The Adjoint State Method: A Tutorial

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Abstract

While numerical algorithms based on the Adjoint State Method (ASM) are becoming increasingly more popular in the geophysical community, the underlying mathematics is much less understood. The ideas behind the algorithm are hidden in complicated algebraic manipulations of differential equations. The purpose of this document is to provide an easy–to–understand introduction of the fundamentals of the ASM and show derivations based on implicit differentiation and Lagrange multipliers. Once understood, I demonstrate how to apply the ASM algorithm to Geophysical problems under more complicated and realistic situations.

1 Introduction

When I took courses in Inversion Theory, we learned about the linear inversion problem

$$Au = f \tag{1.1}$$

where A is a matrix and u is a vector. At that time, I understood that if we knew A and f then we could find u. If A is non–singular then

$$u = A^{-1} f.$$

But in general A is not even a square matrix. After this we learned about the least square method to solve 1.1, and solutions based on the steepest descent, conjugate gradients and other methods.

We were taught that u belongs to the model space and f to the data space.

Now, working on a Full Waveform Inversion (FWI) problem I found that u is in the data space. Where is the model?

The problem that we are trying to solve here is a bit more interesting than the problem on equation 1.1. It is

$$A(p)u = f \tag{1.2}$$

where now $A(p)$ is a matrix function of some model parameters p. Now, in problem 1.2 the data space is the space of u's and the model space is the space of p's.

Whether A is a matrix or a more general operator the problem in equation 1.2 in abstract is the same. I present the problem in two ways, the matrix version (section 2) and a differential–equation based version(section 3). From this presentation a general template is extracted that could be used in general. representation, a generally–applicable template is extracted that can be applied to practical applications currently deployed by the seismic exploration community. Finally, some numerical computations demonstrate the validity of the method. Two appendices are included to make the tutorial self–contained. One on the Fréchet and Gâteaux derivatives, which might not be familiar to geophysicists, and another in adjoint operators. The results on both of the appendices are used frequently in the main part of the document.

According to Yedlin, [11] the ASM started with Lagrange as early as 1760, who introduced the adjoint operator. We show here how the method can be derived from Lagrange multipliers. Among many contributors to the invention of the method we acknowledge Maurice René Fréchet and René Gâteaux (see Appendix A which shows an important part of their contributions). The method as we know it today was developed by Marchuk [9].

In Geophysics, the first important work relevant to seismic exploration is by Lailly [10] in 1983. Lailly's paper was framed in a mathematical language which is not well suited for geophysicists. Tarantola, [1] published the method of inversion using the ASM method in a simpler language. After this, it was clear that finding the gradient of descent was much like performing Reverse Time Migration (RTM) on residual data. However it took significant advances in computer science and hardware to make this approach practical. Only recently, more than 20 years after the first derivation of the seismic inversion problem, can we apply this compute–intensive method in both time

and frequency domain implementations. Pratt, [6], provides a good overview of publications since Lailly's original work. There are many publications more recent contributions, but in this context, I only mention Plessix [4], and Fichtner et. al., [5] who present some good theoretical foundations.

2 The Matrix Version

In this section, I show how obtain an approximate solution for equation 1.2 for p, provided we know A and f and a physical realization of the experiment that is captured by equation 1.2. The solution of this problem illustrates the ASM.

We focus in the problem

$$A(p)u = f \tag{2.3}$$

where f is a source term, u is a forward modeled field and $A(p)$ is a modeling equation. For this document we assume that the scalars are all real (no complex). So we think of $A(p)$ as a matrix in the space $\mathbb{R}^{m\times n}$, $u \in \mathbb{R}^n$, and $f \in \mathbb{R}^m$. We assume that a physical system records data d which corresponds to this modeling experiment and we only have one instance of that data d. We want to know how to find p with the knowledge of A, f and the data realization d.

For example, we can say that $A(p)$ is given in $\mathbb{R}^{2\times 2}$

$$A(p) = \begin{pmatrix} 3p_1 & \exp(p_2) \\ \log p_3 & 5 \end{pmatrix}$$

and equation 2.3 takes the specific form

$$\begin{pmatrix} 3\,p_1 & \exp(p_2) \\ \log p_3 & 5 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \end{pmatrix} \tag{2.4}$$

The question here is that without knowing u, we try to find $p = (p_1, p_2, p_3)$. At first glance, this looks hopeless, but recall that we also have some data measurements $d = (d_1, d_2)^T$ obtained from the correct model p. These data should be close to the forward modeled field u, assuming the modeling equations captured in A are correct.

- Does this system has a solution for p?

- If it does, is it unique?

It is obvious that even in this particular toy example, the system is highly non–linear as a function of p. It is a short toy matrix. We observe that if a system is linear, then there would be a unique solution (non–singular matrix of coefficients), no solution (the right term is not in the range of the matrix) or an infinite number of solutions (the null space has dimension 1 or larger). Geometrically, planes can intersect along one point (like a corner in an office room); in a line, like an edge in an office room, or not intersect at all (like two parallel walls in an office room). However when the equation is non–linear, the planes and lines turn to curved surfaces and wiggles. These objects can intersect in a finite discrete set of points, in only 1 point, in a discrete infinite set of points or in a continuum set of points. The concept of existence and uniqueness is not obvious in this context. Non–linear equations are not as well understood as linear equations.

The problem is more complex when the dimension of the spaces under consideration grow. Typical geophysical problems deal with vector spaces of dimensions of the order of millions and more.

For problems this complicated, unfortunately, we only can say that since we have some instance d of a physical realization, we can play with the u's and find some parameters p which are consistent, up to a "small" error, with system 2.3.

In this way we want to set up an optimization problem. The most obvious optimization problem is the least square problem where the objective (cost) function is given by

$$\mathcal{C}(p) = \frac{1}{2} \left\| u(p) - d \ , \ u(p) - d \right\|^2 = \frac{1}{2} \left\langle u(p) - d \ , \ u(p) - d \right\rangle. \tag{2.5}$$

where it is obvious that u depends (implicitly) on p in equation 2.3 and the data space is a Hilbert space where we can take inner products.

So, the most we can do (assuming no other constraints) is to minimize the objective function $\mathcal{C}(p)$. But the question here is

- Is the objective function $\mathcal{C}(p)$ convex?

Convexity of the objective function translates into uniqueness of the solution (which would be good news). Unfortunately since in general u is non–linear as function of p, then we can foresee that $\mathcal{C}(p)$ is highly non–linear as a function of p. Non–linearity creates wiggles with peaks and valleys. Clearly

$\mathcal{C}(p)$ is now non–convex and does not have an obvious unique minimum. Additional constraints help to reduce the space of solutions. One special situation we want to comment on is a sinusoidal dependency of the modeling equation on a parameter p, for example terms such as $\sin \omega p_i$. This is bad news, because sinusoidal functions wiggle for ever and could oscillate very rapidly (for high frequencies). Fortunately for our geophysical applications the parameters in the analytical representations are low–order polynomials or simple algebraic multipliers or dividers.

From calculus, if we want to find a minimum, we take the gradient and make it zero. That is, we find the Fréchet derivative (see Appendix A) of the cost function 2.5 and make it zero, or

$$\frac{d\mathcal{C}(p)}{dp} = \nabla_p \mathcal{C}(p) = \langle u_p \ , \ u - d \rangle = 0.$$

with $u_p = du/dp$.

However in practice the data are noisy,the modeling equations inadequately describe the physical system and the computer evaluations have limited accuracy. In other words, we cannot match the data perfectly to the modeled field u. Besides, we do not know p to start with, and if we use an initial guess of p_0, the chances to get this p_0 to fit the data are small, so the best we can do is a descent method, where we start somewhere along the hypersurface representing the cost function and descent toward the minimum. If that minimum happens to be the wrong local minimum we are out of luck and should perturb the initial guess p_0 to move to another convex zone. Of course, this assumes that the surface (or hypersurface) does not oscillate too rapidly as for example close to zero for a function of the form $\sin(1/x)$. Fortunately, this is typically not the case.

Once the gradient $\nabla_p \mathcal{C}(p_0)$ is found, then it can be used to move our initial guess p_0 to a "closer" point p_1 by using optimized descent methods which are outside of the scope of this document. We will only focus on the gradient and the process of how to obtain it.

So, let us forget about the gradient being zero and compute

$$\frac{d\mathcal{C}(p)}{dp} = \nabla_p \mathcal{C}(p) = \langle u_p \ , \ u - d \rangle. \tag{2.6}$$

To find the gradient, we need to know u_p. We can find u_p in two different ways

- Find u from equation 2.3. That is, if $A(p)$ is non–singular (if $A^{-1}(p)$ exists)

$$u = A(p)^{-1} f$$

and from here take the derivative of du/dp. However $A(p)$ could be singular, so we have no way to directly compute u_p. In wave propagation we can find u as a solution of the wave equation using finite differences or ray tracing methods. However u has a domain which in practice is a huge grid and each grid point allocates a component of the parameter vector p. If we want to compute the gradient, we need to know the change along each individual cell, but this change needs to be computed by modeling at least two instances (for the central finite difference star) per cell. A 2D velocity model of 1000×1000 a million cells will need 2 million modeling experiments. New parameters (such as density ρ for example) will increase the size of these computations linearly with the number of parameters. A 3D experiment would be prohibitively expensive. We need to find alternative methods to find the gradient and this is the main motivation behind the ASM. Which we illustrate next.

- Take the implicit derivative in 2.3. This should always work. That is

$$A_p u + A u_p = 0,$$

so

$$A u_p = -A_p u.$$

In this equation we are free to take inner product with whatever function we want in the Hilbert space of u's. That is, we can think about a "test" function v such that

$$\langle A u_p \ , \ v \rangle = \langle -A_p u \ , \ v \rangle$$

and if the adjoint of A exists (it is the transposed in the case of real matrices), and we call it A^* then

$$\langle \, u_p \ , \ A^* v \rangle = \langle -A_p u \ , \ v \rangle \tag{2.7}$$

So, by looking to the gradient in equation 2.6, we reduce the problem to

(i) Find u such that

$$A\,u = f.$$

The forward propagating problem.

(ii) Find v such that

$$A^* v = u - d \tag{2.8}$$

The backwards propagating problem. This is the key step in the Adjoint State method. If we can solve this system, then we can completely avoid the computation of the costly derivative u_p. Instead, we evaluate the right side of equation 2.7

(iii) and apply this v to

$$\langle -A_p u\ ,\ v \rangle. \tag{2.9}$$

Note that since $p = (p_1, \cdots, p_n)$ is a vector, we have that

$$\nabla_p A = A_p = \begin{pmatrix} A_{p_1} \\ A_{p_2} \\ \vdots \\ A_{p_n} \end{pmatrix}$$

Here only two systems of the same order of the system $Au = f$ have to be solved (instead of 2 million for the 1000×1000 2D velocity model. Note that the least amount of terms to compute a derivative using central finite differences is 2.). In section 5 I show an implementation of the algorithm using the acoustic wave equation with constant density which demonstrates numerically the validity of the method.

