right) \int_0^\infty \Pi_2(\tau) d\mathbb{P}_{\xi_1-\xi_2}\{\chi < \tau\} \\
&\quad \leq C\delta^2 \widetilde{C}\delta^{-\varepsilon} + C\left(\ln \delta^{-1}\right) \psi^2\left(\left(\psi\rho\right)^{-1}\left(\delta\right)\right) \widetilde{C} \\
&\quad =C\widetilde{C}\delta^{2-\varepsilon} + C\widetilde{C}\left(\ln \delta^{-1}\right) \psi^2\left(\left(\psi\rho\right)^{-1}\left(\delta\right)\right) \\
&\quad \leq \overline{C}\left(\ln \delta^{-1}\right) \psi^2\left(\left(\psi\rho\right)^{-1}\left(\delta\right)\right)
\end{aligned}
$$

The last inequality holds because we chose ε in such a way that $\delta^{1-\varepsilon/2}$ decreases at least as fast as $\psi\left(\left(\psi\rho\right)^{-1}\left(\delta\right)\right)$. The whole inequality is exactly our assertion which consequently holds. q.e.d.

5.3.2 Severely Ill-Posed Case

The theorem and the proof are analogous to the ordinary ill-posed case:

Theorem 5.30

Assume that our problem is severely ill-posed with stochastical noise and polynomial smoothness of the solution ψ.

We assume three non-regularized input data sets Z, Z_1 and Z_2 as given, which are biased in the same way. Assume furthermore that Z_1 is uncorrelated to Z_2 and $Z_1 - Z_2$ is uncorrelated to Z which is the input we want to regularize.
Assume for our convenience that $\rho(n) = n^{-\mu}\exp(an^{\beta})$, at least asymptotically, β shall be known exactly.
Then denote the estimates we got from the last theorems for δ as $\tilde{\delta}$, for μ as $\tilde{\mu}$ and for a as $\tilde{a}$; there exists an approximation level which is sufficiently high to guarantee the later result (see proof of this theorem). Using $\tilde{\mu}$ and $\tilde{a}$ we get an estimated version $\tilde{\rho}(n)$.
If δ is small enough one can choose $\kappa = 4\ln\ln\tilde{\delta}^{-1}$
Now choose the cutting point as :

$$n_* = \min\left\{n: \ ||X_n - X_m|| \leq \frac{4\kappa\tilde{\delta}}{\tilde{\rho}(m)}, \ N = \tilde{\rho}^{-1}(\tilde{\delta}) > m > n\right\}$$

Then we have for δ small enough:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_{\xi}||X - X^{\delta}_{n_*}||^2\right) \leq \overline{C}\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

for an appropriate constant $\overline{C}$.

Proof

The noise on Z is uncorrelated to the one on $Z_1 - Z_2$ and hence the noise on $X_{1,m} - X_{2,m}$ is uncorrelated to the one on X_n which implies that the noise on X_n, i.e. η^{ξ}_n is *uncorrelated* to χ holding for all pairs (n, m).
χ was just considered as an arbitrary variable in the theorems estimating $\mathbb{E}_{\xi}||X - X^{\delta}_{n_*}||^2$. Hence using the uncorrelatedness to ξ we can consider the following term which is an expectation in $\xi_1 - \xi_2$ and so in χ:

$$\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_{\xi}||X - X^{\delta}_{n_*}||^2\right) \leq \mathbb{E}_{\xi_1-\xi_2}\left(\Pi(\chi)\right)$$

where the function $\Pi(\chi)$ is defined as

$$\Pi(\chi) = C\left(\ln\delta^{-1}\right)^{\frac{1}{\beta}-\chi^2\ln\ln\delta^{-1}} + \chi^2\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)$$

as in the theorem estimating $\mathbb{E}_{\xi}||X - X^{\delta}_{n_*}||^2$ in the severely ill-posed case.
In the severely ill-posed case we have that $(\ln\delta^{-1})^{-\frac{r}{\beta}}$ is descending at least as fast as $\psi((\psi\rho)^{-1}(\delta))$. Now, as in the ordinarily ill-posed case we introduce functions $\Pi_{\boxdot}$:

$$\Pi_1(\chi) = \left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}-\chi^2\ln\ln\delta^{-1}}$$
$$\Pi_2(\chi) = \chi^2$$

and hence

$$\Pi(\chi) = C\left(\ln\delta^{-1}\right)^{-2\frac{r}{\beta}}\ \Pi_1(\chi) + C\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)\ \Pi_2(\chi)$$

Now we want to get an estimate for

$$\begin{aligned}
&\mathbb{E}_{\xi_1-\xi_2}\left(\Pi(\chi)\right)\\
&\quad=\int_0^\infty \Pi(\tau)\, d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}\\
&\quad=C\left(\ln\delta^{-1}\right)^{-2\frac{r}{\beta}}\int_0^\infty \Pi_1(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}\\
&\qquad+C\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)\int_0^\infty \Pi_2(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}
\end{aligned}$$

So it suffices to estimate the parts $\int_0^\infty \Pi_\boxdot(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}$ separately. We will now assume δ to be small enough, i.e. such that $\ln\ln\delta^{-1}>1$ and furthermore $2\frac{r}{\beta}+\frac{1}{\beta}-\frac{1}{4}\ln\ln\delta^{-1}<0$ and hence get:

$$\begin{aligned}
&\int_0^\infty \Pi_1(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\}\\
&\qquad=\int_\infty^0 \Pi_1(\tau^{-1})d\mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\\
&\qquad=\Pi_1\left(\tau^{-1}\right)\mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\Big|_\infty^0\\
&\qquad\quad-\int_\infty^0 \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}d\Pi_1(\tau^{-1})\\
&\qquad=0-0+\int_0^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}d\Pi_1(\tau^{-1})\\
&\qquad=\int_0^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\frac{\partial}{\partial\tau}\Pi_1(\tau^{-1})d\tau\\
&\qquad\le\int_0^2 \frac{\partial}{\partial\tau}\Pi_1(\tau^{-1})d\tau\\
&\qquad\quad+\int_2^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\\
&\qquad\qquad\qquad 2\left(\ln\ln\delta^{-1}\right)^2\tau^{-3}\left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}-\tau^{-2}\ln\ln\delta^{-1}}d\tau\\
&\qquad\le\Pi_1\left(\frac{1}{2}\right)-0\\
&\qquad\quad+2\left(\ln\ln\delta^{-1}\right)^2\left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}-0\ln\ln\delta^{-1}}\\
&\qquad\qquad\qquad\int_2^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\tau^{-3}d\tau
\end{aligned}$$

$$
\begin{aligned}
&\leq \left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}-\frac{1}{4}\ln\ln\delta^{-1}} \\
&\quad + 2\left(\ln\ln\delta^{-1}\right)^2\left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}-0\ln\ln\delta^{-1}} \\
&\qquad\qquad \int_2^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi^{-1}>\tau\}\tau^{-3}d\tau \\
&\leq 1+2\left(\ln\ln\delta^{-1}\right)^2\left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}} \\
&\qquad\qquad \int_2^\infty c_1\exp\left(-c_2\left(\tau-1\right)\right)\tau^{-3}d\tau \\
&\leq 1+2\left(\ln\ln\delta^{-1}\right)^2\left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}}\int_2^\infty c_1\exp\left(-c_2\left(\tau-1\right)\right)d\tau \\
&\leq 1+2\left(\ln\ln\delta^{-1}\right)^2\left(\ln\delta^{-1}\right)^{2\frac{r}{\beta}+\frac{1}{\beta}}c_1c_2^{-1}\exp(-c_2) \\
&\leq \widetilde{C}
\end{aligned}
$$

where $\widetilde{C}$ is a constant which can be bounded intendant of δ because we are free to choose c_2 as high as we want, like remarked beforehand.
The second term can be evaluated in a similar way:

$$
\begin{aligned}
&\int_0^\infty \Pi_2(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\} \\
&\qquad = \int_0^\infty \tau^2 d\left(1-\mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\}\right) \\
&\qquad = -\int_0^\infty \tau^2 d\mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\} \\
&\qquad = -\tau^2\mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\}\Big|_0^\infty + \int_0^\infty \mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\}d\tau^2 \\
&\qquad = 0-0+\int_0^\infty 2\tau\mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\}d\tau \\
&\qquad = \int_0^2 2\tau\mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\}d\tau + \int_2^\infty 2\tau\mathbb{P}_{\xi_1-\xi_2}\{\chi>\tau\}d\tau \\
&\qquad \leq \int_0^2 2\tau d\tau + \int_2^\infty 2\tau c_1\exp\left(-c_2\left(\tau-1\right)\right)d\tau \\
&\qquad = 4+2c_1c_2^{-2}(1+2c_2)\exp\left(-c_2\right) \\
&\qquad \leq \widetilde{C}
\end{aligned}
$$

which can be assured when c_2 is chosen big enough.
Hence we get using these results:

$$
\begin{aligned}
&\mathbb{E}_{\xi_1-\xi_2}\left(\mathbb{E}_\xi||X-X_{n_*}^\delta||^2\right) \\
&\quad = C\left(\ln\delta^{-1}\right)^{-2\frac{r}{\beta}}\int_0^\infty \Pi_1(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\} \\
&\qquad + C\left(\ln\ln\delta^{-1}\right)^2\psi^2\left((\psi\rho)^{-1}(\delta)\right)\int_0^\infty \Pi_2(\tau)d\mathbb{P}_{\xi_1-\xi_2}\{\chi<\tau\} \\
&\quad \leq C\left(\ln\delta^{-1}\right)^{-2\frac{r}{\beta}}\widetilde{C}
\end{aligned}
$$

$$
\begin{aligned}
&+ C \left(\ln\ln\delta^{-1}\right)^2 \psi^2 \left((\psi\rho)^{-1}(\delta)\right) \widetilde{C} \\
\leq &\overline{C} \left(\ln\ln\delta^{-1}\right) \psi^2 \left((\psi\rho)^{-1}(\delta)\right)
\end{aligned}
$$

The last inequality holds because $(\ln\delta^{-1})^{-\frac{r}{\beta}}$ is descending at least as fast as the term $\psi((\psi\rho)^{-1}(\delta))$. This whole inequality is exactly our assertion which consequently holds. q.e.d.

