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Split Operations for Oblique Boundary Value Problems

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Abstract

In the field of gravity determination a special kind of boundary value problem respectively ill-posed satellite problem occurs; the data and hence side condition of our PDE are oblique second order derivatives of the gravitational potential.

In mathematical terms this means that our gravitational potential v fulfills $\Delta v = 0$ in the exterior space of the Earth Σ_{ext} and $\mathcal{D}v = f$ on the discrete data location which is on the Earth's surface Σ for terrestrial measurements and on a satellite track in Σ_{ext} for spaceborne measurement campaigns. \mathcal{D} is a first order derivative for methods like geometric astronomic levelling and satellite-to-satellite tracking (e.g. CHAMP); it is a second order derivative for other methods like terrestrial gradiometry and satellite gravity gradiometry (e.g. GOCE).

Classically one can handle first order side conditions which are not tangential to the Σ and second derivatives pointing in the radial direction employing integral and pseudo differential equation methods. We will present a different approach: We classify all first and purely second order operators \mathcal{D} which fulfill $\Delta \mathcal{D}v = 0$ if $\Delta v = 0$. This allows us to solve the problem with oblique side conditions as if we had ordinary i.e. non-derived side conditions. The only additional work which has to be done is an inversion of \mathcal{D} , i.e. integration.

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1 Introduction

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. 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. Quite often we cannot decide which direction of the derivatives can be obtained.

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.

A prominent example is the gravitational field which fulfills the Laplace equation in the outer space of the Earth Σ_{ext} . A modern approach to this topic is measuring the derivatives of this quantity by satellites. Among others there are two very important measurement procedures. The first one is Satellite-to-Satellite Tracking (SST, e.g. the satellite CHAMP) which returns the first derivatives and Satellite Gravity Gradiometry (SGG, e.g. the satellite GOCE) which returns the second derivatives.

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 [4,6].
- First and second order radial derivatives in radial direction, e.g., in [3].

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. Much deeper insight into this classical approaches can be found in [5] and the references therein.

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.

2 General Problem Setup

Now we will rewrite the oblique derivative problem in a more functional analytic context in which it is easier to attack. The proofs in this section are straight forward but can also be found in [1].

Question 2.1 (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 $U : \mathcal{S} \rightarrow \mathcal{T}_1$ and $D : \mathcal{S} \rightarrow \mathcal{T}_2$ be linear operators. Assume furthermore $t_2 \in \mathcal{T}_2$.

We search all $v \in \mathcal{S}$ fulfilling

$$\begin{aligned} Uv &= 0 \\ (Dv)|_{\Sigma_D} &= t_2|_{\Sigma_D} \end{aligned}$$

Remark. This is our oblique derivative problem in the geoscientific case if we set Σ_{ext} to the exterior of the Earth, Σ_D to the data location (satellite track), $U = \Delta$ and $D = \mathcal{D}$ to an oblique derivative Σ_D .

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 $(Dv)|_{\Sigma_D} = t_2|_{\Sigma_D}$. The problem would simplify considerably if we could remove this additional operator D .

Definition 2.2 (Split Operator). $U_D : \mathcal{T}_2 \rightarrow \mathcal{T}_1$ is called split operator for U with respect to D if it fulfills the following property:

$$Uv = 0 \Rightarrow U_D Dv = 0 \quad \text{for all } v \in \mathcal{S}$$

Remark. It is also sensible to introduce a bidirectional version of the split operator with “ \Leftrightarrow ” instead of “ \Rightarrow ”, cf. [1]

Lemma 2.3 (Split Lemma). Let U_D be a split operator for U with respect to D .

If v is a solution of the problem

$$\begin{aligned} Uv &= 0 \\ (Dv)|_{\Sigma_D} &= t_2|_{\Sigma_D} \end{aligned}$$

then it is also a solution of the problem

$$\begin{aligned} U_D v_D &= 0 \\ v_D|_{\Sigma_D} &= t_2|_{\Sigma_D} \\ Dv &= v_D \end{aligned}$$

This means that we split the original problem with a non-standard side condition $(Dv)|_{\Sigma_D} = t_2|_{\Sigma_D}$ into a problem with a standard side condition $v_D|_{\Sigma_D} = t_2|_{\Sigma_D}$ and an additional integration problem $Dv = v_D$. This was the motivation for calling U_D split operator.