In example 2.4, all the elements to compute du/dp are easy to find. For example

$$A_{p_2} = \begin{pmatrix} 0 & \exp(p_2) \\ 0 & 0 \end{pmatrix}$$

and

$$A^*(p) = \begin{pmatrix} 3p_1 & \log p_3 \\ \exp(p_2) & 5 \end{pmatrix}$$

So we need to solve first for v in

$$A^*(p)u = \begin{pmatrix} 3p_1 & \log p_3 \\ \exp(p_2) & 5 \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \begin{pmatrix} u_1 - d_1 \\ u_2 - d_2 \end{pmatrix}$$

and then compute the gradient as

$$\frac{\partial \mathcal{C}}{\partial p_i} = \langle -A_{p_i} u \ , \ v \rangle.$$

2.1 The Lagrange Multipliers Approach

We can write the optimization problem as follows:

$$\begin{aligned} &\text{minimize for } p \\ &\mathcal{C}_L(p, \lambda) \ = \ \alpha \langle u(p) - d \ , \ u(p) - d \rangle + \beta \langle L(p) \ , \ \lambda \rangle \end{aligned} \tag{2.10}$$

$$L(p) = A(p)u - f \equiv 0. \tag{2.11}$$

Since $L(p) \equiv 0$, β and λ could have any value. Now, any value of p, which minimizes a function, should minimize that function when scaled by $\alpha > 0$. So we are not changing the solution by imposing the constants $\alpha > 0$ and β. However, as we show below, we are changing the gradient (up to a scale factor).

Then, the stationary condition on the extended objective function implies that

$$\frac{\partial \mathcal{C}_L}{\partial p} \ = \ 0 \quad , \quad \frac{\partial \mathcal{C}_L}{\partial \lambda} = 0.$$

The right equation does not provide any new information. It just produces $L(p) = f$ which we already know. From the left equation we find

$$\alpha \langle u_p \ , \ u - d \rangle + \beta \langle A_p u \ , \ \lambda \rangle + \beta \langle A u_p \ , \ \lambda \rangle = 0. \tag{2.12}$$

Because we have freedom to choose λ, we can choose λ such that

$$A^*\lambda = u - d \tag{2.13}$$

then from the previous two equations:

$$\begin{aligned} 0 &= \alpha\langle u_p\ ,\ u-d\rangle + \beta\langle A_p u\ ,\ \lambda\rangle + \beta\langle u_p\ ,\ A^*\lambda\rangle \\ &= (\alpha+\beta)\langle u_p\ ,\ u-d\rangle + \beta\langle A_p u\ ,\ \lambda\rangle \end{aligned}$$

so

$$\langle u_p\ ,\ u-d\rangle = -\frac{\alpha}{\alpha+\beta}\,\langle A_p u\ ,\ \lambda\rangle. \tag{2.14}$$

When $\alpha = 1/2$, $\beta = 0$ we have the original optimization problem, and this equation matches equation 2.9. Different combinations of $\alpha > 0$ and β produces different gradients but all of them have the same direction and different magnitude. In this sense the Lagrange multipliers analysis sets up a more general framework for the same problem which leads to a gamma of gradients.

In summary, the algorithm is as follows:

(i) Solve equation 2.11

$$Au = f.$$

(ii) Solve the adjoint state equation 2.13

$$A^*\lambda = u - d,$$

for λ and

(iii) find

$$-\frac{\alpha}{\alpha+\beta}\,\langle A_p u\ ,\ \lambda\rangle, \tag{2.15}$$

which according to equation 2.14 is the same as

$$\langle u_p\ ,\ u-d\rangle = \nabla_p \mathcal{C}$$

So we found that the Lagrange multipliers λ correspond with the adjoint state variable v above. By comparing equations 2.15 and 2.9. We see that 2.9 can be obtained by simply choosing $\alpha = 1/2, \beta = 0$ in the cost function $\mathcal{C}_{\mathcal{L}}$ defined in equation 2.10.

In what follows we will use the optimization function 2.10 with $\alpha = 1/2$ and $\beta = 0$.

In practice Lagrange multipliers are used when additional constraints are added to the cost function. For example constraints on smoothness, mask functions or preconditioning; such as for example, adding well logs information to the seismic (Wang et. at., [3]).

3 The Differential Equation Version

3.1 The ASM by Example

Here is the simplest example I can think of. Imagine we have a machine that can model some data d provided some source s on an object with some unknown parameters p. Let us assume that the experiment can be mathematically described by the equation

$$p(x)\frac{du(x)}{dx} = s(x). \tag{3.16}$$

with boundary conditions

$$u(a) = u(b) = 0.$$

where $a < x < b$.

Now, whatever the physics behind this toy problem, the idea is to perturb the parameter p so that with one instance of the measured data d we can estimate the actual p in the real model. This is an optimization problem. We define a simple objective (cost) function

$$\mathcal{C}(p) = \frac{1}{2}\left\|u(p) - d\right\|^2 = \frac{1}{2}\left\langle u(p) - d\ ,\ u(p) - d\right\rangle.$$

Which represents the misfit between the acquired data d and the synthetic data $u(p)$ for a model with parameters p. Note that we eliminate the dependence on x and show that u will depend on the model parameter p, through

the differential equation 3.16. This does not mean that u does not depend on x but the optimization is with respect to p and not with respect to x.

Optimization problems are seen usually as minimization problems. We want to minimize the cost function $\mathcal{C}(p)$ as a function of p. If we can get $\mathcal{C}(p) = 0$ that be would ideal, we have found a set of parameters p such that they model the data perfectly. In reality this does not happen, so we start with some initial parameter p_0 and through a gradient technique (the gradient of $\mathcal{C}(p)$) perturb it as a sequence of linear perturbations until find the best match (the minimum of $\mathcal{C}(p)$).

Note that $\mathcal{C}$ is a functional. That is, $\mathcal{C}$ is a function from the parameter space of functions to the real numbers. Here

$$\begin{aligned} p : A = [a, b] \subset \mathbb{R} &\rightarrow \mathbb{R} \\ x &\mapsto p(x). \end{aligned}$$

For example p could represent the linear density along a string, and

$$\begin{aligned} \mathcal{C} : U &\rightarrow \mathbb{R} \\ p &\mapsto \mathcal{C}(p) \end{aligned}$$

where U is the space of p functions of a one–dimensional real variable into the reals. So $\mathcal{C}$ lies in a space of functionals. Taking the derivative of u with respect to a point $p \in \mathcal{C}$ is not a common derivative with respect to a simple variable in $\mathbb{R}$. That is why we need the Fréchet derivative extension in Banach spaces. Appendix A shows some basic theory on Fréchet and Gâteaux derivatives, for which we will refer often in this document and are not assumed to be known by geophysicists.

We want to evaluate, the Fréchet derivative

$$D\mathcal{C}(p) = \frac{d\mathcal{C}}{dp} = \frac{1}{2}\langle u_p \, , \, u - d \rangle + \frac{1}{2}\langle u - d \, , \, u_p \rangle = \langle u_p \, , \, u - d \rangle \qquad (3.17)$$

with

$$u_p = \frac{\partial u}{\partial p} \quad {}^{1}$$

as the Gâteaux derivative of u seen as a function of p, and we use commu-

[1]Note that I choose the partial derivative sign instead of the total derivative. Not, because u depends on p and x. They leave in different spaces. The reason is that in practice p is a vector of parameters and we should think about partial derivatives with respect to p_i.

tation of the inner product of functionals in the real space (in the complex space we would need to conjugate numbers, but again, I want to simplify as much as possible).

So the evaluation of the gradient rest upon the evaluation of the Gâteaux derivative u_p at each point of the model. This operation (if computed by finite differences for example) is very expensive because the model space is usually large and we need to solve for u every time. Section 5 illustrates the details about why the computation of the Gâteaux derivative is so expensive.

The implicit derivative is a powerful tool in calculus because we can find derivatives in complicated relations (equations) without having to solve for the dependent variable (y) as a function of the independent variable (x). If solving algebraic equations could be hard, think about solving differential equations. This is precisely the point. We will find the derivative u_p without having to solve the differential equation for u and then take the derivative of this u. We look at u as a function of p where p is seen as a real variable (when indeed it is a function) and since the definition of the Gâteaux and Fréchet derivatives has the same functional structure as those in real variables, we can use all the nice properties that we learned in calculus about taking implicit derivatives including the chain rule, the product rule, etc.

Then, to find u_p, we use equation 3.16 and take implicit differentiation by defining

$$f(p) = p\frac{du(p)}{dx} - s \equiv 0.$$

So

$$\frac{df}{dp} = \frac{du(p)}{dx} + p\,\frac{du_p(p)}{dx} = 0 \tag{3.18}$$

As in implicit differentiation in algebraic equations, we still have to solve an equation after the implicit differentiation and, there, we hoped for an easier equation. Here we have to solve equation 3.18 for u_p, and it is apparent that we converted a relatively simple problem into a more complicated one. Here is where the ASM plays the protagonist role.

Let us assume a differentiable function $\phi = \phi(x)$. This function is the adjoint state. We take the inner product of equation 3.18 with $\phi(x)$ and obtain

$$\left\langle \frac{du(p)(x)}{dx}\ ,\ \phi(x) \right\rangle + \left\langle p\,\frac{du_p(p)(x)}{dx}\ ,\ \phi(x) \right\rangle = 0,$$

where now we look at $u(p)(x)$ as a function of x for each parameter p. Here I will drop the argument p when referring to u and to u_p. The inner product in function spaces is an integral with respect to x. Doing integration by parts (this is the way to find the adjoint) along the interval $[a, b]$, (and since $u(a) = u(b) = 0$) we find

$$-\left\langle u(x)\ ,\ \frac{d\phi(x)}{dx}\right\rangle - \left\langle u_p(x)\ ,\ \frac{d}{dx}[p(x)\,\phi(x)]\right\rangle = 0 \tag{3.19}$$

Since the function $\phi(x)$ is differentiable, but other than that, arbitrary; we can assume that

$$-\frac{d}{dx}[p(x)\,\phi(x)] = u(x) - d,$$

Now from equation 3.19, finally we have an explicit equation in u_p. Even better, compare the second term on this equation with the gradient of the cost function 3.17 and we find

$$D\mathcal{C}(p) = \nabla_P \mathcal{C} = \langle u_p\ ,\ u - d\rangle = \left\langle u\ ,\ \frac{d\phi}{dx}\right\rangle. \tag{3.20}$$

In conclusion, the gradient of the objective function is the inner product (zero lag cross–correlation) of the solution of the differential equation with the derivative of the solution ϕ of the equation

$$-\frac{d}{dx}[p(x)\,\phi(x)] = u(x) - d,$$

We see that for the differential operator $Lu = p(x)du(x)/dx$, with the operator $L(p) = p$, the adjoint operator is $L^*u = -d/dx[u(x)p(x)]$, so the factor function ϕ is determined by solving the problem

$$L^*\phi(x) = u(x) - d.$$

(the adjoint state equation)

Now, the operator acting on $\phi = \phi(x)$ is d/dx (for this toy problem), which in general is

$$d/dx = dL/dp,$$

so in this case we can write that the ASM

$$L(p)u = s$$

in three steps

- Solve the adjoint equation $L^*\phi(x) = u(x) - d$
- find the solution of $Lu = s$
- Find the inner product $\left\langle u \ , \ \frac{dL}{dp}\phi \right\rangle$.

I show next that this is the case in general.

3.2 The Problem in Abstract

The problem can be divided in several subproblems

- Set up the modeling equation with boundary conditions.
- Define the objective function.
- Find the gradient of the objective function in several steps.
  - Take implicit differentiation.
  - Instead of solving explicit for the partial derivatives in a complicated implicit equation, use the adjoint method to move the differential operators into test functions and so uncover the desired operator u_p from its derivatives.

We will follow those steps in what follows.

3.3 The modeling equations

The problem is posted by some differential equation, call it

$$Lu(x) = s(x), \tag{3.21}$$

where L is

$$L \equiv L\left((\partial_x)^{(k)}, p(x)\right),$$

Here k, the order of the derivative, can be any positive integer, but for the wave equation it is $k = 2$, $p(x)$ is a vector of scalar functions representing the model parameters, and $s(x)$ is a source term. The vector x contains the spatial coordinates and time; that is, x is located in the $n + 1$ dimensional real space $\mathbb{R}^{n+1}$.