Remark

The usage of three different input data sets Z_1, Z_2 and additionally Z in reality is inconvenient and impracticable. However we propose the following way out of this dilemma.
We use the following property of $Z := \frac{1}{2}(Z_1 + Z_2)$:

$$\mathbb{E}\langle Z_1 - Z_2, Z\rangle = \frac{1}{2}\left(\mathbb{E}||Z_1||^2 - \mathbb{E}||Z_2||^2\right) = 0$$

because we assumed the same distribution for the Z_1 and Z_2.
This implies that as long as Z_1 and Z_2 are biased with Gaussian white noise that Z and $Z_1 - Z_2$ are uncorrelated.
Because we are dealing with linear problems the computation of $\frac{1}{2}(Z_1 + Z_2)$, $Z_1 - Z_2$ and the corresponding regularized solutions can be done in a negligible time out of the ones of Z_1 and Z_2. Although the above argument is not rigorous the proposal seems to be the method of choice.

5.4 Conclusion

Now we want to summarize the results of this chapter shortly and explain their relevance to our satellite missions. We could show the following points:

- It is reasonable to assume that our data in the frequency domain are biased with stochastical noise rather than deterministic noise. Our regularization method has to be suitable for this harder case.
- Out of one set of spectral data one cannot get an optimal regularization. (Lemma of Bakushinskii).
- If one adds some knowledge to one set of spectral data (e.g., error behavior) one can get an optimal regularization.
- Out of two sets of spectral data one can get a reasonable estimate on the overall error and error behavior in the spectral data.
- Using such an error model we obtain a regularization procedure which is asymptotically near to optimal, even under the hard assumption of stochastical noise.

This means in particular that we were able to obtain the results we demanded in the begin of the chapter.

Chapter 6

Combining Data in a Unified Setup

How can one combine data from different sources , e.g., different differential components of the satellite and/or different measurement campaigns, in a sensible way? What conditions do we have to impose on the data?

Of course, one can calculate a solution for each input data set and afterwards just averaging the results. However, this does not need to be the most efficient method and does not necessarily possess a good behavior towards measurement errors. If we want to do it otherwise we are facing two major problems:

- Different satellites are flying at different heights with different (unknown) error levels in their measurements. Therefore it is at least problematic to combine these data without preprocessing.
- Not every differential component one can choose actually yields the possibility to do a complete reconstruction of the geopotential field, i.e., the differential maps some non-zero functions to zero and hence we have a non-zero kernel.

6.1 Order of the Solution Scheme

In the face of the above obstacles we have to decide in what order we will have to do the following solution steps:

- Approximation of data at the height of the satellite track.
- Inverting the differentiation operator (integration).
- Downward-continuation.
- Data combination.

6.1.1 Approximation

As any other mathematical task including integration and downward-continuation requires data in the spectral domain as input in our ansatz we need to transform the discrete input data to a spectral version. This solution of the oblique boundary value problem (if at Earth's height) or oblique satellite problem (if at satellite height) has to be done by approximation with an appropriate system of trial functions.

We explicitly do not want to mix the approximation process with integration or downward-continuation. So we have to perform this step at first place. As a result we get differentiated data in spectral representation.

6.1.2 Downward-Continuation

There are two major arguments which strongly recommend that we should do the downward-continuation directly after the approximation step.

- After the downward continuation all data are all on the Earth's and hence the *same* surface Σ and as a consequence much easier to combine.
- The total error level gets smaller. This is due to the following simplified argument: (just given as an illustration, a more rigorous treatment of the background in functional analysis can be found in the preceding chapter)

  We are dealing with a severely ill posed problem, hence an error level of δ results (asymptotically) in an error level of $(\ln(\delta^{-1}))^{-k}$ after regularization. For convenience assume $k = 1$. (Similar arguments will hold for any other k and for non-severely ill-posed problems). Assume that we are having 4 independent data sets with error level δ.

  If we combine them beforehand, our error level will get $\delta/2$ before and $(\ln 2 + \ln(\delta^{-1}))^{-1}$ after regularization. In comparison, a combination afterwards will yield an error level of $(2\ln(\delta^{-1}))^{-1}$ which is almost twice as good if δ is not extremely large.

6.1.3 Integration

Obviously, the integration now needs to be done in the last place. This has the particular advantage that this is the first place, where we actually need to take care if our differential operator $\mathfrak{D}$ has a non-zero kernel because we were just dealing with ordinary functions beforehand.

6.2 The Combination

Our situation is the following, now: We assume that we have approximated and regularized data given at the height of the Earth's surface Σ. The data are assumed to be given in the spectral domain, i.e., as a sum of weighted (basis) functions.

Note that differentiation and integration are linear operators. Hence if we have "incomplete" information (non-zero kernel of the operator, for example; ground based campaign over small regions) from several sources we may combine them with a least squares approach. In particular this would enable us to use differential operators which are tangential to the satellite orbit.

These remarks directly give rise to the following mathematical problem setup:

Problem 6.1

Let $\mathcal{U}$ and $(\mathcal{V}_k)_{k=1\ldots n}$ be separable Hilbert spaces and $(\mathfrak{D}_k)_{k=1\ldots n}$ be a set of continuous linear operators mapping

$$\mathfrak{D}_k : \mathcal{U} \to \mathcal{V}_k$$

Assume $V \in \mathcal{U}$ and assume that we have given the data $\mathfrak{D}_k V = Data_k \in \mathcal{V}_k$ in spectral representation for each k.
What does V look like?

Remark

In our case $\mathcal{U}$ is the space of harmonics $Pot(\overline{\Sigma_{ext}})$ and $\mathfrak{D}_k$ the set of observables, e.g., differential operators. Then the $\mathcal{V}_k$ are the corresponding Sobolev spaces. Having the $Data_k$ we want to determine the gravitational potential V.

Observe that we can rewrite the above problem in the following way (the operator $\oplus$ shall denote the Euclidean direct sum in every place):

$$\mathfrak{D}V = \begin{pmatrix} \mathfrak{D}_1 \\ \mathfrak{D}_2 \\ \vdots \\ \mathfrak{D}_n \end{pmatrix} V = \begin{pmatrix} \mathfrak{D}_1 V \\ \mathfrak{D}_2 V \\ \vdots \\ \mathfrak{D}_n V \end{pmatrix} = \begin{pmatrix} Data_1 \\ Data_2 \\ \vdots \\ Data_n \end{pmatrix} = Data$$

where the operator $\mathfrak{D} = \bigoplus_{k=1}^{n} \mathfrak{D}_k$ maps from the space $\mathcal{U}$ to the separable Hilbert space $\mathcal{V} = \bigoplus_{k=1}^{n} \mathcal{V}_k$.

$$\mathfrak{D} : \mathcal{U} \to \mathcal{V}$$

Furthermore define $Data = \bigoplus_{k=1}^{n} Data_k$.

This is obviously an overdetermined system for most cases. The standard solution technique for such kind of problems is a least squares approach (with a diagonal weight operator $\mathfrak{W}$ assigning one weight to each solution):

$$(\mathfrak{D}^T \mathfrak{W} \mathfrak{D})V = \left(\sum_{k=1}^{n} W_k \mathfrak{D}_k^T \mathfrak{D}_k \right) V = \sum_{k=1}^{n} W_k \mathfrak{D}_k^T Data_k = \mathfrak{D}^T \mathfrak{W} Data$$

Observe that this is an operator equation and hence not finite dimensional.

In order to get this approach in a finite dimensional setup we need to impose some more requirements on our original problem. The reformulated version gets:

Problem 6.2

Let $\mathcal{U}$ and $(\mathcal{V}_k)_{k=1\ldots n}$ be separable Hilbert spaces and $(\mathfrak{D}_k)_{k=1\ldots n}$ be a set of continuous linear operators mapping

$$\mathfrak{D}_k : \mathcal{U} \to \mathcal{V}_k$$

Assume $V \in \mathcal{U}$ and assume that we have given the data $\mathfrak{D}_k V = Data_k \in \mathcal{V}_k$ in spectral representation for each k.