Obviously this approach just makes sense if U_D exists and if we can compute it. This will turn out to be a very hard problem. Furthermore the most simple example for a split operator is 0, however not a sensible one. We are mainly interested in other, non-trivial split operators.

Particularly important are the following two properties of split operators:

Lemma 2.4 (Composition of Split Operators). Assume $D = D_2 D_1$ and let U_{D_2} and $(U_{D_2})_{D_1}$ be the corresponding split operators. If v is a solution of the problem

$$\begin{aligned} Uv &= 0 \\ (Dv)|_{\Sigma_D} &= t_2|_{\Sigma_D} \end{aligned}$$

then it is also a solution of the problem

$$\begin{aligned}(U_{D_2})_{D_1} v_D &= 0 \\ v_D|_{\Sigma_D} &= t_2|_{\Sigma_D} \\ Dv &= v_D\end{aligned}$$

In other words, we have the equality

$$(U_{D_2})_{D_1} = U_{(D_2 D_1)} = U_D$$

Thus we are able to handle any finite compositions of operators D . In particular, the second derivatives we observe as data in our satellite problem are covered. Similarly we have a linearity result.

Lemma 2.5 (Linearity of Split Operators). Assume $U_{D_1} = U_{D_2}$ are (bidirectional) split operators with respect to D_1 and D_2 respectively.

Then $U_D := U_{D_1}$ is a split operator with respect to the operator

$$D = \alpha_1 D_1 + \alpha_2 D_2 \quad \text{where } \alpha_1, \alpha_2 \in \mathbb{R}$$

After having introduced split operators in a general setting we will return to the geoscientifically relevant case. First we will examine first order, later second order operators as boundary conditions.

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.

In order to keep the notation simple a_{\square} 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 that we denote the derivative in the Euclidean direction x_i by ∂_i .

3 Split Operators wrt. a First Order Operator Condition

First we want to state our exact problem, where the geoscientific problem with $\bar{\Delta} = \Delta$ is a special case:

Question 3.1. Assume

$$\bar{\Delta} = \sum_{i \leq j} a_{ij} \partial_i \partial_j + \sum_i a_i \partial_i + a$$

where the $a_{\square} \in C^\infty(\overline{\Sigma_{ext}})$ denote smooth functions and all matrices $\mathbf{A}_{ij} = \begin{pmatrix} a_{ii} & a_{ij} \\ 0 & a_{jj} \end{pmatrix}$ are definite. (I.e., $(v^T \mathbf{A}_{ij} v)(x) \neq 0$ for all $v \in \mathbb{R}^2 \setminus \{0\}$ for all $x \in \overline{\Sigma_{ext}}$)

Additionally $\bar{\Delta}$ should fulfill the following technical condition. For all differential operators $\{1, \partial_i, \partial_j \partial_k, \partial_i \partial_j \partial_k\}$ with $1 \leq i \leq j \leq k \leq 3$ 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):

- $h_\mu \in C^3(\overline{\Sigma_{ext}})$ for all μ
- $\bar{\Delta} h_\mu = 0$ for all μ
- $\partial_\nu h_\mu = 0$ for all $\nu \blacktriangleright \mu$

- $\partial_\nu h_\nu = \bar{h}_\nu \neq 0$ for all ν

Assume furthermore

$$\mathcal{D} = \sum_k d_k \partial_k + d$$

where the $d_\square \in C^\infty(\overline{\Sigma_{ext}})$ 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 $\bar{\Delta}_\mathcal{D}$ for $\bar{\Delta}$ with respect to \mathcal{D} with smooth coefficient functions? How does it look like? Which conditions does \mathcal{D} have to fulfill?

Note that in terms of the operator notation in the last section we would have $U = \bar{\Delta}$, $D = \mathcal{D}$ and hence $U_D = \bar{\Delta}_\mathcal{D}$.

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_\square .

Alternatively to $1 \leq i \leq j \leq k \leq 3$ 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 the way how we deal with it.

Lemma 3.2. The Laplace operator $\Delta = \sum_i \partial_i \partial_i$ fulfills the requirements imposed by the above question.

The proof is simply stating the corresponding h_\square which can be found in [1]

3.1 First Order Split Operators

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

Lemma 3.3. Let $\bar{\Delta}$ and \mathcal{D} be as defined in the above problem.