This differential equation is subjected to some boundary and initial conditions

$$B_i(\Sigma(x)) = 0$$

$i = 1, \cdots n$, where Σ is some manifold wrapping the domain volume, in time and space and B_i is a function of the first n partial derivatives and $p(x)$. That is,

$$B_i = B_i(\partial_x^i, p(x)).$$

3.4 The Objective Function

Equation 3.21 implicitly defines u as a function of the vector of parameter scalar functions p. That is, $u = u(p)$.

Since we know the modeling problem $Lu = s$, we can create synthetic data u and match it with some acquired data d in order to minimize the mismatch error. We choose the following simple objective (cost) function

$$\mathcal{C}(p) = \frac{1}{2}\langle\, u(p) - d\ ,\ u(p) - d\,\rangle.$$

which solves the least squares minimization problem. In practice the data d are limited in many aspects. For example:

- To fit the problem, data should be recorded in a closed volume. In the case of surface seismic, data are acquired in only one of 6 faces of an imaginary rectangular prism of earth. This lack of aperture reduces spatial resolution on the seismic images.

- Even if data are collected in a closed surface, they are collected in samples and no continuously. Loss of resolution due to coarse sampling is an inherent problem to any inversion. It can be addressed by constraints and interative application, but this is out–of–scope for this tutorial.

- The amount of data could be insufficient to solve for the parameters p. This could increase the space of possible solutions. To remedy this problem, additional constraints should be added. These could be added by including a weight into the norm definition. This is the role of the

covariance matrix into the least squares weight for matrices. Preconditioning in the form of additional terms into the cost function further could reduce the space of solutions. For example adding smoothness to the solution implies simultaneous minimization of the function and its derivatives up to a certain order. That is, we think about a norm in a Sobolev space. This new problem with constraints can be seen as a Lagrange Multiplier's problem. We discussed this in section 2.1.

To find the minimum usually a descent method is used, and this implies finding the Fréchet derivative of $\mathcal{C}$ as a function of the parameter vector p. Since the cost function is a functional (its range is in the real numbers) this Fréchet derivative is a gradient.

3.5 The Gradient of the Objective Function

$$D\mathcal{C}(p) = \nabla_p \mathcal{C}(p) = \langle\, u_p \,,\; u(p) - d \,\rangle, \tag{3.22}$$

where we used the rules of differentiation for inner products. The problem here is that we need to find u_p and a naive approach could be to solve the differential equation $Lu = s$ for p and then take the Gâteux derivative of u as a function of p. As discussed above, this could be a very expensive process due to the large dimension of the parameter space for practical problems.

We will take implicit differentiation of the objective function, which does not imply to solve any system.

3.5.1 Implicit Differentiation

To compute $u_p(p)$ we build the following operator

$$F(u(p), p) = Lu - s \equiv 0$$

and take the total (Fréchet) derivative of F with respect to p. That is

$$\frac{dF}{dp} = \frac{\partial L}{\partial p} u + L\, u_p = 0. \tag{3.23}$$

So we see that u_p is under the operator L. To remove the operator L from u_p we use the ASM.

3.5.2 The Adjoint Method

To find the gradient of the objective function, we take the inner product of equation 3.23 with a differentiable function $\phi = \phi(x)$. That is

$$\left\langle \frac{\partial L}{\partial p} u \ , \ \phi \right\rangle + \langle L u_p \ , \ \phi \rangle = 0,$$

and from the definition of adjoint applied to the second term on the left, we rewrite this equation as

$$\left\langle \frac{\partial L}{\partial p} u \ , \ \phi \right\rangle + \langle u_p \ , \ L^* \phi \rangle = 0. \tag{3.24}$$

where L^* is the adjoint of the operator L.

The key trick now is to specify a test function. Since, to find the gradient in equation 3.22 we need to evaluate

$$\langle \, u_p, u(p) - d \, \rangle$$

by finding ϕ such that

$$L^* \phi = u(p) - d,$$

and from equation 3.24 we see that

$$D\mathcal{C}(p) = \nabla_p \mathcal{C}(p) = \langle u_p \ , \ u(p) - d \rangle = - \left\langle \frac{\partial L}{\partial p} u \ , \ \phi \right\rangle$$

So the recipe to find the gradient is as follows

3.5.2.1 Template

(i) Find the adjoint L^* and from this ϕ such that

$$L^* \phi = u(p) - d \tag{3.25}$$

This, in waveform inversion, is the reverse propagation from the residual between the synthetic data u and the acquired data d.

(ii) Find the forward solution u of the equation

$$Lu = s$$

and then compute

$$\frac{\partial L}{\partial p} u.$$

(iii) Find the negative of the zero lag cross–correlation between the forward field solution under the operator $(\partial L/\partial p)$ and the adjoint state variable ϕ. That is

$$D\mathcal{C}(p) = \nabla_p \mathcal{C}(p) = -\left\langle \frac{\partial L}{\partial p}\, u \ ,\ \phi \right\rangle. \tag{3.26}$$

In the next section I show a few classical examples and how they can be solved in a simple way by applying the template 3.5.2.1.

4 Examples

In all the examples shown here, we follow the same template shown in the section 3.5.2.1.

4.1 The homogeneous–isotropic wave equation

Let us assume density $\rho = 1$, and write the wave equation as

$$Lu = \left(\frac{1}{v^2} \frac{\partial}{\partial t^2} - \nabla^2 \right) u = s.$$

We should write the corresponding equations with 3.25 and 3.26. Here $p = v$.

We impose the boundary and initial conditions

$$\begin{aligned} u(\boldsymbol{x}, 0) &= 0 \\ \frac{\partial u(\boldsymbol{x}, 0)}{\partial t} &= 0 \end{aligned}$$

and the Sommerfeld radiation conditions

$$u(\boldsymbol{x},t)\Big|_{\boldsymbol{x}\to\infty} \longrightarrow 0.$$

(i) The operator

$$L = \frac{1}{v^2}\frac{\partial}{\partial t^2} - \nabla^2$$

is self–adjoint since v is independent of time, so $L = L^*$. Now we should find $\phi(\boldsymbol{x},t)$ such that

$$L^*\phi(\boldsymbol{x},t) = u(\boldsymbol{x},t) - d(\boldsymbol{x},t)$$

(ii) Step two is

$$\frac{\partial L}{\partial v} = -\frac{2}{v^3}\ \frac{\partial}{\partial t^2}$$

and step three

(iii)

$$D\mathcal{C}(v) = \nabla_v \mathcal{C}(v) = -\left\langle \frac{\partial L}{\partial v}u\ ,\ \phi(\boldsymbol{x},t)\right\rangle = \frac{2}{v^3}\ \left\langle \frac{\partial^2 u}{\partial t^2}\ ,\ \phi(\boldsymbol{x},t)\right\rangle.$$

4.2 Tarantola's 1984 inversion for K, ρ, and source s

Tarantola [1] uses the acoustic wave equation

$$Lu = \left[\frac{1}{K(\boldsymbol{x})}\frac{\partial^2}{\partial t^2} - \nabla.\left(\frac{1}{\rho(\boldsymbol{x})}\nabla\right)\right] u(\boldsymbol{x},t) = s(\boldsymbol{x},t).$$

Where we impose the boundary and initial conditions

$$\begin{aligned} u(\boldsymbol{x},0) &= 0 \\ \frac{\partial u(\boldsymbol{x},0)}{\partial t} &= 0 \end{aligned}$$

and the Sommerfeld radiation conditions

$$u(\boldsymbol{x},t)\Big|_{\boldsymbol{x}\ \to\ \infty} \longrightarrow 0.$$

(i) As we showed in equation B.51 the operator L is self–adjoint. That is,

$$L = L^*$$

From the point of view of analysis, self–adjoint operators have great advantages over non–self adjoint operators. For example the eigenvalues are real and the operator can be diagonalized. However, this is aside from the flow in this document. From the point of view of numerical implementations self–adjoint operators have a great advantage, since the same code used to compute the forward wavefield through L can be recycled to use the backward propagation wavefield through L^*.

Solve for

$$L^*\phi = L\phi = u(\boldsymbol{x}, t) - d(\boldsymbol{x}, t).$$

(ii) Step two: Find $u(\boldsymbol{x}, t)$ such

$$Lu(\boldsymbol{x}, t) = s(\boldsymbol{x}, t).$$

The gradient of L with respect to the model parameters.

$$\begin{aligned}
\frac{\partial L}{\partial K} &= -\frac{1}{K^2}\frac{\partial^2}{\partial t^2} \\
\frac{\partial L}{\partial \rho} &= \frac{\partial}{\partial \rho}\left[\nabla\left(\frac{1}{\rho}\right)\cdot\nabla\right] = -\nabla\frac{1}{\rho^2}\cdot\nabla
\end{aligned}$$

(iii) Step three:

$$D\mathcal{C}(v) = \nabla_v \mathcal{C}(v) = \begin{pmatrix} \mathcal{C}_K \\ \mathcal{C}_\rho \end{pmatrix}$$

With

$$\mathcal{C}_K = \left\langle \frac{\partial L}{\partial K} u \ , \ \phi(\boldsymbol{x}, t) \right\rangle = -\frac{1}{K^2}\left\langle \frac{\partial^2 u}{\partial t^2} \ , \ \phi(\boldsymbol{x}, t) \right\rangle \tag{4.27}$$

$$\begin{aligned}
\mathcal{C}_\rho &= \left\langle \frac{\partial L}{\partial \rho} u \ , \ \phi(\boldsymbol{x}, t) \right\rangle = -\left\langle \nabla\frac{1}{\rho^2}\cdot\nabla u \ , \ \phi(\boldsymbol{x}, t) \right\rangle \\
&= -\left\langle u \ , \ \nabla\frac{1}{\rho^2}\cdot\nabla\phi \right\rangle
\end{aligned} \tag{4.28}$$

Where in the last equality we used the fact that the operator acting on u is self–adjoint as shown in Appendix B. See table 1 line 4 (labeled "Mixed").

Equations 4.27 and 4.28 match the first two equation of Tarantola [1] (see his equation (A-6)) except that in Tarantola the density factor $1/\rho^2$ is outside of the ∇ operator and in my case it is inside the ∇ operator. Either Tarantola or myself have an error here.

4.2.0.2 Inversion for Source Signature: Tarantola also inverts for source signature. To invert for source signature we redefine the problem as follows:

$$L(K,\rho)(u) - s = \left[\frac{1}{K(\boldsymbol{x})}\frac{\partial^2}{\partial t^2} - \nabla.\left(\frac{1}{\rho(\boldsymbol{x})}\nabla\right)\right] u(\boldsymbol{x},t) - s(\boldsymbol{x},t) \equiv 0. \tag{4.29}$$

We assume that

$$s(\boldsymbol{x},t) = \delta(\boldsymbol{x}-\boldsymbol{x}_s)w(t)$$

where $w(t)$ is some wavelet that we want to invert for. We rewrite equation 4.29 as

$$\left[\frac{1}{K(\boldsymbol{x})}\frac{\partial^2}{\partial t^2} - \nabla.\left(\frac{1}{\rho(\boldsymbol{x})}\nabla\right)\right] u(\boldsymbol{x},t) - \delta(\boldsymbol{x}-\boldsymbol{x}_s)w(t) \equiv 0.$$

Doing implicit differentiation in this equation with respect to w we find

$$\left[\frac{1}{K(\boldsymbol{x})}\frac{\partial^2}{\partial t^2} - \nabla.\left(\frac{1}{\rho(\boldsymbol{x})}\nabla\right)\right] u_w - \delta(\boldsymbol{x}-\boldsymbol{x}_s) = 0$$

As done before, we take inner product with a differentiable function ϕ

$$\langle Lu_w(\boldsymbol{x},t)\ ,\ \phi(\boldsymbol{x},t)\rangle = \langle \delta(\boldsymbol{x}-\boldsymbol{x}_s)\ ,\ \phi(\boldsymbol{x},t)\rangle = \phi(\boldsymbol{x}_s,t).$$

We write

$$\langle u_w(\boldsymbol{x},t)\ ,\ L^*\phi(\boldsymbol{x},t)\rangle = \phi(\boldsymbol{x}_0,t)$$

So the gradient with respect to the source signature $w = w(t)$ is given by

$$D\mathcal{C}(w) = \nabla_w \mathcal{C} = \langle u_w \ , \ u(w) - d \rangle = \phi(\boldsymbol{x}_s, t)$$

where we assume that

$$L^* \phi(\boldsymbol{x}, t) = u(\boldsymbol{x}, t) - d(\boldsymbol{x}, t). \tag{4.30}$$

So to find the source signature, we should just solve the adjoint equation 4.30 and evaluate the solution at $\boldsymbol{x} = \boldsymbol{x}_0$. In fact this makes sense since equation 4.30 is back–propagating the wavefield from the receivers and collapsing at the source location $\boldsymbol{x}_s$. No modeling is required (as in RTM) because the modeling implies some source and we do not care about a synthetic source which has nothing to do with the field data.