Assume furthermore that $\mathcal{U}$, the spaces $\mathcal{V}_k$ and the operators $\mathfrak{D}_k$ decompose in the following way:

$$\mathcal{U} = \bigoplus_{m=1}^{N+1} \mathcal{U}^m \qquad \text{for all } k \in \{1, \ldots, n\}$$
$$\mathcal{V}_k = \bigoplus_{m=1}^{N+1} \mathcal{V}_k^m \qquad \text{for all } k \in \{1, \ldots, n\}$$
$$\mathfrak{D}_k = \bigoplus_{m=1}^{N+1} \mathfrak{D}_k^m \qquad \text{for all } k \in \{1, \ldots, n\}$$

such that

$$\mathfrak{D}_k^m : \mathcal{U}^m \to \mathcal{V}_k^m \qquad \text{for all } k \in \{1, \ldots, n\}$$

This implies that our data have an analogous representation:

$$Data_k = \bigoplus_{m=1}^{N+1} Data_k^m \qquad \text{for all } k \in \{1, \ldots, n\}$$

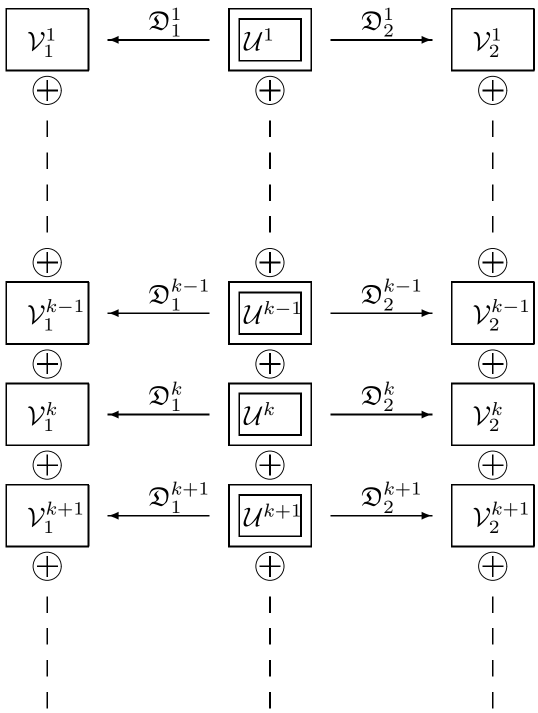
All of the spaces $\mathcal{U}^m$ and $\mathfrak{D}_k^m$ shall be finite dimensional up to N. (This immediately implies $\mathfrak{D}_k^m$ to be finite dimensional operators, i.e., matrices).

What does V look like?

Remark

In practice we can just consider finite dimensional spaces. So the last point is not a severe restriction. For our practical case a possible division along the spaces of homogeneous harmonic polynomials of same degree $\mathcal{U}^m = Harm_m$ (see [FGS98]).

Generally one can state the smaller the subdivision gets the smaller are the computational efforts. In order to get a better idea we just give a sketch about the above situation for two different operators:



Hence we can split our problem and just need to solve the following problem for *each* of the spaces $\mathcal{U}^m$.

$$\mathfrak{D}^m V = \begin{pmatrix} \mathfrak{D}_1^m \\ \mathfrak{D}_2^m \\ \vdots \\ \mathfrak{D}_n^m \end{pmatrix} V = \begin{pmatrix} \mathfrak{D}_1^m V \\ \mathfrak{D}_2^m V \\ \vdots \\ \mathfrak{D}_n^m V \end{pmatrix} = \begin{pmatrix} Data_1^m \\ Data_2^m \\ \vdots \\ Data_n^m \end{pmatrix} = Data^m \qquad \text{for all } \ m \le N$$

Again this gets a least squares problem, but now for each subspace $\mathcal{U}^m$:

$$\left(\sum_{k=1}^{n} W_k^m (\mathfrak{D}_k^m)^T \mathfrak{D}_k^m \right) V = \sum_{k=1}^{n} W_k^m (\mathfrak{D}_k^m)^T Data_k^m \qquad \text{for all } \ m \le N$$

Please note that the solvability of the above equations depends on the kernels of the matrices $\mathfrak{D}_k^m$. We will discuss this point again when we are having some more specific information on these.

Another important point is the possibility to use different weights W_k^m for each of the subspaces $\mathcal{U}_m$ and operators $\mathfrak{D}^k$. This allows us to incorporate valuable information into our solution process.

6.3 Error and Weights

Now we want to take a closer look on the interplay between error and optimal corresponding weight. Assume that we know that our $Data_k^m$ are biased with an error of ε_k^m. I.e., we have

$$\varepsilon_k^m = \sqrt{\mathbb{E} \left(Data_k^m - \mathbb{E} \left(Data_k^m \right) \right)^2}$$

The combined error gets when we use our weights introduced above [BD96]:

$$\varepsilon^m = \sqrt{\left(\sum_{k=1}^{n} W_k^m\right)^{-2} \sum_{k=1}^{n} (W_k^m \varepsilon_k^m)^2}$$

Then we minimize the error for each subspace $\mathcal{U}_m$ when choosing :

$$W_k^m = (\varepsilon_k^m)^{-2}$$

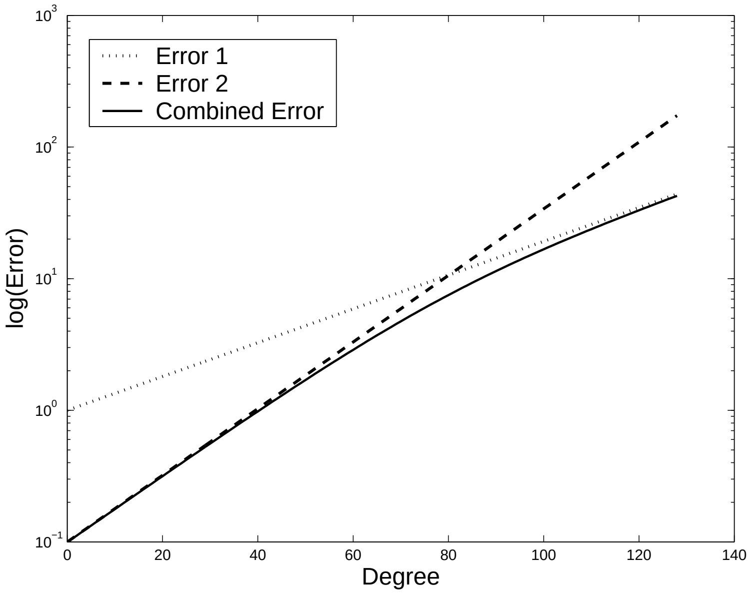
Hence the combined error gets:

$$\varepsilon^m = \left(\sum_{k=1}^{n} W_k^m\right)^{-1/2} = \left(\sum_{k=1}^{n} (\varepsilon_k^m)^{-2}\right)^{-1/2}$$

The subspaces $\mathcal{U}^m$ are orthogonal to each other, hence we also minimize the overall error.

These weights get particularly important for our satellite case. Assume that the $\mathcal{U}^m$ are the spaces of homogeneous harmonic polynomials of degree m and assume that we observe data originating from satellites flying at different heights. Hence the error for each degree m can be roughly described by $\delta \left(\frac{\text{Radius of Satellite Orbit}}{\text{Radius of Earth}}\right)^m$.

Choose for example $\varepsilon_1^m = 1 \cdot 1.03^m$ and $\varepsilon_2^m = 0.1 \cdot 1.06^m$ which results in



In the picture we observe the behavior indicated by the formula for the error, the combined error always behaves like the smallest error function.

6.4 Final Algorithm

Concluding we end up with the following still rather rough algorithm:

1. Approximate or interpolate the differentiated data with respect to $\mathfrak{D}_k$ at the height of the satellite track.

2. Determine a weight factors which should represent the reliability of the above approximation for each space $\mathcal{U}^m$.
3. Solve the inverse problem “downward-continuation”. Using the error level will enhance the reliability considerably.
4. Solve the least squares problem for each of the subspaces $\mathcal{U}^m$ which is posed by the inversion of the differential operators $\mathfrak{D}_k^m$ (integration) and combination of the data $Data_k^m$ from different sources.

6.5 Conclusion and Demands

Now we want to summarize the results of this chapter shortly and explain their relevance to our problem of determining V. Roughly we could show the following points.

- Out of mathematical considerations we obtain a good order for the mathematical treatment of the data, namely:
    1. Approximation
    2. Regularization
    3. Combination
- Combination should be done with a least squares approach using a reasonable error estimates on the data.

Chapter 7

Aspects of Scientific Computing

> *Does the method proposed in the solutions above actually work on data, derived from a geophysically relevant modell?*

In particular we want to show the following points separately:

- The auto-regularization works and is competitive to other known methods
- A problem with second order oblique derivatives can be solved.
- The combination of data from different sources is possible.

Note that it is not our goal to provide a numerically competitive solution but to give a proof of concept. Program sources and numerical results may be obtained electronically from the author.

7.1 Restrictions and Model

In order to be able to give a proof of concept we restricted ourselves to an easier scenario, where we could do some numerical experiments which are on the one hand sufficiently near to the real world situation and on the other hand still in our control.

7.1.1 Satellite Data

We have decided not to use satellite data because of several reasons. The first and perhaps most simple reason is just a lack of resources and knowledge in high performance computing. Therefore we would not have been able to provide a numerically competitive solution, neither in speed nor in accuracy.

Furthermore the computation with “real” data has another severe mathematical implication. We cannot judge anymore if a solution is actually good or bad because one never knows who used the “better” method when we compare two solutions.

7.1.2 Approximation

The choice of an appropriate basis system is a very difficult topic because both global (e.g., spherical harmonics) and local (e.g., splines, wavelets) ones have particular advantages and disadvantages. We just intend to do a proof of concept and hence chose the old but very well understood orthonormal system of spherical harmonics which is easy to use in numerical terms.