Then there does not exist a nontrivial split operator in the form $\bar{\Delta}_\mathcal{D} = \sum_i b_i \partial_i + b$, where the b_i and b denote smooth functions, i.e., $b_\square \in C^\infty(\overline{\Sigma_{ext}})$.

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 $\bar{\Delta}_\mathcal{D} \mathcal{D}$. Using the chain rule we obtain:

$$\begin{aligned} \bar{\Delta}_\mathcal{D} \mathcal{D} &= \sum_i b_i \sum_j ((\partial_i d_j) \partial_j + d_j \partial_i \partial_j) + \sum_j b d_j \partial_j + \sum_i b_i (\partial_i d + d \partial_i) + b d \\ &= \sum_{i,j} b_i d_j \partial_i \partial_j + \sum_i \left(\left(\sum_j b_i \partial_j d_j \right) + b d_i + b_i d \right) \partial_i + b d + \sum_i b_i \partial_i d \end{aligned}$$

Now we want to use the technical condition concerning the functions h_\square . 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 $\bar{\Delta} v = 0$ and hence $\bar{\Delta}_\mathcal{D} \mathcal{D} v = 0$. So subtracting $\frac{d_3 b_3}{a_{33}} \bar{\Delta}$ ($a_{33} \neq 0$ 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:

$$\begin{aligned}
0 &= \left(\bar{\Delta}_{\mathcal{D}} \mathcal{D} - \frac{d_3 b_3 \bar{\Delta}}{a_{33}} \right) v \\
&= \left(\sum_i \left(d_i b_i - \frac{d_3 b_3}{a_{33}} a_{ii} \right) \partial_i \partial_i + \sum_{i < j} \left(d_j b_i + d_i b_j - \frac{d_3 b_3}{a_{33}} a_{ij} \right) \partial_i \partial_j \right. \\
&\quad \left. + \sum_i \left(\left(\sum_j b_j \partial_j d_i \right) + b d_i + b_i d - \frac{d_3 b_3}{a_{33}} a_i \right) \partial_i + b d + \sum_i b_i \partial_i d - \frac{d_3 b_3}{a_{33}} a \right) v
\end{aligned}$$

Now we can apply the technical condition we required to hold. Using $\nu_1 \blacktriangleleft \nu_2 \blacktriangleleft \dots \blacktriangleleft \nu_9$ (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:

$$\begin{aligned}
0 &= \left(\sum_{i=1}^9 c_{\nu_i} \partial_{\nu_i} \right) h_{\nu_k} = \left(\sum_{1 \leq i < k} c_{\nu_i} \partial_{\nu_i} h_{\nu_k} \right) + c_{\nu_k} \bar{h}_{\nu_k} + \left(\sum_{k < i \leq 9} c_{\nu_i} \partial_{\nu_i} h_{\nu_k} \right) \\
&= \left(\sum_{1 \leq i < k} c_{\nu_i} \partial_{\nu_i} h_{\nu_k} \right) + c_{\nu_k} \bar{h}_{\nu_k}
\end{aligned}$$

which is structurally seen a triangular homogeneous linear system of linear equations. Using $\bar{h}_{\nu_k} \neq 0$ 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:

$$\begin{aligned}
0 &= b d + \sum_i b_i \partial_i d - \frac{d_3 b_3}{a_{33}} a \\
0 &= \left(\sum_j b_j \partial_j d_i \right) + b d_i + b_i d - \frac{d_3 b_3}{a_{33}} a_i && \text{for all } i \\
0 &= b_i d_j + b_j d_i - \frac{d_3 b_3}{a_{33}} a_{ij} && \text{for all } i < j \\
0 &= b_i d_i - \frac{d_3 b_3}{a_{33}} a_{ii} && \text{for all } i
\end{aligned}$$

Using the last two sets of equations we get:

$$\begin{aligned}
0 &= d_i d_j \left(b_i d_j + b_j d_i - \frac{d_3 b_3}{a_{33}} a_{ij} \right) = b_i d_i d_j^2 + b_j d_j d_i^2 - d_i d_j \frac{d_3 b_3}{a_{33}} a_{ij} \\
&= \frac{d_3 b_3}{a_{33}} (a_{ii} d_j^2 + a_{jj} d_i^2 - a_{ij} d_i d_j) = -\frac{d_3 b_3}{a_{33}} \begin{pmatrix} -d_j & d_i \end{pmatrix} \begin{pmatrix} a_{ii} & a_{ij} \\ 0 & a_{jj} \end{pmatrix} \begin{pmatrix} -d_j \\ d_i \end{pmatrix} \\
&= -\frac{d_3 b_3}{a_{33}} \begin{pmatrix} -d_j & d_i \end{pmatrix} \mathbf{A}_{ij} \begin{pmatrix} -d_j \\ d_i \end{pmatrix}
\end{aligned}$$

We assumed every matrix of the type \mathbf{A}_{ij} to be definite. In particular this means that $0 = \frac{d_3 b_3}{a_{33}}$ 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 $b d_3 = 0$ and thus $b = 0$.