Since the field ϕ in all cases is the solution to the wave operator

$$L^* \phi(\boldsymbol{x}, t) = u(\boldsymbol{x}, t) - d(\boldsymbol{x}, t)$$

The inversion for all parameters could be done simultaneously. The cross–correlation or signature extraction of the field changes on each case and could be done individually to build the global gradient with respect to all model parameters. The perturbation could be done individually (for each parameter) or simultaneously. These are details that pertain to the code implementation and will not be discussed here.

4.3 Elastic Wave Equation

The general anisotropic elastic wave equation is represented by the operators

$$L_{ik} u_k = \left[\rho \frac{\partial^2}{\partial t^2} - \frac{\partial}{\partial x_j} \left(c_{ijkl} \frac{\partial}{\partial x_l} \right) \right] u_k = f_i$$

Where we can label L_{ik} as the operator acting on the wavefield component u_k, excited by the source function f_i. Usually the source is written in terms of Dirac delta distributions, such as for example $A_i \delta(t - t_0) \delta(\boldsymbol{x} - \boldsymbol{x}_s)$ for a point source starting at time $t = t_0$ and located at the point $x = x_s$. Sometimes, instead of $\delta(t - t)$ we find the use of wavelets (Ricker or other).

The arguments for the wavefield u are $\boldsymbol{x}$ and t and the arguments for the density ρ and the stiffness tensor components c_{ijkl} are $\boldsymbol{x}$. We assume

Einstein's notation of sum over repeated indices. For the derivation of this equation see Aki and Richards [2].

For the adjoint operator we use zero boundary conditions

$$\begin{aligned} u_k(\boldsymbol{x}, 0) &= 0 \\ \frac{\partial u_k(\boldsymbol{x}, 0)}{\partial t} &= 0 \end{aligned}$$

and the Sommerfeld radiation conditions

$$u_k(\boldsymbol{x}, t)\Big|_{\boldsymbol{x} \Rightarrow \infty} \longrightarrow 0.$$

Before we apply the template 3.5.2.1 to solve the problem let us note that L_{ik} is really a 3×3 matrix of operators. Each operator L_{ik} solves a problem of a source f_i polarized in some direction e_i, for a receiver u_k recorded with a sensor responding to another direction e_k. The u_k are known as 9–component data, because the 9 possible combinations. Now, due to reciprocity only 6 combinations are independet. There should be a total of 9 data sets that we can use to compute the gradient. For the description below, each data set could be treated as a separated problem. Having a gradient for the 6 possible independent combinations of source and receiver polarization directions is still an expensive process in terms of the dimension of the combined vector space for all components. The signal–to–noise ratio of all data sets is different. Usually the best signal to ratio is for vertical components both at the source and at the receiver location. If done individually, then we can find 9 different gradients with respect to the same parameters. Indeed each cost function is different, because both the data and the modeling equations are different. Hence we do not have to expect the same gradients. However after updating the parameters they should be close to each other in all the 9 set of parameters. Redundancy is statistically good, but the stacking of those might have to be done with a weighted average. A problem of averages is that they tend to eliminate the hight frequencies and in WFI we want to enhance the high frequencies of the parameters. Hence, even though the one–by–one treatment is easier to understand, to formulate and perhaps to implement, I will treat all the L_{ij}s as a part of a single operator L.

We write the problem in matrix form as

$$Lu = \begin{pmatrix} L_{11} & L_{12} & L_{13} \\ L_{21} & L_{22} & L_{23} \\ L_{31} & L_{32} & L_{33} \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ f_3 \end{pmatrix} = f$$

This is an interesting problem because involves the matrix approach and the differential operator approach simultaneously. Here the inner product is both discrete and continuous. That is, for example for two functions f and g in the space of solutions, the inner product is given by

$$\langle f \ , \ g \rangle = \int_V f_i g_i \, d\boldsymbol{x} dt$$

(see equation B.44), where the sum along the dummy i index is from 1 to 3. Let us choose a test function $\Phi(\boldsymbol{x}, t) = (\phi_1(\boldsymbol{x}, t), \phi_2(\boldsymbol{x}, t), \phi_3(\boldsymbol{x}, t))^T$.

$$\langle Lu \ , \ \Phi \rangle = \langle L_{ik} u_k \ , \ \phi_i \rangle = \langle u_k \ , \ L^*_{ik} \phi_i \rangle = \langle u \ , \ L^* \Phi \rangle$$

where

$$(L^*)_{ik} = L^*_{ki} = L_{ki}.$$

Note that L_{ik} does not have to be equal to L_{ki} since c_{ijkl} is not necessarily equal to c_{kjil}. However from the properties shown in appendix B (see table 1) we see that L_{ik} is self–adjoint. That is

$$L_{ik} = L^*_{ik}.$$

Let us apply the template:

(i) Find $\phi_k = \phi_k(x, t)$, $k = 1, 2, 3$ such that

$$L^*_{ik} \phi_i = L_{ik} \phi_i = u_k(x, t) - d(x, t).$$

(ii) Find $u_k(x, t)$ such that

$$L_{ik} u_k(x, t) = f_i(x, t).$$

The gradient of L_{ik} with respect to the model parameter ρ is given by

$$\frac{\partial L_{ik}}{\partial \rho} = \frac{\partial}{\partial t^2}$$

Next, we want to find the gradient with respect to the stiffness parameters c_{ijkl}. If the c_{ijkl} were mutually independent then the operator $\partial L_{ik}/\partial c_{mnop}$ would be easy to find. That would be

$$\frac{\partial L_{ik}}{\partial c_{mnop}} = -\frac{\partial}{\partial x_j}\left(\delta_{im}\delta_{jn}\delta_{ko}\delta_{lp}\,\frac{\partial}{\partial x_l}\right) = -\frac{\partial}{\partial x_n}\left(\delta_{im}\delta_{ko}\frac{\partial}{\partial x_p}\right)$$

which is relatively simple as compared, for example, with the corresponding orthorombic equations. However we know that these parameters are not independent due to symmetries on the elastic tensor.

For the reader who is not familiar with Kronecker delta manipulations under Einstein's contraction notation, here is a tip that could be useful for syntax debugging. Dummy indices should appear exactly twice. If they appear either one, three or more times, check your derivation. Dummy indices should disappear after contraction with Kronecker deltas. In all analysis from here down, the free variables are only k (for u_k) and i (for the source f_i). Free variables only appear once. If two or three check your algebra. This is like dimensional analysis, here for indices, instead of units.

There are up to only 21 independent stiffness constants which can be independent, so a maximum of 22 gradient components [2]

In general for a given parameter p we should find:

$$\frac{\partial L_{ik}}{\partial p} = -\frac{\partial}{\partial x_j}\left(\frac{\partial c_{ijkl}}{\partial p}\frac{\partial}{\partial x_l}\right)$$

For example, for isotropic media (Aki and Richards, [2])

$$c_{ijkl} = \lambda\delta_{ij}\delta_{kl} + \mu(\delta_{ik}\,\delta_{jl} + \delta_{il}\delta_{jk}), \tag{4.31}$$

[2]When we make the model discrete, these 22 translate into 22 nx*ny*nz where nx, ny, nz are the dimensions of the velocity model.

hence

$$\begin{aligned}\frac{\partial L_{ik}}{\partial \lambda} &= -\frac{\partial}{\partial x_j}\delta_{ij}\delta_{kl}\frac{\partial}{\partial x_l} = -\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k} \\ \frac{\partial L_{ik}}{\partial \mu} &= -\frac{\partial}{\partial x_j}(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk})\frac{\partial}{\partial x_l} = -\delta_{ik}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l} - \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k}.\end{aligned}$$

(iii) For any medium

$$\mathcal{C}_\rho = \left\langle \frac{\partial L_{ik}}{\partial \rho}u_k \ , \ \phi_i \right\rangle = \left\langle \frac{\partial^2 u_i}{\partial^2 t} \ , \ \phi_i \right\rangle$$

For the isotropic case we found

$$\begin{aligned}\mathcal{C}_\lambda &= -\left\langle \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k}u_k \ , \ \phi_i \right\rangle \\ \mathcal{C}_\mu &= -\left\langle \delta_{ik}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l}u_k \ , \ \phi_i \right\rangle - \left\langle \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k}u_k \ , \ \phi_i \right\rangle.\end{aligned}$$

4.4 Transversely Isotropic Media with a Vertical axis of Symmetry: VTI

It is common to define the stiffness tensor in terms of the Voigt coefficients. Here $C_{IJ} = c_{ijkl}$ with the mapping

$$\begin{aligned} ij \mapsto I \quad , \quad kl \mapsto J: & \\ 11 \ \mapsto \ 1 \quad , \quad 22 \mapsto 2 \quad , \quad 33 \mapsto 3 & \\ 23, 32 \ \mapsto \ 4, \quad 13 \quad \text{and} \quad 31 \mapsto 5, \quad \text{and} \quad 12 \text{ and } 21 \mapsto 6, & \end{aligned}$$

The Voigt notation has the advantage of reducing the number of coefficients from 81 to 36 (from which at most 21 are different). The new matrix C_{IJ} is symmetric.

The relation between the stiffness coefficients c_{ijlk} and the Voigt coefficients C_{IJ} for VTI is given by

$$\begin{aligned} c_{ijkl} &= \lambda_{_{VTI}}\,\delta_{ij}\delta_{kl} + \mu_{_{VTI}}\,(\delta_{ik}\delta_{jl}+\delta_{il}\delta_{jk}) \\ &+ (C_{11}+C_{33}-2C_{13}-4C_{44})\,\delta_{i3}\,\delta_{j3}\,\delta_{k3}\,\delta_{l3} \\ &+ (C_{13}-C_{11}+2C_{66})(\delta_{i3}\,\delta_{j3}\,\delta_{kl}+\delta_{ij}\,\delta_{k3}\,\delta_{l3}) \\ &+ (C_{44}-C_{66})(\delta_{il}\,\delta_{j3}\,\delta_{k3}+\delta_{i3}\,\delta_{l3}\,\delta_{jk}+\delta_{ik}\,\delta_{j3}\,\delta_{l3}+\delta_{i3}\,\delta_{k3}\,\delta_{jl}), \end{aligned} \tag{4.32}$$

with

$$\begin{aligned}\lambda_{VTI} &= C_{11} - 2C_{66} \\ \mu_{VTI} &= C_{66}.\end{aligned}$$

Ikelle and Amundsen, [7]. This equation assumes that x_3 points along the symmetry axis.