However, as remarked in the last chapters, in principle every possible basis system is capable of providing a reasonable structure to use the auto-regularization procedure and the new scheme for dealing with oblique derivatives.

We just calculated our data up to degree 128 which is not a principal restriction but again a sensible constraint completely sufficient for our model assumptions. Any higher degree could be considered but would of course enlarge the requirements for RAM and computation time.

Just for the data combination problem we chose to calculate 150 data points in order to have a better view on the occurring effects.

7.1.3 Data Distribution

We assumed our data to be given on an integration grid on the sphere. This has the advantage that we do not have to bother about the (ill-posed) problem of transferring data from a satellite track to such a grid and consequently evades several sources of additional error. Furthermore this enables us to study our new methods in an unbiased environment.

We used a Driscoll-Healy grid at an orbit height of 3% and 6% of the Earth radius. This roughly corresponds to an average satellite height of 200 km (like GOCE) and 400 km (like CHAMP). We generated the data globally on a grid which allows exact integration up to degree 180. Just for the combination of data from different sources we chose to use a grid which allows exact integration up to degree 300.

Although we just go up to degree 128 (150, respectively) in our computations this higher integration precision seemed to have stabilized the numerics, perhaps due to a suboptimal implementation.

7.1.4 Data Generation

7.1.4.1 Derivative Generation

All second derivatives are computed at each grid point in a satellite's coordinate system (i.e., $\widetilde{x_1}$ in flight direction, $\widetilde{x_2}$ perpendicular to $\widetilde{x_1}$ pointing east and $\widetilde{x_3}$ in the radial direction). This task was done with a stable Clenshaw algorithm which is proposed in the paper of Rod Deakin [Dea98] who also provided the necessary source code which just needed small adaptations to the object oriented implementation.

7.1.4.2 Gravitational Field

We used a stable Clenshaw algorithm [Dea98]. We always used the spectral model EGM96 as input and reference data.

7.1.4.3 Noise

The above data (both potential and derivatives) are modified with some additional stochastical noise which was proposed in the last chapter. We chose a ratio of 1 : 1 (i.e., $c_u = c_c = 0.5$) between the general error and the noise spread with $h = 0.9$ to the neighboring region.

For the error level we chose different scenarios:

- Auto-Regularization Test:

  $\delta = 0.5$ for the 200km case, $\delta = 0.05$ for the 400km case.

- Second Order Oblique Derivatives Test and Combination:

  $\delta = 5 \cdot 10^{-12}$ low noise level,

  $\delta = 1 \cdot 10^{-11}$ middle noise level and

  $\delta = 2 \cdot 10^{-11}$ high noise level,

  all at ∼200 km height

- Combination Test:

  $\delta = 2.5 \cdot 10^{-7}$ for SST-like data at ∼400km

  $\delta = 2 \cdot 10^{-11}$ for SGG-like data at ∼200km

Generally one can say that the error level is in near the order of magnitude as the data we are awaiting (when we neglect the first 3 Fourier coefficients). Note that the relative error is about 3 orders of magnitude lower in the $\partial_{\widetilde{x_1}}\partial_{\widetilde{x_1}}$, $\partial_{\widetilde{x_2}}\partial_{\widetilde{x_2}}$ and $\partial_{\widetilde{x_3}}\partial_{\widetilde{x_3}}$ direction in comparison to the mixed $\partial_{\widetilde{x_1}}\partial_{\widetilde{x_2}}$, $\partial_{\widetilde{x_1}}\partial_{\widetilde{x_3}}$ and $\partial_{\widetilde{x_2}}\partial_{\widetilde{x_3}}$ derivative directions.

7.1.5 Regularization Method

Another difficult topic is the choice of a good regularization method. Although our regularization procedure is capable to handle different types of methods we restricted ourselves to the spectral cut-off scheme because of one single fact: It is the only sensible regularization scheme which leaves the Fourier coefficients unchanged and hence allows some deeper insight in our usage of split operators and allows an easy control over the regularization in our setting.

7.1.6 Auto - Regularization

7.1.6.1 Noise Estimation

We generated a small second data set of degrees 4 – 15 (i.e., about 200 actual data, for the combination case) and another of degrees 8–32 (i.e., about 900 actual data, for the other cases) and compared it with the biased approximation of our noisy data. Note that one could have also used a second noisy approximation. But this would have just increased computation time without giving any mathematical valuable information. We only need to consider more Fourier coefficients to obtain the same accuracy in the estimation (approximately degrees 4 –18, or 8–36 respectively).

7.1.6.2 Parameters

We did the downward continuation and the regularization by the method proposed in the last chapter. The important parameter is κ, which was chosen by experience. For our purposes we observed that a $\kappa = 0.25$ ($\kappa = 0.276$ for the older oblique derivative part) seems to be a good choice which corresponds (roughly) to an accepted Signal/Noise ratio of 1:1 at the cutting point.

7.1.7 Data Combination

The data combination is done like proposed in the unified setup chapter. Please note that for the combination of SST like and SGG like "data" we made two small alterations:

- We used the data even after the cut-off point for combination. (If they are biased with high noise they will have a low weight, and hence improve the solution). Relevant at this point is just the highest cut-off point.

- We had to normalize the error estimate of the SST like data in comparison to the SGG like data with a factor of $2n + 1$ for each degree in order to counter the error amplification due to the different derivative.

7.1.8 Implementation, Time and Accuracy

A limitation on our experiments is imposed by the available computer equipment. The maximal sensible degree of spherical harmonics we are capable to consider is around 128 (with our newest machine 150). In order to study the auto-regularization we therefore needed to use a rather big error which was assumed to be near the order of magnitude of the data we actually wanted to study.

The implementation of our program was done with KDevelop in C++ on a Linux machine running the gcc2.96 compiler series. The program was executed on several Pentium III/IV machines in the 1GHz region with at least 512Mb RAM. The combination was done on a 3.2GHz Pentium with 2GB Ram.

Because the program was written for the ease of use (i.e., object oriented) we think that we are at least a factor of 2 away from a time efficient implementation. For each experiment (which considers all possible derivatives) we can expect an execution time of roughly 18 – 24 h depending on the machine in use; for the combination roughly three days.

7.2 Numerical Tests

We performed three kinds of completely different experiments. In the first one we wanted to assess the new auto-regularization. In the second test series we were interested in the information we can retrieve out of the oblique derivatives and how well the auto-regularization works for these examples. In the third one we had an emphasis on the data combination.

7.2.1 Auto-Regularization

For the test of the auto-regularization we generated a biased potential field at satellite height and did the downward continuation. In order to compare this method with another stop strategy we chose the widely applied L-curve method [Fen02].

In order to test two differently severely ill-posed problems we chose to use two different satellite heights, the first data set generated for 3% (roughly 200km) and the second for 6% (roughly 400km) of the Earth's radius. The noise was chosen in a way such that theoretically the noise to error ratio had to pass 1.0 around the degree of 80.

Further note that the noise is chosen at random and hence every run gives different results. For this numerical test an averaging over several runs is not sensible, which left us with choosing the examples to present. In general we can say that in every run our new method performed much better than the L-curve method and almost every time the regularization parameter was chosen in the region, where the degree-wise noise to signal ratio was between 0.5 and 1.5.

7.2.1.1 Some Notation and the L-curve method

The given data at satellite height (projected to $Harm_{128}$) shall be called d, our regularized solution x and the upward continuation operator A. Hence the size of x gets $||x||_2$ and the error occurring when choosing x gets $||Ax - d||_2$.

The L-curve method now tries to estimate the point, where the curve $(||x||_2, ||Ax - d||_2)$ is bending the most. As we will see in the next pictures this point is rather hard to obtain, especially because there are a big number of possible points nearby. Within these limitations we want to see our guess for an appropriate regularization parameter using the L-curve method. The point $\circ$ marked in the following pictures could also mark another degree in the range of 35–45 without really changing too much. But this also signifies that in the choice of the regularization parameter via this method is a rather big random element.

For a better readability of both the table and the pictures we rescaled the occurring values by a factor of $(10^5, 10^6)$.

The $\frac{\text{Noise}}{\text{Signal}}$ ratio is displayed for each degree of the solution. The optimal regularization point is, where this value changes to values greater than 1.

7.2.1.2 Data

First we will present the L-curves corresponding to our two input data sets:

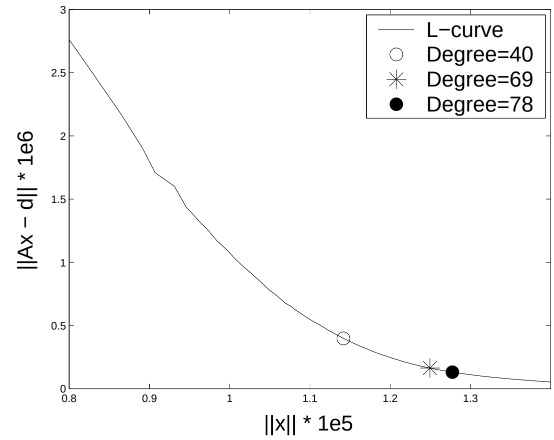


Figure 7.1: Data set at 200km

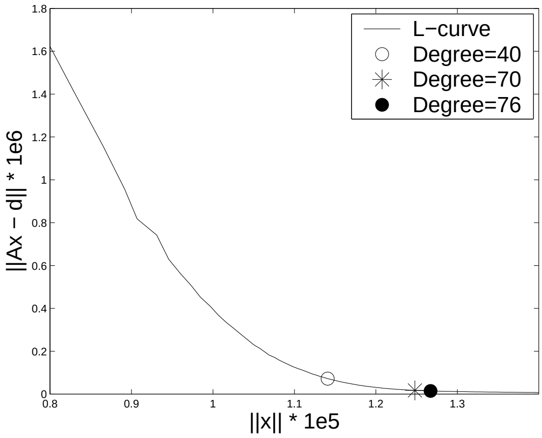


Figure 7.2: Data set at 400km

We displayed the optimal regularization point (i.e., $\frac{noise}{signal} = 1$) by $\bullet$, the regularization point proposed by the L-curve method by $\circ$ and the regularization point found by the auto-regularization method by $*$.