These arguments hold for all points in $\overline{\Sigma_{ext}}$ and hence the operator $\overline{\Delta}_{\mathcal{D}} = 0$ is the trivial operator. \square

3.2 Second Order Split Operators

Definition 3.4. The second order differential operator $\tilde{\Delta}$ is defined as

$$\tilde{\Delta} = \sum_{i \leq j} b_{ij} \partial_i \partial_j + \sum_i b_i \partial_i + b$$

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

$\tilde{\Delta}$ shall be our candidate for the split operator $\overline{\Delta}_{\mathcal{D}}$ as described in the last question. 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.

The proofs and following computations are lengthy but work exactly along the lines of the last lemma. Therefore we omit them and refer to [1].

Lemma 3.5. Let $\overline{\Delta}$, \mathcal{D} and $\tilde{\Delta}$ be as defined beforehand. Then the second order parts of $\overline{\Delta}$ and $\tilde{\Delta}$ are essentially the same, i.e. there exists $c \in C^\infty(\overline{\Sigma_{ext}})$ with

$$\tilde{\Delta} = c \sum_{i \leq j} a_{ij} \partial_i \partial_j + \sum_i b_i \partial_i + b$$

Remark. c has to be different from 0 at every point because otherwise using the preceding lemma the split operator gets trivial. Therefore we can divide by c and put this factor into the b_{\square} which is equivalent to $c = 1$.

As we are mainly interested in the Laplace operator and general considerations get too complicated we restrict our attention on the case $\overline{\Delta} = \Delta$ and hence $\tilde{\Delta} = \Delta + \sum_i b_i \partial_i + b$.

Lemma 3.6. We have the following equations which have to be fulfilled:

$$\begin{aligned} 0 &= \tilde{\Delta} d_i + 2\partial_i d + b_i d && \text{for all } i \\ 0 &= 2\partial_i d_j + b_i d_j + 2\partial_j d_i + b_j d_i && \text{for all } i \neq j \\ 0 &= 2\partial_i d_i + b_i d_i - 2\partial_j d_j - b_j d_j && \text{for all } i \neq j \\ 0 &= \tilde{\Delta} d \end{aligned}$$

Now we want to solve the above system of differential equations. This will be done in two different steps. The first one is determining a set of possible solutions, the second step is showing that these are all. In order to do the second step we will translate the above system of PDE's to the language of algebra.

However, the above system is extremely symmetric and hence poses hard problems when we try to solve it this way (this was done in collaboration with V. Levandovskyy [9] with a non-commutative version of Singular [7]).

Therefore we had to change to the language of commutative algebra which meant in particular that we had to restrict our attention on constant b_{\square} .

3.3 Solving the System of PDE's

We need to do some preparatory steps to solve this system using a method proposed in [11]. 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. The other coefficients stay right the same.

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 $(\partial_1, \partial_2, \partial_3, b_1, b_2, b_3, b)$. 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 [8], the program used is Singular [7].

When we transfer this standard basis back in the language of PDE's we obtain a system without hidden integrability conditions [11].

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 [7]. For further instructions on the possible orderings, their advantages and disadvantages we want to refer the reader to [8].

The number of solutions will now be obtained by regarding the corresponding Reid diagrams [11]. The proof of the following theorem is lengthy and technical and we want to refer therefore to [1].