While equation 4.32 is long, it is very convenient. It shows a linear relationship between the Voigt coefficients C_{IJ} and the stiffness coefficients c_{ijkl}. This will make the algebra simple when finding $\partial L_{ik}/\partial p$. In fact the gradient for the 5 VTI parameters: $C_{11}, C_{13}, C_{33}, C_{44}$ and C_{66} is found from the following simple derivations:

$$\begin{aligned}
\frac{\partial L_{ik}}{\partial C_{11}} &= -\frac{\partial}{\partial x_j}(\delta_{ij}\,\delta_{kl} + \delta_{i3}\,\delta_{j3}\,\delta_{k3}\,\delta_{l3} - \delta_{i3}\,\delta_{j3}\,\delta_{kl} - \delta_{ij}\,\delta_{k3}\delta_{l3})\frac{\partial}{\partial x_l} \\
&= -\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k} - \delta_{i3}\delta_{k3}\frac{\partial^2}{\partial^3 x_3} + \delta_{i3}\frac{\partial}{\partial x_3}\frac{\partial}{\partial x_k} + \delta_{k3}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_3} \\
\frac{\partial L_{ik}}{\partial C_{13}} &= -\frac{\partial}{\partial x_j}(-2\delta_{i3}\,\delta_{j3}\,\delta_{k3}\,\delta_{l3} + \delta_{i3}\,\delta_{j3}\,\delta_{kl} + \delta_{ij}\,\delta_{k3}\,\delta_{l3})\frac{\partial}{\partial x_l} \\
&= 2\delta_{i3}\delta_{k3}\,\frac{\partial^2}{\partial^2 x_3} - \delta_{i3}\frac{\partial}{\partial x_3}\frac{\partial}{\partial x_k} - \delta_{k3}\frac{\partial}{x_i}\frac{\partial}{\partial x_3} \\
\frac{\partial L_{ik}}{\partial C_{33}} &= -\frac{\partial}{\partial x_j}(\delta_{i3}\,\delta_{j3}\,\delta_{k3}\,\delta_{l3})\frac{\partial}{\partial x_l} = -\frac{\partial^2}{\partial^2 x_3} \\
\frac{\partial L_{ik}}{\partial C_{44}} &= -\frac{\partial}{\partial x_j}((\delta_{il}\,\delta_{j3}\,\delta_{k3} + \delta_{i3}\,\delta_{l3}\,\delta_{jk} + \delta_{ik}\,\delta_{j3}\,\delta_{l3} + \delta_{i3}\,\delta_{k3}\,\delta_{jl})\frac{\partial}{\partial x_l} \\
&= -\delta_{k3}\,\frac{\partial}{x_3}\frac{\partial}{\partial x_i} - \delta_{i3}\,\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_3} - \delta_{ik}\,\frac{\partial^2}{\partial^2 x_3} - \delta_{i3}\delta_{k3}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l} \\
\frac{\partial L_{ik}}{\partial C_{66}} &= -\frac{\partial}{\partial x_j}(\delta_{ik}\delta_{jl} - \delta_{il}\,\delta_{j3}\,\delta_{k3} - \delta_{i3}\,\delta_{l3}\,\delta_{jk} - \delta_{ik}\,\delta_{j3}\,\delta_{l3} - \delta_{i3}\,\delta_{k3}\,\delta_{jl})\frac{\partial}{\partial x_l} \\
&= \delta_{k3}\,\frac{\partial}{x_3}\frac{\partial}{\partial x_i} + \delta_{i3}\,\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_3} + \delta_{ik}\,\frac{\partial^2}{\partial^2 x_3} + \delta_{i3}\delta_{k3}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l} - \delta_{ik}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l} \\
&= \delta_{k3}\,\frac{\partial}{x_3}\frac{\partial}{\partial x_i} + \delta_{i3}\,\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_3} + \delta_{ik}\,\frac{\partial^2}{\partial^2 x_3} + (\delta_{i3}\delta_{k3} - \delta_{ik})\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l}.
\end{aligned}$$

These relationships are relatively simple since all derivatives are taken on linear relations. Modeling in terms of the c_{ijkl} or the C_{ij} coefficients is simpler than using other coefficients (such as Thomsen [8] parameters for example).

In addition, the gradient computation turn out to be simpler this way, since the relationship between the c_{ijkl} and the C_{IJ} is linear while the relationship between any of these and Thomsen's parameters (for example) is not. Here are the relations between the C_{IJ}'s and the Thomsen's parameters.

$$\begin{aligned} V_{PO} &= \sqrt{\frac{C_{33}}{\rho}} \\ V_{SO} &= \sqrt{\frac{C_{44}}{\rho}} \\ \epsilon &= \frac{C_{11} - C_{33}}{2\,C_{33}} \\ \delta &= \frac{(C_{13} + C_{44})^2 - (C_{33} - C_{44})^2}{2C_{33}(C_{33} - C_{44})} \\ \gamma &= \frac{C_{66} - C_{44}}{2\,C_{44}}. \end{aligned}$$

The success on Thomsen's notation comes from the geophysical interpretation of his parameters, however for numerical purposes the relation between the stiffness and the Voigt coefficients is more convenient. Thomsen's equations are easy to invert for C_{IJ} in terms of $V_{PO}, V_{S0}, \epsilon, \delta$ and γ. If those are the data that are given to FWI, then they can be converted simply to C_{IJ} form (using for example Seismic Unix "suop" and "suop2")

The final example is the transversely isotropic media with a horizontal axis of symmetry.

4.5 Transversely Isotropic Media with a Horizontal Axis of Symmetry: HTI

The relation between the stiffness coefficients c_{ijlk} and the Voigt coefficients C_{IJ} for HTI with the symmetry axis pointing in the x_1 direction is given by

$$\begin{aligned} c_{ijkl} &= \lambda_{_{HTI}}\,\delta_{ij}\delta_{kl} + \mu_{_{HTI}}\,(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk}) \\ &+ (C_{11} + C_{33} - 2C_{13} - 4C_{66})\,\delta_{i1}\,\delta_{j1}\,\delta_{k1}\,\delta_{l1} \\ &+ (C_{13} - C_{33} + 2C_{44})(\delta_{i1}\,\delta_{j1}\,\delta_{kl} + \delta_{ij}\,\delta_{k1}\,\delta_{l1}) \\ &+ (C_{66} - C_{44})(\delta_{il}\,\delta_{j1}\,\delta_{k3} + \delta_{i1}\,\delta_{l1}\,\delta_{jk} + \delta_{ik}\,\delta_{j1}\,\delta_{l1} + \delta_{i1}\,\delta_{k1}\,\delta_{jl}), \end{aligned}$$

with

$$\begin{aligned}\lambda_{_{HTI}} &= C_{33} - 2\,C_{44}\\ \mu_{_{HTI}} &= C_{44},\end{aligned}$$

which look almost like the VTI but switching the index 3 by the index 1 (Ikelle and Amundsen [7]). As with the previous example the gradient computation is obtained after finding the partial Gâteaux derivatives:

$$\begin{aligned}
\frac{\partial L_{ik}}{\partial C_{11}} &= -\frac{\partial}{\partial x_j}(\delta_{i1}\,\delta_{j1}\,\delta_{k1}\,\delta_{l1})\frac{\partial}{\partial x_l} = -\delta_{i1}\,\delta_{k1}\frac{\partial^2}{\partial^2 x_1}\\
\frac{\partial L_{ik}}{\partial C_{13}} &= -\frac{\partial}{\partial x_j}(-2\delta_{i1}\,\delta_{j1}\,\delta_{k1}\,\delta_{l1}) + \delta_{i1}\,\delta_{j1}\,\delta_{kl} + \delta_{ij}\,\delta_{k1}\,\delta_{l1})\frac{\partial}{\partial x_l}\\
&= 2\delta_{i1}\,\delta_{k1}\frac{\partial^2}{\partial^2 x_1} - \delta_{i1}\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_k} - \delta_{k1}\,\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_1}\\
\frac{\partial L_{ik}}{\partial C_{33}} &= -\frac{\partial}{\partial x_j}(\delta_{i1}\,\delta_{j1}\,\delta_{k1}\,\delta_{l1} - \delta_{i1}\,\delta_{j1}\,\delta_{kl} - \delta_{ij}\,\delta_{k1}\,\delta_{l1} + \delta_{ij}\delta_{kl})\frac{\partial}{\partial x_l}\\
&= -\delta_{i1}\delta_{k1}\frac{\partial^2}{\partial^2 x_1} + \delta_{i1}\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_k} + \delta_{k1}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_1} + \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k}\\
\frac{\partial L_{ik}}{\partial C_{44}} &= -\frac{\partial}{\partial x_j}(2(\delta_{i1}\,\delta_{j1}\,\delta_{kl} + \delta_{ij}\,\delta_{k1}\,\delta_{l1}) - (\delta_{il}\,\delta_{j1}\,\delta_{k3} +\\
&\quad \delta_{i1}\,\delta_{l1}\delta_{jk} + \delta_{ik}\,\delta_{j1}\,\delta_{l1} + \delta_{i1}\,\delta_{l1}\,\delta_{jl} + \delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk})\frac{\partial}{\partial x_l}\\
&= \delta_{k3}\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_i} + \delta_{i1}\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_k} + \delta_{ik}\frac{\partial^2}{\partial^2 x_1} + \delta_{i1}\frac{\partial^2}{\partial^2 x_1}\\
&\quad \delta_{ik}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l} + \frac{\partial}{\partial x_i}\frac{\partial}{\partial x_k} - 2\delta_{i1}\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_k} - 2\delta_{k1}\frac{\partial}{\partial x_i}\frac{\partial}{\partial x_1}\\
\frac{\partial L_{ik}}{\partial C_{66}} &= -\frac{\partial}{\partial x_j}(\delta_{il}\,\delta_{u1}\,\delta_{k3} + \delta_{i1}\,\delta_{k1}\,\delta_{jk} + \delta_{ik}\,\delta_{j1}\,\delta_{l1}\\
&\quad + \delta_{i1}\,\delta_{k1}\,\delta_{jl} - 4\,\delta_{i1}\,\delta_{j1}\,\delta_{k1}\,\delta_{l1})\frac{\partial}{\partial x_l}\\
&= 4\delta_{i1}\delta_{k1}\frac{\partial^2}{\partial^2 x_1} - \delta_{k3}\frac{\partial}{\partial x_1}\frac{\partial}{\partial x_i} - \delta_{i1}\frac{\partial}{\partial x_k}\frac{\partial}{\partial x_1} - \delta_{ik}\frac{\partial^2}{\partial^2 x_1} - \delta_{i1}\delta_{k1}\frac{\partial}{\partial x_l}\frac{\partial}{\partial x_l}.
\end{aligned}$$

Since the wave operators are self–adjoint then the steps to compute ϕ and u are done with the same anisotropic modeling equation. The only algebraic computations that we have to do are those for $\partial L_{ik}/\partial p$ as shown here.

The same type of computations could be carried out for orthorombic media, but the algebra is more complex.

Next, I show a numerical example on the acoustic wave equation to test the validity of the results proved on this document.

5 Numerical Test

For the numerical tests, I evaluate the gradient of the objective function corresponding to the acoustic isotropic, constant density wave equation, a generalization of the homogeneous case discussed in section 4.1.

The information that we need is an initial guess p_0 which in this case is the initial velocity model shown in Figure 1.