The noise/signal behavior is shown in the next curve. For a better observability we chose a log scale.

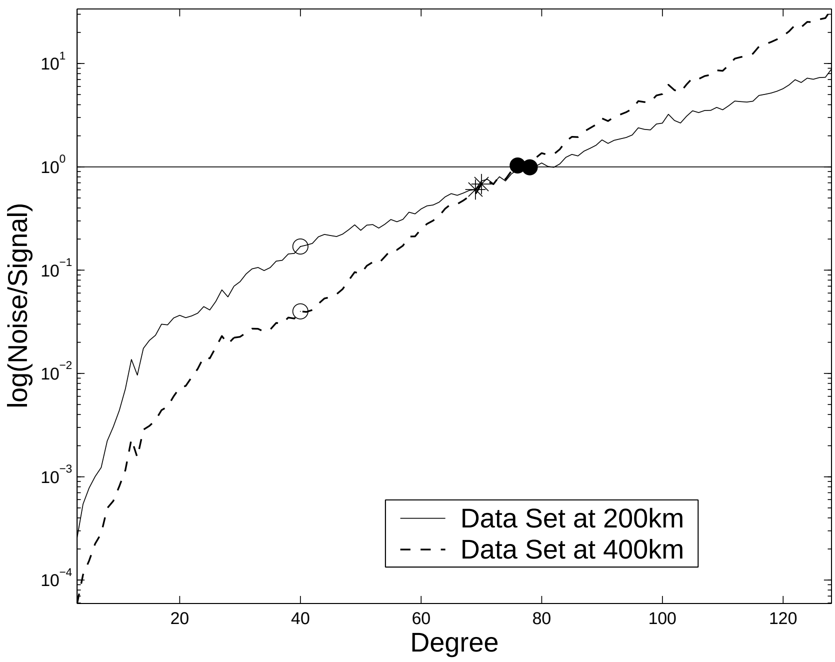


Figure 7.3: Noise/Signal ratio with respect to the degrees

Now we will present the table of data values. Due to space restrictions we chose the most interesting region:

Degree	Data Set 1 $\|\|x\|\|_2$	Data Set 1 $\|\|Ax-d\|\|_2$	Data Set 1 $\frac{\text{Noise}}{\text{Signal}}$	Data Set 2 $\|\|x\|\|_2$	Data Set 2 $\|\|Ax-d\|\|_2$	Data Set 2 $\frac{\text{Noise}}{\text{Signal}}$
3	0.2970	9.3820	0.0003	0.2970	7.4766	0.0001
4	0.4557	6.6642	0.0005	0.4557	4.9830	0.0001
...	...	...	...	...	...	...
38	1.1321	0.4295	0.1433	1.1315	0.0823	0.0348
39	1.1372	0.4137	0.1452	1.1364	0.0771	0.0340
40	1.1417	0.3977	**0.1695**	1.1408	0.0721	**0.0399**
41	1.1462	0.3840	0.1747	1.1452	0.0679	0.0393
42	1.1508	0.3704	0.1817	1.1498	0.0638	0.0411
43	1.1552	0.3571	0.2100	1.1540	0.0598	0.0472
...	...	...	...	...	...	...
61	1.2241	0.2011	0.4196	1.2208	0.0236	0.2808
62	1.2271	0.1956	0.4277	1.2239	0.0227	0.3016
63	1.2304	0.1907	0.4542	1.2270	0.0219	0.3348
64	1.2335	0.1855	0.5121	1.2300	0.0211	0.3940
65	1.2365	0.1809	0.5500	1.2328	0.0204	0.4376
66	1.2397	0.1766	0.5301	1.2357	0.0197	0.4363
67	1.2429	0.1719	0.5576	1.2388	0.0191	0.4727
68	1.2460	0.1676	0.5925	1.2418	0.0185	0.5192
69	1.2495	0.1634	**0.6020**	1.2451	0.0179	0.5430
70	1.2523	0.1589	0.7311	1.2479	0.0173	**0.6805**
71	1.2553	0.1553	0.7592	1.2510	0.0169	0.7270
72	1.2586	0.1516	0.6886	1.2540	0.0164	0.6788
73	1.2616	0.1477	0.8026	1.2571	0.0159	0.8126
74	1.2648	0.1442	0.7290	1.2607	0.0155	0.7578
75	1.2681	0.1406	0.8573	1.2640	0.0150	0.9144
76	1.2711	0.1371	0.9374	1.2671	0.0146	**1.0299**
77	1.2742	0.1339	0.9501	1.2705	0.0142	1.0720
78	1.2774	0.1307	**0.9901**	1.2739	0.0138	1.1522
79	1.2806	0.1274	1.0123	1.2775	0.0135	1.2194
80	1.2838	0.1244	1.0903	1.2811	0.0131	1.3589
81	1.2872	0.1214	1.0126	1.2849	0.0128	1.3088
82	1.2905	0.1183	0.9891	1.2891	0.0124	1.3241
83	1.2943	0.1153	1.0683	1.2934	0.0121	1.4802
84	1.2976	0.1121	1.2364	1.2977	0.0117	1.7747
85	1.3010	0.1093	1.3210	1.3022	0.0114	1.9532
86	1.3045	0.1066	1.2775	1.3070	0.0111	1.9411
87	1.3080	0.1038	1.4173	1.3120	0.0108	2.1954
88	1.3117	0.1012	1.5114	1.3172	0.0104	2.3725
89	1.3153	0.0984	1.6167	1.3226	0.0101	2.5698
90	1.3191	0.0958	1.8239	1.3281	0.0098	2.9426
...	...	...	...	...	...	...
127	1.5560	0.0049	7.3559	1.9532	0.0005	27.5285
128	1.5666	0.0024	8.8348	1.9936	0.0002	33.8520

7.2.1.3 Discussion

The data above indicate that the auto-regularization method is at least not worse and perhaps even superior to the L-curve method, which itself has been proven to be reliable in a wide number of cases.

Furthermore we will see in the next section when we post-process the data that even under these suboptimal conditions the new auto-regularization cuts quite reliably in the range $\frac{\text{Noise}}{\text{Signal}} \in [0.5, 1.5]$.

Both facts indicate that the new method should be the method of choice for such regularization problems.

7.2.2 Oblique Derivatives

7.2.2.1 Directions of Derivatives

In order to get a broad overview we utilized a large of vector fields to test our new method. In particular we used all the ones proposed in the chapter on split operators.

At this point we get our first problem. As remarked beforehand, not every possible vector field actually enables us to do a reconstruction on its own, because of its small but nevertheless non-zero kernels. In order to get an idea of the behavior of such a single vector field, we therefore added a very small perturbation (10^{-7}) of the identity, which now enabled us to invert the occurring matrices.

Note that this is just necessary if one wants to get information concerning one particular direction. The combination of the results was done by using the error levels we observed in the regularization part.

7.2.2.2 Data Selection

Beside the look on single directions which were just incorporated for testing purposes we also looked at the combinations we proposed in the general strategy section. At this point one faces a severe problem. Which solutions to choose? Of course one could use the ones with the smallest error level, but perhaps one looses valuable information. One could just block the data of a certain kind and have a look. Or one could use all possible approximations and hope the best.

Particularly, we decided to incorporate the following quantities (notation as in the chapter on split operators):

$\sum_{i\leq j} \mathsf{d}_{x_i}\mathsf{d}_{x_j}$, $\sum_i \mathsf{d}_{\neg x_i}\mathsf{d}_{x_i}$, $\sum_i \mathsf{d}_r\mathsf{d}_{x_i}$, $\sum_i \mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_i}$ and $\sum$ *ALL*

These sums are of course not actually the sum of the particular derivatives, but this shall denote that we considered the *weighted* sum of the results standing within the sum. As given in the “Combining Data in a Unified Setup” chapter we use the inverse of the square of the error as weight factor.

The combination was done with the integration matrices obtained in the chapter on “Integration”, of course. The “trash” parts of the solutions were not considered.

Please note in particular the comparison to the solution in the two times radial derivative direction.

7.2.2.3 Notation

Now we want to present the actual numerical results. For each noise level we did seven runs. For each direction we will give the following data (average always means average over the seven runs):

- deg := average degree at what point we cut
- deg_{min} := minimal degree at which we cut
- err := average relative error
- $err_{\boxdot}$:= average relative error at degree (high noise: $\boxdot = 33$,middle noise: $\boxdot = 55$, low noise: $\boxdot = 85$); if it is not possible to give this result: —
- err_{last} := average relative error of the last considered degree

Note that the error was computed neglecting the first three degrees every time. The error at a degree is the error at the degree specified, i.e.,

$$err_n := \frac{\sqrt{\sum_{k=-n}^{n} \left(a_n^k - \tilde{a}_n^k\right)^2}}{\sqrt{\sum_{k=-n}^{n} \left(a_n^k\right)^2}}$$

when a_n^k denote the unbiased Fourier coefficients corresponding to Y_n^k, $\tilde{a}_n^k$ the computed ones. This can be also seen as the noise to signal ratio at this specific degree. The value $err_{\boxdot}$ was picked to give a better comparison between the particular results, because all of them have a different degree considered and hence are not easily comparable.