Theorem 3.7. Assume $\mathcal{D} = \sum_k d_k \partial_k + d$. A split operator of the form $\Delta_{\mathcal{D}} = \Delta + \sum_k b_k \partial_k + b$ for Δ with constant b_{\square} just exists in the case when $\Delta_{\mathcal{D}}$ fulfils:

$$b = \frac{1}{4} (b_1^2 + b_2^2 + b_3^2)$$

and \mathcal{D} is member of the 14 dimensional space which is constituted by

$$\begin{aligned} d &= s(c_{q1}x_1 + c_{q2}x_2 + c_{q3}x_3 + c) \\ d_1 &= s(c_1 + c_r x_1 + c_{-3}x_2 + c_{-2}x_3 + c_{q1}(x_1^2 - x_2^2 - x_3^2) + 2c_{q2}x_1x_2 + 2c_{q3}x_1x_3) \\ d_2 &= s(c_2 - c_{-3}x_1 + c_r x_2 + c_{-1}x_3 + c_{q1}x_1x_2 + c_{q2}(-x_1^2 + x_2^2 - x_3^2) + 2c_{q3}x_2x_3) \\ d_3 &= s(c_3 - c_{-2}x_1 - c_{-1}x_2 + c_r x_3 + c_{q1}x_1x_3 + 2c_{q2}x_2x_3 + c_{q3}(-x_1^2 - x_2^2 + x_3^2)) \end{aligned}$$

where the c_{\square} are real constants we are free to choose and

$$s = e^{-2(b_1x_1 + b_2x_2 + b_3x_3)}$$

These are all solutions of our problem under these conditions.

We observe that the common prefactor $e^{-(\bar{b}_1x_1 + \bar{b}_2x_2 + \bar{b}_3x_3)}$ just changes the length, but not the direction of our differential operator. Therefore we will drop it from now on by setting $b = b_1 = b_2 = b_3 = 0$ and hence $\Delta_{\mathcal{D}} = \Delta$. This results in a 11 dimensional vector space of solutions.

4 Compositions

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

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 4.1. Define the following differential operators

$$\begin{aligned}
D_{id} &= 1 \\
D_{x_1} &= \partial_1, & D_{x_2} &= \partial_2, & D_{x_3} &= \partial_3 \\
D_{-x_1} &= x_3 \partial_2 - x_2 \partial_3, & D_{-x_2} &= x_3 \partial_1 - x_1 \partial_3, & D_{-x_3} &= x_2 \partial_1 - x_1 \partial_2 \\
D_r &= x_1 \partial_1 + x_2 \partial_2 + x_3 \partial_3, & D_{\bar{r}} &= x_1 \partial_1 + x_2 \partial_2 + x_3 \partial_3 - 1
\end{aligned}$$

Lemma 4.2. The differential operators shown below are pure second order operators which read the following way: ($\overline{i+k}$ shall denote $(i+k \bmod 3) + 1$)

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

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

$$\begin{aligned}
& \left(D_r D_{x_i} = x_1 \partial_1 \partial_i + x_2 \partial_2 \partial_i + x_3 \partial_3 \partial_i \quad \forall i \right) \\
D_{\bar{r}} D_{-x_i} &= (-x_{\overline{i+1}}^2 + x_{\overline{i+2}}^2) \partial_{\overline{i+1}} \partial_{\overline{i+2}} + x_{\overline{i+2}} x_i \partial_{\overline{i+1}} \partial_i - x_{\overline{i+1}} x_i \partial_{\overline{i+2}} \partial_i \\
& \quad + x_{\overline{i+1}} x_{\overline{i+2}} \partial_{\overline{i+1}} \partial_{\overline{i+1}} - x_{\overline{i+1}} x_{\overline{i+2}} \partial_{\overline{i+2}} \partial_{\overline{i+2}} \quad \forall i \\
D_{\bar{r}} D_r &= x_1^2 \partial_1 \partial_1 + x_2^2 \partial_2 \partial_2 + x_3^2 \partial_3 \partial_3 \\
& \quad + 2x_1 x_2 \partial_1 \partial_2 + 2x_1 x_3 \partial_1 \partial_3 + 2x_2 x_3 \partial_2 \partial_3
\end{aligned}$$

All of them have the split operator $\Delta_{\mathcal{D}} = \Delta$ for the operator Δ .

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.

5 Split Operators wrt. a 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 \mathcal{D} are the same as in the last section.

Question. Assume

$$\overline{\Delta} = \Delta + \sum_i a_i \partial_i + a$$

where the $a_{\square} \in C^\infty(\overline{\Sigma_{ext}})$ 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 $1 \leq i \leq j \leq k \leq l \leq 3$ and $k \neq 3$ 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 $\nu \blacktriangleright \mu$

- $\partial_\nu h_\nu = \bar{h}_\nu \neq 0$ for all ν

Assume furthermore

$$\mathcal{D} = \sum_{i \leq j} d_{ij} \partial_i \partial_j$$

where the $d_{\square} \in C^\infty(\overline{\Sigma_{ext}})$ are smooth functions.