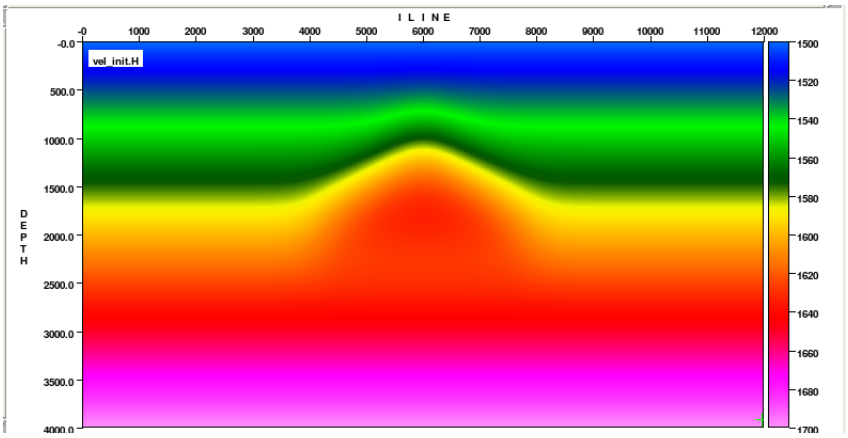

Figure 1: Initial Guess

For reference only, the exact velocity model is shown in Figure 2

I modeled 79 shot gathers, each with 240 receivers. On each receiver I computed a synthetic trace with 1000 samples, each sample with a sampling rate of 1 millisecond. Figure 3 shows a shot record simulated on the right side of the model. The distance between shots is 100 m, the distance between receivers is 50 meters in a split–spread acquisition pattern. The source used for the modeling is a Ricker wavelet with 10 Hz central frequency and a maximum frequency of 20 Hz. The grid size for the modeling is of $10 \times 10\,\mathrm{m}^2$.

I computed directional derivatives using two different methods and compare the results. One of the methods is the ASM, which is the topic of this

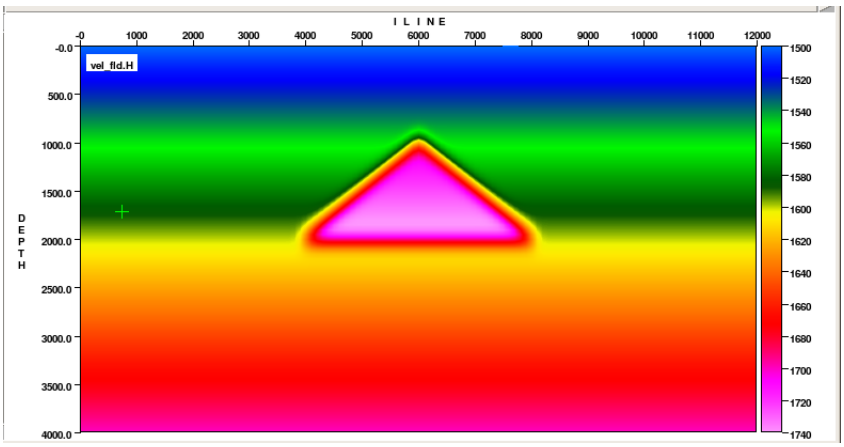

Figure 2: True Velocity

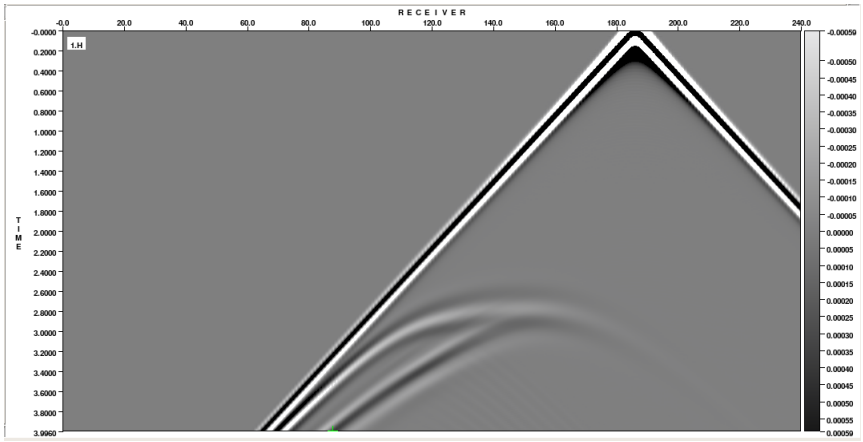

Figure 3: A shot gather simulated on the right side of the model

document.

Figure 4 shows the result of computing the gradient using the ASM.

The other method is to use a Gâteaux central difference equation

$$\frac{\mathcal{C}(v + s\,\delta\,v_i) - \mathcal{C}(v - s\,\delta\,v_i)}{2s} \tag{5.33}$$

where v is the initial guess shown in Figure 1 and δv_i is the following vector

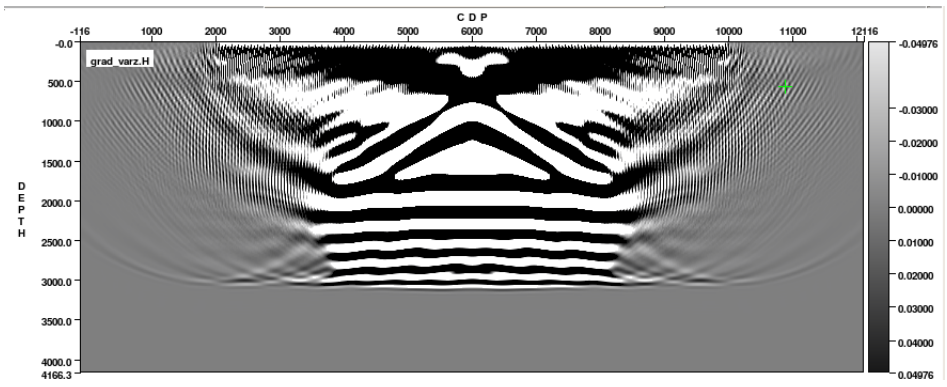

Figure 4: Gradient from the ASM: The Fréchet derivative.

(matrix, or better, the tensor direction)

$$\delta\, v_i = \begin{pmatrix} 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \tag{5.34}$$

The number of columns is `nx=120` (the number of traces of the velocity model, sampled at 100 m) and the number of rows is `nz=400`(number of depth samples with sampling rate of 10 m each). The only raw with a 1 in each column is the i–th row. All other rows are zero. We need `nz` of these vectors to expand our space of interest.

Ideally we would like to use a perturbation matrix δv_{jk} with entries δ_{jk}, tht is, all zeroes except for a single 1 in the `jk` entry. However this would imply that to compute all central derivatives we would need to run `4*nx*nz,`that is, `192000` modeling problems (the cost of 96000 RTMs).

Precisely, we want to test the validity of the following formula

$$D\mathcal{C}(v)(\delta v_i) \approx \frac{\mathcal{C}(v + s\,\delta\, v_i) - \mathcal{C}(v - s\,\delta\, v_i)}{2s}$$

where the left symbol $D\mathcal{C}(v)(\delta v_i)$ represents the Fréchet derivative of the cost function $\mathcal{C}(v)$ on the initial guess velocity model v in Figure 1 and evaluated (inner product with) at the increment vector δv_i in equation 5.34,

while the right expression is the central difference Gâteaux derivative. We choose $s = 1, 10, 20, 30, 40$ in this experiment. In order to compare the two differential approaches we need to take the dot product of the Fréchet derivative shown in Figure 4 with the vector δv_i for each depth. This will provides us with 401 points (to cover depths from 0 to 4000 m). At each point the value is the differential computed by the two methods. Figure 5 shows the comparison of the differential found using the Fréchet derivative (the dark brown circles) with the Gâteaux derivative for $s = 1$ (red crosses), $s = 10$ (green "x"s), $s = 20$ (dark blue stars *) $s = 30$ (purple squares) and $s = 40$ (light blue solid squares).

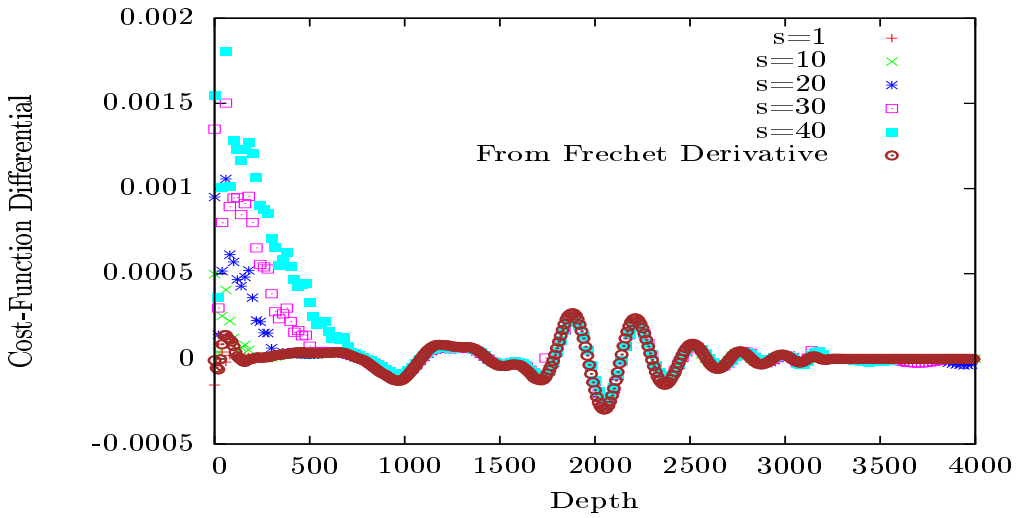

Figure 5: Differential along the vector δv, evaluated using the central differences 5.33 (Gâteaux derivative) for $s = 1, 10, 20, 30, 40$ and from the Fréchet derivative.

More precisely, here is a pseudo–code of the procedure to compute the data in Figure 5.

```
Compute the Frechet derivative (Gradient) in Figure 4

for each z (index i=0,400)
{
    /* inner product of tensors Frechet with dvi=(0,0,....1,1,....0,0) */
    left[i] = DC(V) . dv[i] /* sum DC[V[i]) along row "i"
```

```
    for each s (1,10,20,30,40)
    {
         /* compute the Gateaux Derivative */
         right[i][s] = ( C(V + s dv[i]) - C(V)/(2 s)
    }
}
```

The plot corresponds to the 401 points `left[i]` of the Fréchet derivative and the same number of points `right[i][s]` for each $s = 1, 10, 20, 30$ and 40 on the Gâteaux derivatives.

While the Fréchet derivative in this example is a tensor of rank 2, we are more familiar with gradients which are tensors of rank 1. That is, we know that the partial derivative could be computed from the formula

$$\frac{\partial \mathcal{C}}{\partial v_i} = \lim_{s \to 0} \frac{\mathcal{C}(V + s e_i) - \mathcal{C}(V - s e_i)}{2\, s}.$$

where $e_i = (0, \cdots 0, 1, 0 \cdots 0)$. Where the "1" is in the i–th position. If we have the gradient (Fréchet), then another way of computing the partial derivative is by taking the dot product with the gradient. That is,

$$\frac{\partial \mathcal{C}}{\partial v_i} = \nabla C(v) \cdot e_i.$$

However the gradient allows us to compute more than that. We can find the derivative along any arbitrary direction u by just having the dot product of the gradient with this u. That is, the directional derivative along u can be written as

$$\frac{\partial \mathcal{C}}{\partial u} = \lim_{s \to 0} \frac{\mathcal{C}(V + s u) - \mathcal{C}(V - s u)}{2\, s}.$$

where u is a direction vector in the parameter space, or

$$\frac{\partial \mathcal{C}}{\partial u} = \nabla C(v) \cdot u.$$

For parameters defined in a 3D space, the Fréchet derivative is a rank 3 tensor and the directional (Gâteaux) derivative is a tensor contraction.