The results we considered as most important are printed in bold letters.

7.2.2.4 Combination

The data combination was done using the regularized solutions without considering degrees which were cut. This approach was chosen because it allowed best to compare combined data with non-combined ones. However, for a more realistic example one has to think about another more elaborate strategy for choosing the data and for the cut-off point of the combined data.

7.2.2.5 Low Noise

Derivative	deg	deg_{min}	err	err_{85}	err_{last}
$\mathsf{d}_{x_1}\mathsf{d}_{x_1}$	117.00	112	0.0524	0.8228	2.0195
$\mathsf{d}_{x_1}\mathsf{d}_{x_2}$	120.57	116	0.0233	0.2880	0.8379
$\mathsf{d}_{x_1}\mathsf{d}_{x_3}$	109.00	96	0.0263	0.2578	0.4824
$\mathsf{d}_{x_2}\mathsf{d}_{x_2}$	120.43	115	0.0516	0.8410	2.2474
$\mathsf{d}_{x_2}\mathsf{d}_{x_3}$	118.43	112	0.0218	0.2532	0.5230
$\mathsf{d}_{x_3}\mathsf{d}_{x_3}$	117.00	111	0.0206	0.1214	0.2450
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_1}$	114.43	105	0.0631	0.8050	2.0586
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_2}$	117.57	109	0.1648	2.7000	6.3670
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_3}$	116.57	108	0.0607	0.8846	1.7476
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_1}$	111.14	104	0.1698	3.0976	5.6204
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_2}$	113.43	102	0.0577	0.5821	2.1693
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_3}$	105.00	88	0.0675	0.9721	1.6252
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_1}$	126.57	126	0.0304	0.3493	0.9348
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_2}$	126.71	126	0.0287	0.3785	1.0143
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_3}$	125.86	125	0.0191	0.1819	0.3844
$\mathsf{d}_{r}\mathsf{d}_{x_1}$	115.86	108	0.0242	0.2590	0.5615
$\mathsf{d}_{r}\mathsf{d}_{x_2}$	122.43	118	0.0201	0.2555	0.5938
$\mathsf{d}_{r}\mathsf{d}_{x_3}$	120.00	115	0.0174	0.1085	0.2347
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_1}$	119.57	112	0.0645	0.8993	1.9926
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_2}$	109.00	94	0.0746	1.1165	2.0630
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_3}$	127.71	127	0.0171	0.1820	0.4356
$\mathbf{d}_{\overline{r}}\mathbf{d}_{r}$	**123.29**	**120**	**0.0153**	**0.1052**	**0.2456**
$\sum_{i\le j} \mathbf{d}_{x_i}\mathbf{d}_{x_j}$	**107.86**	**96**	**0.0092**	**0.0742**	**0.1211**
$\sum_i \mathsf{d}_{\neg x_i}\mathsf{d}_{x_i}$	113.43	102	0.0183	0.2031	0.4913
$\sum_i \mathsf{d}_{r}\mathsf{d}_{x_i}$	115.00	108	0.0105	0.0898	0.1668
$\sum_i \mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_i}$	107.86	94	0.0128	0.1190	0.1982
$\sum \boldsymbol{ALL}$	**102.43**	**88**	**0.0089**	**0.0756**	**0.1066**

7.2.2.6 Middle Noise

Derivative	deg	deg_{min}	err	err_{55}	err_{last}
$\mathsf{d}_{x_1}\mathsf{d}_{x_1}$	98.43	77	0.0994	0.7884	2.6715
$\mathsf{d}_{x_1}\mathsf{d}_{x_2}$	98.14	80	0.0462	0.3549	0.8786
$\mathsf{d}_{x_1}\mathsf{d}_{x_3}$	102.29	90	0.0442	0.2878	0.8394
$\mathsf{d}_{x_2}\mathsf{d}_{x_2}$	97.86	81	0.0901	0.7443	2.4191
$\mathsf{d}_{x_2}\mathsf{d}_{x_3}$	91.29	69	0.0519	0.2720	0.5498
$\mathsf{d}_{x_3}\mathsf{d}_{x_3}$	101.43	78	0.0444	0.1357	0.3485
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_1}$	83.43	59	0.1237	0.7709	1.8627
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_2}$	89.29	67	0.3400	3.4458	8.6777
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_3}$	86.14	61	0.1131	0.8022	1.8005
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_1}$	89.43	61	0.2973	2.1247	7.3039
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_2}$	80.57	58	0.1260	0.7961	2.0600
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_3}$	97.43	82	0.1040	0.9597	2.2164
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_1}$	123.86	121	0.0588	0.4265	1.9956
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_2}$	124.43	122	0.0551	0.4203	1.5748
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_3}$	120.57	118	0.0370	0.2041	0.8450
$\mathsf{d}_{r}\mathsf{d}_{x_1}$	110.71	102	0.0418	0.2836	1.0223
$\mathsf{d}_{r}\mathsf{d}_{x_2}$	100.71	78	0.0465	0.2714	0.6833
$\mathsf{d}_{r}\mathsf{d}_{x_3}$	106.14	88	0.0372	0.1263	0.3383
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_1}$	91.14	64	0.1214	0.7891	2.2205
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_2}$	102.86	89	0.1118	1.2004	2.6853
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_3}$	125.71	125	0.0350	0.1892	0.9184
$\boldsymbol{\mathsf{d}_{\overline{r}}\mathsf{d}_{r}}$	**112.57**	**100**	**0.0321**	**0.1240**	**0.3633**
$\boldsymbol{\sum_{i\leq j} \mathsf{d}_{x_i}\mathsf{d}_{x_j}}$	**84.43**	**69**	**0.0193**	**0.0901**	**0.1497**
$\sum_i \mathsf{d}_{\neg x_i}\mathsf{d}_{x_i}$	80.43	58	0.0328	0.2548	0.4066
$\sum_i \mathsf{d}_{r}\mathsf{d}_{x_i}$	98.00	78	0.0213	0.1080	0.2230
$\sum_i \mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_i}$	91.00	64	0.0277	0.1468	0.2654
$\boldsymbol{\sum ALL}$	**72.57**	**58**	**0.0187**	**0.0933**	**0.1160**

7.2.2.7 High Noise

Derivative	deg	deg_{min}	err	err_{33}	err_{last}
$\mathsf{d}_{x_1}\mathsf{d}_{x_1}$	79.29	56	0.1728	0.8688	4.0037
$\mathsf{d}_{x_1}\mathsf{d}_{x_2}$	86.43	69	0.0858	0.3848	1.2796
$\mathsf{d}_{x_1}\mathsf{d}_{x_3}$	68.43	34	0.1008	0.3695	0.7593
$\mathsf{d}_{x_2}\mathsf{d}_{x_2}$	78.71	57	0.1546	0.6871	2.6736
$\mathsf{d}_{x_2}\mathsf{d}_{x_3}$	76.43	58	0.0886	0.3857	0.8506
$\mathsf{d}_{x_3}\mathsf{d}_{x_3}$	84.00	64	0.0818	0.2261	0.4541
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_1}$	71.86	51	0.2000	1.2588	2.5687
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_2}$	70.86	43	0.5335	2.5049	8.6636
$\mathsf{d}_{\neg x_1}\mathsf{d}_{x_3}$	70.71	51	0.1988	1.0510	2.7945
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_1}$	70.29	41	0.5201	2.9703	11.5575
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_2}$	71.43	50	0.2083	1.1070	2.2107
$\mathsf{d}_{\neg x_2}\mathsf{d}_{x_3}$	61.29	28	0.2453	—	2.3011
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_1}$	117.43	114	0.1029	0.6796	2.9495
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_2}$	117.29	105	0.1080	0.6163	3.8420
$\mathsf{d}_{\neg x_3}\mathsf{d}_{x_3}$	110.71	103	0.0684	0.3447	1.2096
$\mathsf{d}_{r}\mathsf{d}_{x_1}$	80.00	47	0.0875	0.3430	0.8329
$\mathsf{d}_{r}\mathsf{d}_{x_2}$	85.00	68	0.0805	0.3835	1.0773
$\mathsf{d}_{r}\mathsf{d}_{x_3}$	90.14	70	0.0672	0.2067	0.4515
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_1}$	75.14	55	0.2183	1.0513	3.0887
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_2}$	68.14	35	0.2505	0.9609	2.6787
$\mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_3}$	121.43	116	0.0648	0.3066	1.7171
$\mathbf{d}_{\overline{r}}\mathbf{d}_{r}$	**98.29**	**79**	**0.0594**	**0.1951**	**0.5194**
$\sum_{i\le j}\mathbf{d}_{x_i}\mathbf{d}_{x_j}$	**56.86**	**34**	**0.0423**	**0.1329**	**0.1788**
$\sum_i \mathsf{d}_{\neg x_i}\mathsf{d}_{x_i}$	69.86	50	0.0636	0.2950	0.6364
$\sum_i \mathsf{d}_{r}\mathsf{d}_{x_i}$	70.00	47	0.0465	0.1557	0.2733
$\sum_i \mathsf{d}_{\overline{r}}\mathsf{d}_{\neg x_i}$	62.43	35	0.0480	0.2040	0.2981
$\sum \boldsymbol{ALL}$	**48.00**	**28**	**0.0380**	—	**0.1563**

7.2.2.8 Noise/Signal

For the first two cases we also want to include a more detailed picture about the noise/signal behavior in each degree.