Furthermore we demand that for a fixed α at every point there is at least one of the $d_{ij} - \alpha \delta_{ij} \neq 0$. (Due to $\bar{\Delta}v = 0$ we can replace \mathcal{D} by $\mathcal{D} - \alpha \bar{\Delta}$ without facing problems).

Does there exist a sensible (non-zero) split operator $\bar{\Delta}_{\mathcal{D}}$ for $\bar{\Delta}$ with respect to \mathcal{D} ? How does it look like? Which conditions has \mathcal{D} to fulfill?

Lemma 5.1. The Laplace operator $\Delta = \sum_i \partial_i \partial_i$ fulfills the requirements imposed by the above question.

Definition 5.2. The second order differential operator $\tilde{\Delta}$ is defined as

$$\tilde{\Delta} = \sum_{i \leq j} b_{ij} \partial_i \partial_j + \sum_i b_i \partial_i + b$$

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

$\tilde{\Delta}$ shall be the candidate for the split operator $\bar{\Delta}_{\mathcal{D}}$ as described in the last question. Again we are having the following result

Lemma 5.3. Let $\bar{\Delta}$, \mathcal{D} and $\tilde{\Delta}$ be as defined beforehand. Then the second order parts of $\bar{\Delta}$ and $\tilde{\Delta}$ are essentially the same, i.e. there exists $c \in C^\infty(\overline{\Sigma_{ext}})$ with

$$\tilde{\Delta} = c\Delta + \sum_i b_i \partial_i + b$$

Remark. Again we can set $c = 1$ w.l.o.g. The proof is working as shown beforehand, but rather technical.

As we are mainly interested in the Laplace operator and general considerations get to complicated we restrict our attention on the case $\bar{\Delta} = \Delta$.

Lemma 5.4. We have the following equations which have to be fulfilled:

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

The proof of the following theorem is done using the same algebraic methods as for the first order differential case.

Theorem 5.5. Assume $\mathcal{D} = \sum_{i \leq j} d_{ij} \partial_i \partial_j$. A split operator $\Delta_{\mathcal{D}} = \Delta$ for Δ with constant b_{\square} just exists when \mathcal{D} is member of the 17 dimensional space which is constituted by (the c_{\square} are

real constants we are free to choose)

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

These are all solutions of our problem under these conditions.

Remark. Because $\Delta_{\mathcal{D}} = \Delta$ we can set $c_{3,3} = 0$ w.l.o.g. The resulting space is exactly the one given in Lemma 4.2.

6 Derivatives

When we want to use the result presented beforehand we need to know how one can invert the differentials presented beforehand. These calculations are lengthy and very technical [1]. However the result can be verified rather easily. Therefore we just present the result. Please note that at least for the D_{-x_i} we can find these differentials in books about quantum mechanics [2, 10], where D_{-x_i} can be interpreted as an angular momentum. Additionally the result for D_r is well known and can be found e.g., in [3].

Definition 6.1 (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 $\varepsilon_l = \begin{cases} 1 & l = 0 \\ \sqrt{2} & \text{otherwise} \end{cases}$ and P_n^m is the associated Legendre function fulfilling

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

In order to make computations easier we chose a permuted assignment to Cartesian coordinates, namely:

$$\begin{aligned}x_1 &= r \cos \varphi \cos \lambda \\x_2 &= r \sin \varphi \\x_3 &= r \cos \varphi \sin \lambda\end{aligned}$$

Some more details for the following lemma can be found in [1]:

Lemma 6.2. In order to make the formulae simpler we will denote (for $|l| > 1$):

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

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 $D_{id} = 1$

$$D_{id} Y_n^l = 1 \cdot Y_n^l$$

Differential Operator $D_r = x_1 \partial_1 + x_2 \partial_2 + x_3 \partial_3$

$$D_r Y_n^l = -(n + 1) \cdot Y_n^l$$

Differential Operator $D_{x_1} = \partial_1$

$$\begin{aligned}D_{x_1} Y_n^0 &= -\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+1)(n+2)}{2}} \cdot Y_{n+1}^1 \\D_{x_1} Y_n^{-1} &= -\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^{-2} \\D_{x_1} Y_n^1 &= +\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{n(n+1)}{2}} \cdot Y_{n+1}^0 - \sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^2 \\D_{x_1} Y_n^l &= +\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n-|l|+1)(n-|l|+2)}{4}} \cdot Y_{n+1}^{l_-} \\&\quad - \sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+|l|+1)(n+|l|+2)}{4}} \cdot Y_{n+1}^{l_+}\end{aligned}$$