The power of the Fréchet derivative (gradient) is that it needs to be computed only once, and then we can find derivatives along any vectorial or tensor direction. However to compute the Gâteaux derivative without the use of the gradient, the problem has to be solved every time. In this way, finding

the gradient is like finding a Green's function in a differential equation, where we just need to convolve with a source term to get a new solution without having to solve the differential equation again. It is like having A^{-1} when solving for $Ax = b$. We only have to pre–multiply the source b with A^{-1}. The gradient is the "genetic code" of any descent/ascent method. The power of the ASM is that it provides a way to find the actual Fréchet derivative which fits all directional derivatives with only two modeling–like computations (one "forward" and one "backwards"). It is a one–fits–all solution.

We have several observations on the numerical results of this experiment:

- I had to scale down the Fréchet derivative computation by 10^{-6}. The sampling rate is 10^{-3} seconds and a second derivative with respect to time would have 10^{-6} unit scaling. However, ignoring this scaling would make the data only 10^6 smaller, no larger. So, I am not sure if there is an error in the source code or there is something in the mathematical physics that I am not accounting for. Still, we are more interested on the direction of the gradient and not its magnitude, since the optimization problem will scale the gradient based on its own criteria.

- The gradient computation using the ASM (the Fréchet derivative) matches well the computations done using central differences Gâteaux derivatives, except at the top of the model.

- The dispersive error observed closed to the top of the model is worse as s becomes larger. For $s = 1$ the error is very small and the matching between the gradient using the ASM and that using the central differences Gâteaux derivatives is excellent.

- Since the gradient using the ASM was computed for a grid spacing of 10 m, then it is understandable that the level of precision is higher than that of the Gâteaux derivatives for $s > 10$.

- I believe that the error is larger in the top of the model than at the bottom because close to the source the wave equation does not work correctly.

- It is really amazing that the computation of the differentials through the Fréchet derivative (the ASM) is 96000 faster than the computation of the differentials using the Gâteaux central difference if we really want to perturb each cell individually. The gain is much more, the larger the

model. In fact the cost of computing the Gâteaux derivatives for three–dimensional models is prohibitive. More precisely, in 3D the number of RTM–like processes run, if the Gâteaux derivative will be evaluated (for each grid point) would be `nx*ny*nz` , Where `nx` , `ny` and `nz` are the number of grids on the velocity model along the x, y and z directions respectively. Still the number of RTM–like processes needed to find the Frétchet derivative is 1.

- The experiment proposed here would be of great value in evaluating the fidelity of numerical FWI software, such as computing gradients in HTI models, VTI models or any other anisotropic models.

6 Conclusions

In this document I derived the ASM from simple examples, and then from first principles in general linear partial differential equations, matrices of functions and matrices of operators. The derivation shown here has the advantage the it does not depend on solving complicated differential equations and it is general. It applies to any linear partial differential equation or a matrix of functions or operators. The derivation offers a template that can be used in gradient–based inversion problems. This template is posted in terms of three simple steps. I applied the template to show how to find the gradient using the ASM in the case of two simple acoustic wave equations and two elastic wave equations (VTI and HTI). Because the method is general it can be applied to any operator with explicit dependence on the model parameters and that is solvable for the wavefield u. I also show how the Lagrange multipliers method, which offers a more general framework that the traditional framework of optimizing a least square function, can be reduced to a adjoint state problem. Finally, I showed a numerical example that validates the theory.

In addition, I proposed an experiment that could be of great value for testing development software on FWI. For example a new wave–inversion code for HTI models. The computation of the gradient is the most expensive and complicated part of a FWI algorithm and guaranteeing a good gradient computation is having a big part of code in place.

References

[1] Tarantola A. Inversion of seismic reflection data in the acoustic approximation. *Geophysics*, 49:1259–1266, 1984.

[2] K. Aki and Richards P. *Quantitative Seismology: Theory and Methods*, volume I, pages 156–158. W. H. Freeman and Company, 1980.

[3] Wang C., D. Yingst, P. Leveille, J., and R. Bloor. Anisotropic waveform inversion with well constraints. In *EAGE 73th Conference & Exhibition*, Beijing, 2013.

[4] Plessix R. E. A review of the adjoint–state method for computing the gradient of a functional with geophysical applications. *Geophysical Journal Intenational*, 167(2):495–503, 2006.

[5] A. Fichtner, H. P. Bunge, and H. Igel. The adjoint method in seismology: I. theory. *Physics Of The Earth and Planetary Interiors*, 157:86–104, 2006.

[6] Pratt R. G. Seismic waveform inversion in the frequency domain, part 1: Theory and verification in physical scale model. *Geophysics*, 64(3):888–901, 1999.

[7] Luc T. Ikelle and Lasse Amundsen. *Introduction to Petroleum Seismology*, volume 12 of *Investigations in Geophysics*. Society of Exploration Geophysicists, Tulsa, November 2005.

[8] Thomsen L. Weak elastic anisotropy. *Geophysics*, 51(10):1954–1966, 1986.

[9] G. Marchuk. A survey of nuclear-reactor design methods. *Atomic Energy*, 11(4):1000–1016, 1962.

[10] Lailly P. The seismic inversion problem as a sequence of before stack migrations. *Conference on Inverse Scattering: Theory and Applications*, pages 206–220, 1983.

[11] J. Yedlin, M. and G. Van Vorst, D. Tutorial of the continuous and discrete adjoint state method and basic implementation. *CREWES Research Report*, 51(22), 2010.

Appendices

A The Fréchet and Gâteaux derivatives

First, I introduce the concepts of Fréchet derivatives and Gâteaux derivatives starting with the traditional calculus definitions on real variables, then generalize the concept to Banach spaces where the variables can go beyond numbers to functionals.

The concept of derivative (we use the word gradient because our objective functions go from Banach spaces into the real numbers and so, as we will see, the derivatives are actually gradients) is at the heart of linear perturbation theory.

The idea is that we have a function f of some parameters p and want to find out p from perturbing the function and observations of that perturbation away from an initial guessed solution p_0. To the first order

$$f(p + \delta p) = f(p) + f'(p)\,\delta p.$$

that is, the perturbation of the function is, to linear order, that of the parameters times the derivative, or in other words:

$$\delta f(p) = f'(p)\,\delta p.$$

A.1 Review of derivatives in calculus

In real spaces if a function f is defined on A (an open set in $\boldsymbol{R}^n$),

$$\begin{aligned} f : A \subset \mathbb{R}^n &\rightarrow \mathbb{R}^m \\ \boldsymbol{x} &\mapsto f(\boldsymbol{x}). \end{aligned}$$

In calculus we say that if

$$\lim_{\boldsymbol{h} \to 0} \frac{1}{\|h\|}[f(\boldsymbol{x} + \boldsymbol{h}) - f(\boldsymbol{x})] \tag{A.35}$$

for all $\boldsymbol{h}$ near zero exists, then the function is differentiable at the point $\boldsymbol{x}$ and its derivative is given by

$$f'(\boldsymbol{x}) = \lim_{\boldsymbol{h} \to 0} \frac{1}{\|h\|}[f(\boldsymbol{x} + \boldsymbol{h}) - f(\boldsymbol{x})]$$

This definition is not very useful. But it can be shown that if this derivative exists, then by writing

$$\boldsymbol{h} = \sum_j h_j \boldsymbol{e}_j$$

and using the notation

$$f_{i,j} = \frac{\partial f_i}{\partial x_j} = \lim_{h_j \to 0} \frac{1}{h_j}[f_i(\boldsymbol{x} + h_j \boldsymbol{e}_j) - f_i(\boldsymbol{x})],$$

$i = 1, \cdots, m$, $j = 1, \cdots, n$.

Note that we could define the mapping.

$$\begin{aligned} f' : A &\to \mathbb{R}^{m \times n} \\ \boldsymbol{x} &\mapsto f_{i,j}(\boldsymbol{x}) = J(\boldsymbol{x}) \end{aligned}$$

where the notation $J(\boldsymbol{x})$ stands for Jacobian matrix.

However this mapping is not very interesting in practical applications (the Jacobian is, but not the mapping). Usually when solving inverse problems we want to stay in a fixed point $\boldsymbol{x}$, and based on the derivative move along a direction. For this the differential is a more interesting concept. The definition of the differential is given by

$$\begin{aligned} Df(\boldsymbol{x}) : \mathbb{R}^n &\to \mathbb{R}^m \\ \boldsymbol{v} &\mapsto Df(\boldsymbol{x})(v) = J(\boldsymbol{x})\boldsymbol{v} \end{aligned}$$

Note that the symbol $Df(\boldsymbol{x})$ does not show the domain of dependence (the space of $\boldsymbol{v}$s). To see that this operator is well defined we observe that $J(\boldsymbol{x}) \in \mathbb{R}^{m \times n}$ and $\boldsymbol{v} \in \mathbb{R}^n$, so the product is a well defined operation of a matrix times a vector.

The differential has some good attributes. A few of them are:

1. It is a linear operator. That is

$$\begin{aligned} Df(\boldsymbol{x})(\boldsymbol{v} + \boldsymbol{w}) &= Df(\boldsymbol{x})(\boldsymbol{v}) + Df(\boldsymbol{x})(\boldsymbol{w}) \quad \text{and} \\ Df(\boldsymbol{x})(\alpha\, \boldsymbol{v}) &= \alpha Df(\boldsymbol{x})(\boldsymbol{v}). \end{aligned}$$

This can be shown from the definition.

2. It lets us compute some variation of a function along any direction, as we will see below.

3. In integration theory, as well as in sensitivity analysis, $\boldsymbol{v}$ is understood as $d\boldsymbol{x}$ and so we can write

$$Df(\boldsymbol{x})d\boldsymbol{x} = J(\boldsymbol{x})d\boldsymbol{x}$$

which works well to estimate small displacements and differential forms for integration.

4. The differential of a linear function is itself. The proof of this is simple. Assume

$$f(\boldsymbol{x}) = A\boldsymbol{x}$$

(since we are in real spaces A is a matrix and $\boldsymbol{x}$ is a vector.) We know that

$$f_{i,j}(\boldsymbol{x}) = \frac{\partial f_i}{\partial x_j} = a_{ij}$$

Now by definition

$$\begin{aligned} Df(\boldsymbol{x}) : \mathbb{R}^n &\rightarrow \mathbb{R}^m \\ \boldsymbol{v} &\mapsto Df(\boldsymbol{x})(v) = A\boldsymbol{v}, \end{aligned}$$

so $Df(\boldsymbol{x}) = f(\boldsymbol{x})$, for f linear.

5. In 1D, the differential represents the tangent line at the point $(x, f(x))$ of the curve. That is, if we write for a one dimensional space

$$\begin{aligned} Df(x) : \mathbb{R} &\rightarrow \mathbb{R} \\ dx &\mapsto f'(x)dx \end{aligned}$$

It is like saying

$$f(x + h) = f(x) + f'(x)h$$

where the translation from the origin to the point along the curve, is explicitly achieved.

One motivation behind the focus on differentials as going through the $(0,0)$ point is because in general (Hilbert or Banach) spaces linear operators go through the point $(0,0)$.

If $n = 2$ the tangent plane (normal to the gradient vector at the point) and in general it is a tangent hyperspace. So it is the simplest object that approximates (of course linearly) a curve (surface or hypersurface) close to its point of contact. Linearity is important, not only because the integration theory plays with things like $f(x)dx$ and not with things like $f(x)d^2x$ or other monstrosities, but because non–linear problems often are seen as a sequence of linear problems. Also the theory for linear problems is the simplest and most well studied and known of all other (non–linear) theories.

The name of the operator $Df(\boldsymbol{x})$ is the Fréchet derivative, but this name will be more useful when we are not working on real spaces but in spaces of functions where we will extend the concept of derivative with respect to objects different from coordinate points, such as wavefields, vector fields or scalar fields for example.