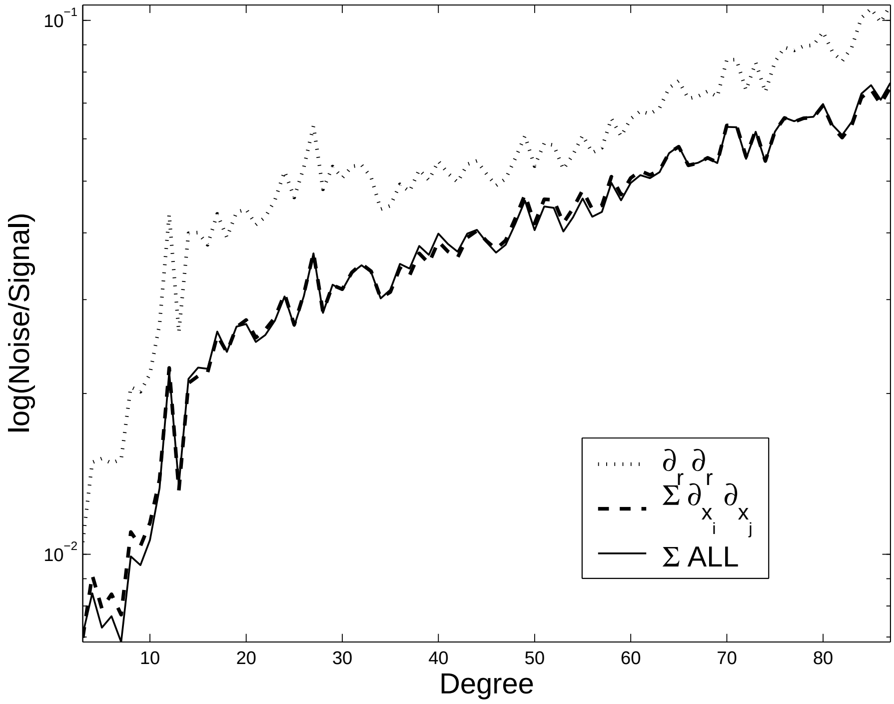


Figure 7.4: Low Noise case: Noise/Signal ratio

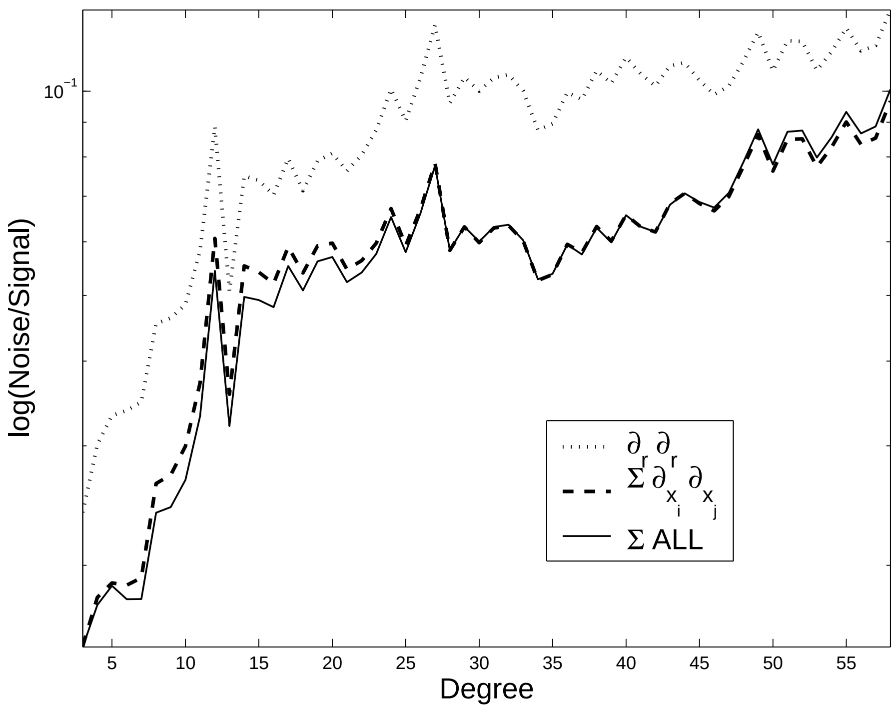


Figure 7.5: Middle Noise case: Noise/Signal ratio

From the pictures above we observe that the inclusion of the data different from the radial direction enhances the reliability of the solution, though the other directions had a quite high bias. Furthermore it seems to be sufficient to restrict our attention to the relatively small set of $\sum_{i\leq j} \mathsf{d}_{x_i}\mathsf{d}_{x_j}$ because even the choice of all considered directions did not lead to significant enhancements in the error level.

Similarly for a state space reconstruction of a low noise model we get the following picture:

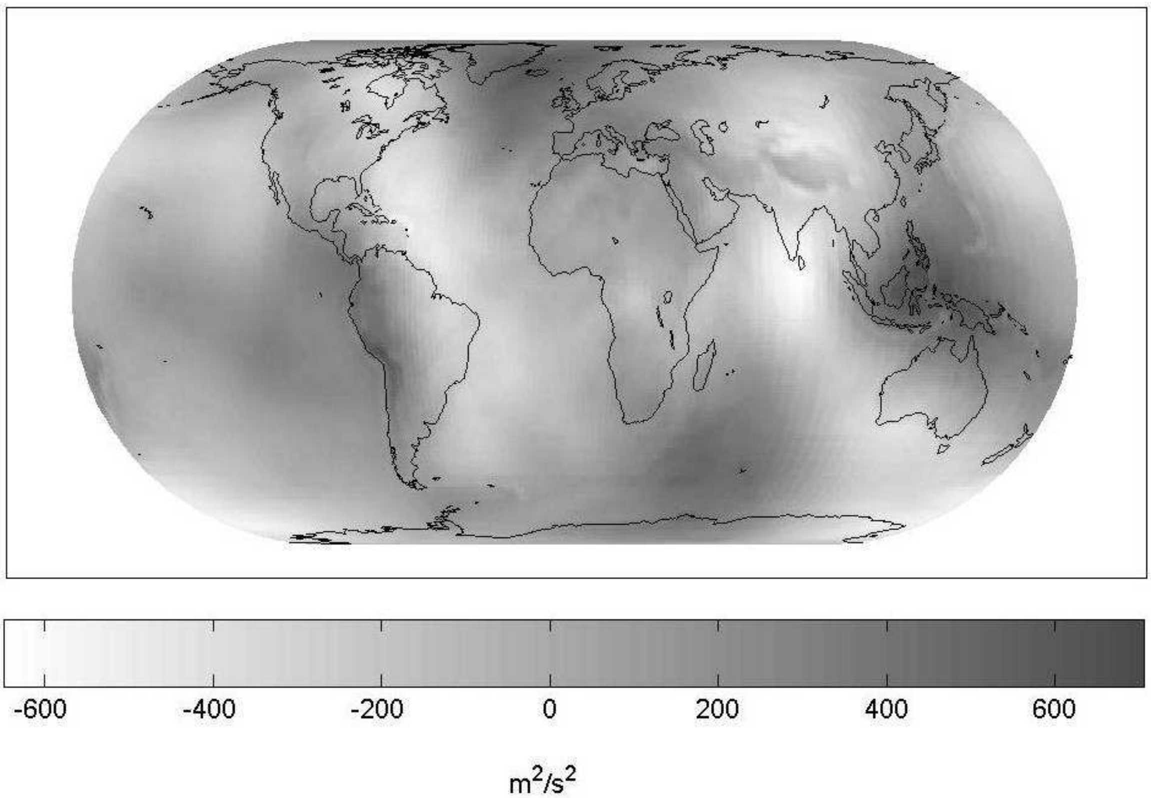


Figure 7.6: Reconstruction

These figures show a very good reconstruction of the EGM96 model (as expected). Only at the pole we have a concentration of the error which is due to the generation of our noise which has a particular higher variance (in comparison to the area) in the polar region. Beside the pole we see that most errors smoothed away.

7.2.2.9 Discussion

Looking at the tables beforehand we observe that the different kinds of derivatives have a particularly different behavior. This is understandable because our error was about three orders of magnitudes higher for the mixed directions than for the pure ones. However it is interesting to note that the radial derivative $\mathsf{d}_{\bar{r}}\mathsf{d}_r$ seems to be quite good in all cases. Particularly bad behaves $\mathsf{d}_{x_i}\mathsf{d}_{x_{\neg j}}$ for $i \neq j$. Additionally it seems that d_{x_3} and $\mathsf{d}_{\neg x_3}$ returns better results than the x_1 and x_2 counterparts.