Differential Operator $D_{x_2} = \partial_2$

$$\begin{aligned}
D_{x_2} Y_n^0 &= -\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+1)(n+2)}{2}} \cdot Y_{n+1}^{-1} \\
D_{x_2} Y_n^1 &= -\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^{-2} \\
D_{x_2} Y_n^{-1} &= +\sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{n(n+1)}{2}} \cdot Y_{n+1}^0 + \sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+2)(n+3)}{4}} \cdot Y_{n+1}^2 \\
D_{x_2} Y_n^l &= l_s \sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n-|l|+1)(n-|l|+2)}{4}} \cdot Y_{n+1}^{-l-} + \\
&\quad l_s \sqrt{\frac{2n+1}{2n+3}} \sqrt{\frac{(n+|l|+1)(n+|l|+2)}{4}} \cdot Y_{n+1}^{-l+}
\end{aligned}$$

Differential Operator $D_{x_3} = \partial_3$

$$D_{x_3} Y_n^l = -\sqrt{\frac{2n+1}{2n+3}} \sqrt{(n+1-l)(n+1+l)} \cdot Y_n^l$$

Differential Operator $D_{-x_1} = x_3 \partial_2 - x_2 \partial_3$

$$\begin{aligned}
D_{-x_1} Y_n^0 &= -\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^{-1} \\
D_{-x_1} Y_n^1 &= -\sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^{-2} \\
D_{-x_1} Y_n^{-1} &= +\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^0 + \sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^2 \\
D_{-x_1} Y_n^l &= l_s \sqrt{\frac{(n-|l|+1)(n+|l|)}{4}} \cdot Y_n^{-l-} + l_s \sqrt{\frac{(n-|l|)(n+|l|+1)}{4}} \cdot Y_{n+1}^{-l+}
\end{aligned}$$

Differential Operator $D_{-x_2} = x_3 \partial_1 - x_1 \partial_3$

$$\begin{aligned}
D_{-x_2} Y_n^0 &= -\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^1 \\
D_{-x_2} Y_n^{-1} &= -\sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^{-2} \\
D_{-x_2} Y_n^1 &= +\sqrt{\frac{n(n+1)}{2}} \cdot Y_n^0 - \sqrt{\frac{(n-1)(n+2)}{4}} \cdot Y_n^2 \\
D_{-x_2} Y_n^l &= +\sqrt{\frac{(n-|l|+1)(n+|l|)}{4}} \cdot Y_n^{l-} - \sqrt{\frac{(n-|l|)(n+|l|+1)}{4}} \cdot Y_{n+1}^{l+}
\end{aligned}$$

Differential Operator $D_{-x_3} = x_2 \partial_1 - x_1 \partial_2$

$$D_{-x_3} Y_n^l = l \cdot Y_n^{-l}$$

7 Numerics

We tested the split operator approach for a set of simulated satellite data. Because there are a number of different mathematical procedures involved which are not part of this article we chose to do a very short presentation. A much more exhaustive treatment can be found in [1].

Looking at the satellite GOCE, it will return the second derivatives of the geopotential field in all possible directions. Currently one just uses the derivative pointing two times in the radial direction. We observed that the bias/variance ratio was reduced significantly by the use of split operators and hence the incorporation of all possible directions. Please note that the bias/variance ratios are increasing in both cases due to the ill-posed nature of the problem and that the both curves are almost parallel because the variance is the same (of course) in both cases.

This suggests that at least for some problems like this one observed in satellite geodesy that the use of split operators is worth a consideration.