But as we know it is not really the strength of the method to get out of a single

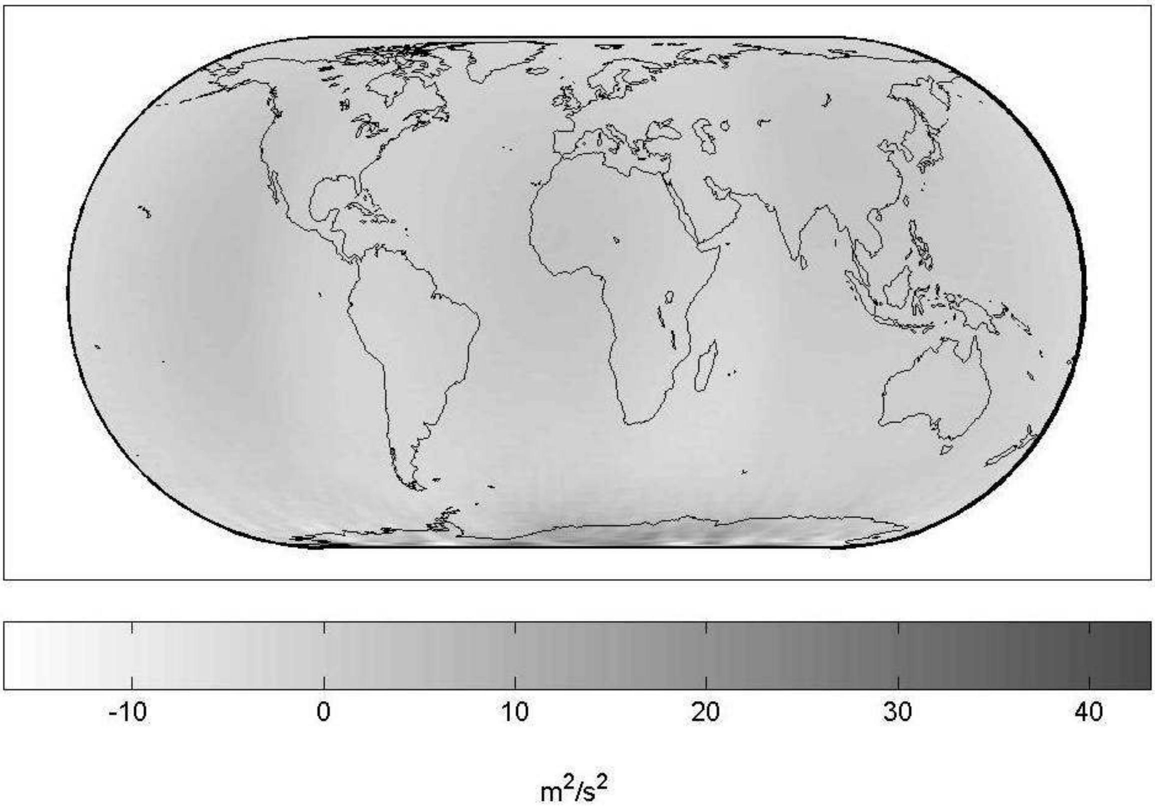


Figure 7.7: Error

direction a really effective approximation, but the interaction of the different solutions is worthwhile to consider.

And there we observe that the combination of all derivatives $\mathsf{d}_{x_i}\mathsf{d}_{x_j}$ yields results which are about 40% better than the ones we would get for the double radial derivative. Equally good (although it incorporates quite a number of really bad solutions) is the weighted combination of all derivatives we computed.

In practice with other noise distributions it might be worth to try a bunch of possible derivatives in order to find the ones which give the best result in the end.

7.2.2.10 Regularization

We were really surprised how well the auto-regularization actually performed in this more realistic environment. As we used a rather low κ we were ready to accept that we cut at a point, where it is quite sure that our data is not dominated by noise. And this job was done really well as long as the noise level was not chosen too high. Just in this case we observed problems, sometimes. These seemed partly to be due to the fact that noise in the first coefficients was jumping so violently that no good noise estimator could be obtained.

As we see in the tables the average last error is in total more or less centered around 1, i.e., we have got the point, where we switch from data to bias. Because we did the averaging process afterwards we see a rather small error there. But this is not the fault of the regularization, but the consequence of more data delivering a better result and smoothing away the error.

This may be countered easily by choosing a larger κ.

7.2.3 Data Combination

Now we want to show the combination of data from different sources, in this case SST like and SGG like data on different satellite heights ($\sim$ 400km and $\sim$ 200km).

7.2.3.1 Directions

For our numerical experiment we chose all possible directional derivatives d_{x_i} for the SST case and $\mathsf{d}_{x_i}\mathsf{d}_{x_j}$ for SGG case because their combination provided the best results for combined data as we saw in the last section.

7.2.3.2 Data

In the sequel we have the picture of the noise/signal ratio for the SST like case, the SGG like case and their combination.

The proposed cut-off points for the single data sets are:

SST

- d_{x_1} : 134
- d_{x_2} : 91
- d_{x_3} : 123

SGG

- $\mathsf{d}_{x_1}\mathsf{d}_{x_1}$: 34
- $\mathsf{d}_{x_1}\mathsf{d}_{x_2}$: 35
- $\mathsf{d}_{x_1}\mathsf{d}_{x_3}$: 51
- $\mathsf{d}_{x_2}\mathsf{d}_{x_2}$: 51
- $\mathsf{d}_{x_2}\mathsf{d}_{x_3}$: 51
- $\mathsf{d}_{x_3}\mathsf{d}_{x_3}$: 131

As the SGG case is expected to give better results for higher degrees due to its lower orbit, it is sensible to assume that the second derivative data are the ones which "decide", where to cut-off in the end. So the cut-off level would be at 131 or slightly lower (because of the other proposed low cut-off's). At degree 131 the noise/signal ratio is 1.594, at 120 it is 1.246. The optimal cut-off point would be degree 111.

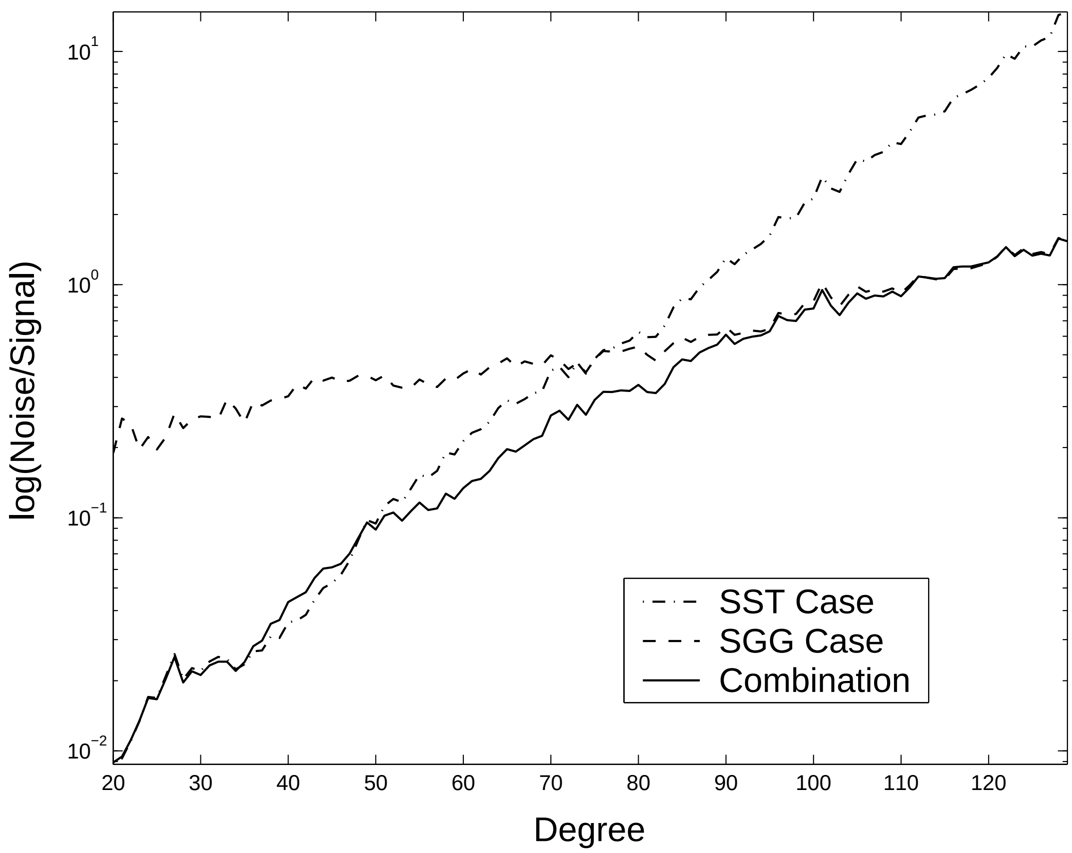


Figure 7.8: Middle Noise case: Noise/Signal ratio

7.2.3.3 Discussion

If we purely look at the data combination it was well done and returned reasonable results, which still leave room to some interpretation.

On the other hand this example shows that at the point of the determination of an optimal κ (with respect to the underlying problem) much work has to be done. However this is not a surprise because the proposed κ is just valid for the error level tending to 0 and hence does not necessarily also provide excellent results for real world problems.

7.3 Conclusion

Our method has passed the numerical tests comparably well. In particular we can remark the following results:

- The reconstruction from the possible set of oblique derivatives works within its specified limitations.

- The auto-regularization works and finds roughly the point, where the data/bias ratio gets 1, although we operated with a simplified error model.

- The combination of different directions results in a considerably better solution.

Consequently we can call our new method promising. Further investigations need to be done in order to determine if this result also transfers to real satellite data. But at least from the mathematical point of view there is no argument to doubt this.

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