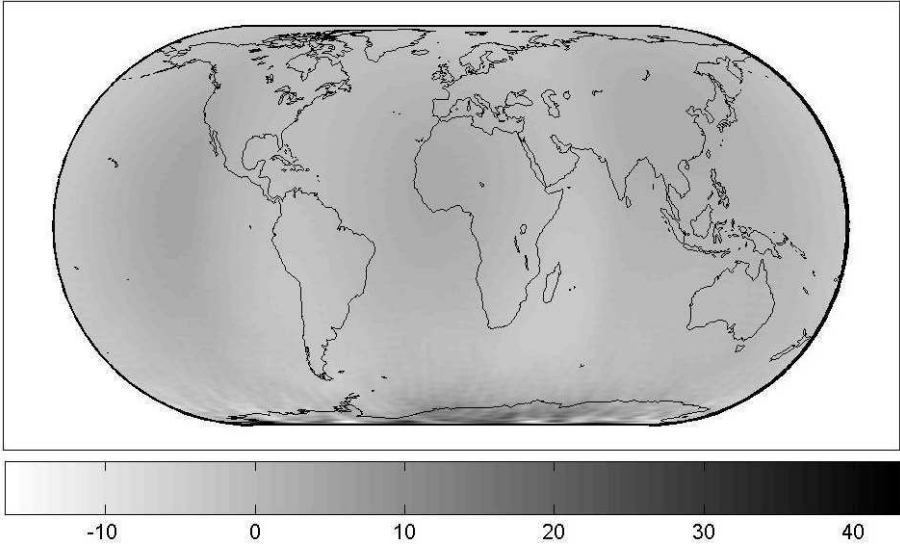


Figure 1: Error using all possible derivatives

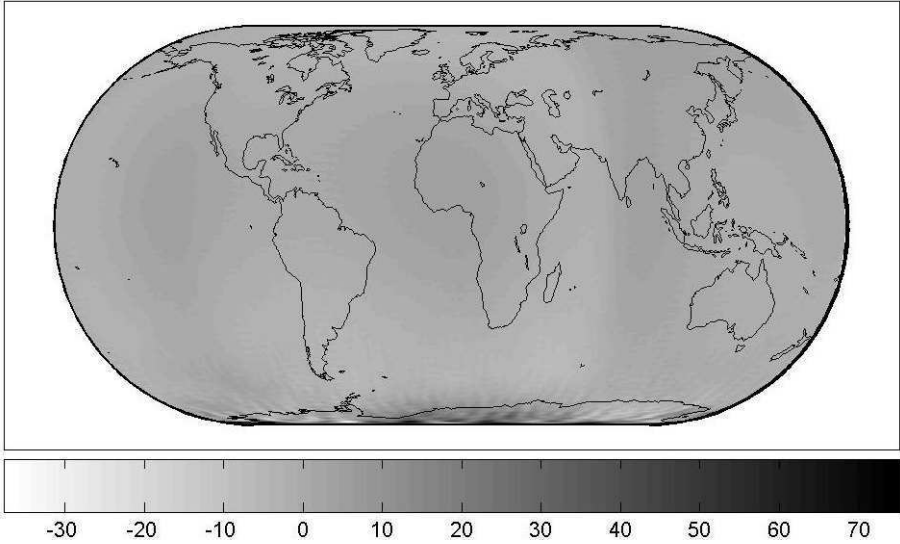


Figure 2: Error just using the radial derivative

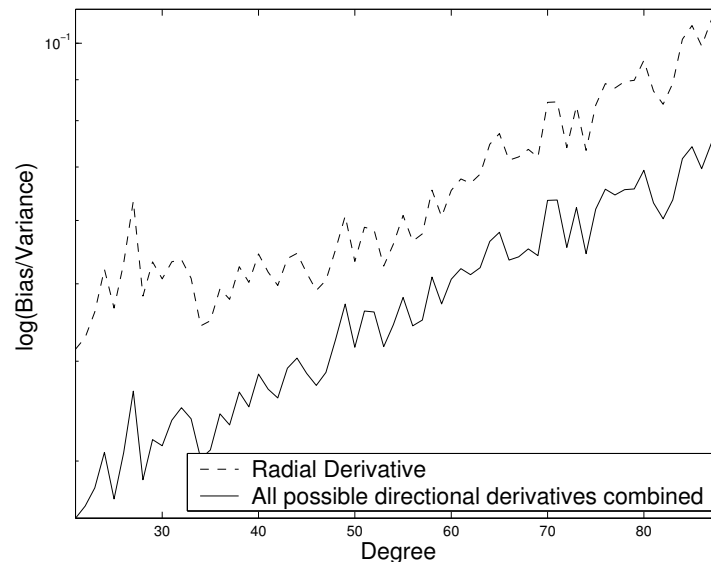
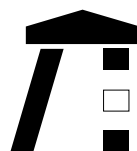


Figure 3: Bias/Variance ratio

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