As a simple example, if $m = 1$ then $Df(\boldsymbol{x})$ is given by

$$\begin{aligned} Df(\boldsymbol{x})d\boldsymbol{x} &= J(\boldsymbol{x})d\boldsymbol{x} \\ &= \sum_i \frac{\partial f}{\partial x_i} dx_i \\ &= \nabla f \cdot d\boldsymbol{x} \end{aligned}$$

which is the well known differential from calculus. So in general for real spaces of the type $\mathbb{R}^{m\times n}$ the Fréchet derivative is the Jacobian matrix $J(\boldsymbol{x})$ and if $m = 1$ it is simply the gradient $\nabla f(\boldsymbol{x})$. The differential at a point $\boldsymbol{v}$ happens to be the product (inner) of the Fréchet derivative with that point $\boldsymbol{v}$ seen as a linear operator acting on $\boldsymbol{v}$. This form of a differential is actually also known as the Gâteaux derivative.

Before we define derivative in more general spaces, let us introduce the concept of directional derivative. This is given by

$$D_{\boldsymbol{v}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{1}{h}[f(\boldsymbol{x} + h\boldsymbol{v}) - f(\boldsymbol{x})] \tag{A.36}$$

where h is a scalar. This is the derivative of f along the direction $\boldsymbol{v}$. Observe that the differential and the Gâteaux derivative coincide.

If f is differentiable, then the directional derivative exists along any direction. The contrary is not true (search for examples in calculus books or the Internet). The directional derivative generalize the concept of partial derivatives. A i–th partial derivative is a directional derivative when $\boldsymbol{u} = \boldsymbol{e}_i$

The directional derivative is known as the Gâteaux derivative, but again this is more important when we move to more general functions which do not depend directly on real variables (such as functionals for example, which are functions from a function space into real variables).

A.2 What is differentiation on general operators?

Now, we have a function

$$\begin{aligned} f : A &\to B \\ x &\mapsto f(x) \end{aligned}$$

Here A and B are more general spaces than just $\mathbb{R}^n$ or $\mathbb{R}^m$. What is the meaning of the derivative of f? what is the meaning of the differential of f? I will not use bold symbols because this is general and if I have to distinguish between scalars and vectors of the space, the context will tell.

We borrow all the elements above to re-formulate the problem in a more general context, but before we do that we have to put some restriction on the spaces A and B. They cannot be, for example, oranges. How close is an orange from another? That is, they cannot be any arbitrary space. We have to be able to measure distances. That is a norm has to be defined on them. The norm does not necessarily have to be the same A that in B, but it should satisfy (of course) the axioms of the norm in functional analysis (positive or zero if vector is zero, scaling, triangular inequality). The context for the spaces A and B is known as Banach spaces. Not only they are normed vector spaces, but they are complete. This means that every Cauchy sequence [3] converge on them.

I start with the Wikipedia [4] definition of Fréchet derivative and show that that that definition reduces to the calculus definition A.35.

[3] A Cauchy sequence is one were the elements get closer together as they get farther from the first element. We will not use this requirement here but it is something needed for the Banach spaces to work "fine".

[4] http://en.wikipedia.org/wiki/Fréchet_derivative

With this the Fréchet derivative is defined as a linear L operator on the same spaces A and B [5] such that

$$\lim_{h\to 0} \frac{\|f(x+h) - f(x) - L(h)\|}{\|h\|} = 0.$$

If such a linear operator L exists then it is the Fréchet derivative and it its noted as $L(h) = Df(x)(h)$.

Another way to say this is that if we define a residual

$$R(x,h) = f(x+h) - f(x) - L(h),$$

such that an L is some linear operator with

$$\lim_{\|h\|\to 0} \frac{R(x,h)}{\|h\|} = 0$$

then that L is the differential explicitly writen as

$$L(h) = f(x+h) - f(x) + R(x,h).$$

This is why in a sloppy way, many authors look at the Fréchet derivative simply as

$$L = \delta f = f(x+\delta x) - f(x).$$

It is, however, correct to say that

$$f(x+h) = f(x) + L(x) + \mathcal{O}(\|h\|^2).$$

So it should be obvious, from here, that

$$\lim_{\|h\|\to 0} \frac{f(x+h) - f(x)}{\|h\|} = L(x) + \cancelto{0}{\lim_{\|h\|\to 0} \mathcal{O}(\|h\|)} = L(x).$$

So the Fréchet derivative reduces to the same definition A.35 used for real spaces. That is, the Fréchet derivative is that linear operator L such that the limit

$$L(x) = \lim_{\|h\|\to 0} \frac{f(x+h) - f(x)}{\|h\|}$$

[5] In practice $B = \mathbb{R}$. If A is the space of functions then any function from A to $B = \mathbb{R}$ is a functional.

exists. This definition is very convenient because the algebraic rules (chain rule, rules for differentiation of sums, products, quotients, etc. are based on this definition and they will inherit the same behavior).

The operator is linear by definition and naming it as

$$L(x) = f'(x)$$

we find the usual expression

$$f(x+h) = f(x) + f'(x)(h) + \mathcal{O}(\|h\|^2) \tag{A.37}$$

The Taylor series theory could be developed in this way defining a second differential, however we will not proceed any further on this direction.

Let us assume that f is linear. That is

$$f(x) = Ax$$

for A independent of x. Then

$$f(x+h) - f(x) = A(x+h) - Ax = Ah$$

so if $L(h) = Ah$ then

$$\lim_{h\to 0} \frac{\|f(x+h) - f(x) - L(h)\|}{\|h\|} = 0,$$

so $L = f = A$. That is, if f is linear then the Fréchet derivative is the same linear operator, as shown above where the spaces A and B are real spaces. If in particular B is a subset of $\mathbb{R}$ then $Df(x)$ is the gradient $\nabla_x f$ and the Fréchet derivative operator is defined as

$$\begin{aligned} Df(x)A &\to B \\ v &\mapsto Df(x)(v) = \langle \nabla_x f, v \rangle \end{aligned}$$

which is the differential as shown above.

It should be clear now that even in spaces which are no real spaces (spaces of functions) we can extend the concept of differentiation, and we can talk about perturbation theory. In exactly the same way in which we perturb functions of a real variable (or complex) we can perturb operators of objects (functions for example) using the same theory with the same algebra, but

being careful of identifying the context. That is, the space that we use to make perturbations. I will be more specific about this in the examples below.

Now, the Gâteaux derivative is defined by the equation A.36

$$D_{\boldsymbol{u}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{1}{h}[f(\boldsymbol{x} + h\boldsymbol{u}) - f(\boldsymbol{x})]$$

[6] which it is an equivalent version of the Gâteaux derivative.

While using the definition could be convenient sometimes, I will stay way from using the definition in the case outlined below. It can be shown (since the definition is the same as in regular calculus, the chain rule, the derivative of products, quotients, sums scalings, they all behave the same) that the algebra used for regular partial derivatives will operate the same here.

B Adjoints of partial differential operators

Given a linear operator L in a Hilbert space, its adjoint is that operator L^* such that for each pair of elements u and v in the Hilbert space

$$\langle Lu\ ,\ v\rangle = \langle u\ ,\ L^* v\rangle.$$

where the inner product $\langle , \rangle$ binary operator is defined on this context by equation B.43. I will not discuss any issues of existence and uniqueness here.

Multi–dimensional differential operators come in many flavors. For example, while in one dimension we only have a first derivative operator, in several dimensions we find for scalar fields gradient (∇) and for vector fields divergence ($\nabla.$) and curl ($\nabla\times$). All of them use first order partial derivatives. In the case of second order I only explore the Laplacian operator (∇^2). The trick to find adjoints is always integration by parts. Integration by parts comes from the derivative of the product of two functions. In symbols, if

$$d(uv) = udv + vdu,$$

then

$$uv = \int (udv + vdu)$$

[6] In the numerical implementation I used the central difference representation

$$D_{\boldsymbol{u}} f(\boldsymbol{x}) = \lim_{h \to 0} \frac{1}{2h}[f(\boldsymbol{x} + h\boldsymbol{u}) - f(\boldsymbol{x} - \boldsymbol{h}\boldsymbol{x})]$$

or

$$\int udv = uv - \int vdu.$$

I will use bold capital letters for vector fields and non–bold non–capital letters for scalar fields. I assume vector fields from $\mathbb{R}^n$ into $\mathbb{R}^m$ (m could be equal to n) and scalar fields from $\mathbb{R}^n$ into $\mathbb{R}$.

Therefore the following set of equations will be of great use in the following sections:

$$\nabla \cdot (f\,\boldsymbol{G}) = \boldsymbol{G} \cdot \nabla f + f\,\nabla \cdot \boldsymbol{G} \tag{B.38}$$

$$\nabla \cdot (\boldsymbol{F} \times \boldsymbol{G}) = \boldsymbol{G} \cdot (\nabla \times \boldsymbol{F}) - \boldsymbol{F} \cdot (\nabla \times \boldsymbol{G}) \tag{B.39}$$

This list could be made larger but what we are shown here is what is most commonly used. The reader could check for example the Wikipedia site. [7] We add that

$$\nabla.\nabla f = \nabla^2 f. \tag{B.40}$$

The Laplacian $\nabla^2 f$ is sometimes noted as Δf. If in equation B.38 we change $\boldsymbol{G}$ by ∇g, we find:

$$\nabla \cdot (f\,\nabla g) = f\,\nabla \cdot \nabla g + \nabla f \cdot \nabla g. \tag{B.41}$$

That is

$$\nabla \cdot (f\,\nabla g) = f\,\nabla^2 g + \nabla f \cdot \nabla g. \tag{B.42}$$

The identities in this section are commonly used to reduce dimensionality of problems. For example to reduce an integral over a volume to the integral over its surface (the boundary). That is the case of the Green's and Stoke's theorems. With Green identities, also built from the identities in this section, Green's functions for wave operators are built. Here we are somehow going the other way around. We want data that vanishes in the boundaries in order to find the adjoint operator in acting on the whole volumes.

Before we start applying the tools at hand, we should understand inner products in functions of several variables. Assume that f and g

$$f, g : V \subseteq \mathbb{R}^n \to \mathbb{R}$$

[7] http://en.wikipedia.org/wiki/Vector_calculus_identities

are scalar differentiable fields, in some open domain V. We define the inner product $\langle\, .\rangle$ of f with g as

$$\langle f\,, g\rangle = \int_V f\, g\, d\boldsymbol{x}, \tag{B.43}$$

where $\boldsymbol{x}$ rolls over all points of the set V, given that this multi–dimensional integral exists.

Now let us define the corresponding inner product for vector fields. Assume that $\boldsymbol{F} = \{f_i\}$ and $\boldsymbol{G} = g_i$, $i = 1, 2, .., n$.

$$\boldsymbol{F}, \boldsymbol{G} : V \subseteq \mathbb{R}^n \to \mathbb{R}^m$$

are vector differentiable fields, in some domain V. We define the inner product $\langle\, .\rangle$ of f with g as

$$\langle \boldsymbol{F}\,, \boldsymbol{G}\rangle = \int_V \sum_{i=1}^{m} f_i\, g_i\, d\boldsymbol{x}, = \int_V \boldsymbol{F}\cdot\boldsymbol{G}\; d\boldsymbol{x}. \tag{B.44}$$

where $\boldsymbol{x}$ rolls over all points of the set V, given that this multi–dimensional integrals exists.

B.0.0.3 The gradient and its adjoint the divergence Assume that f is a scalar differentiable field in $V \subseteq \mathbb{R}^n$. Let us call the Hilbert space $\mathcal{H}_1$ the space of scalar field functions

$$f : V \subseteq \mathbb{R}^n \to \mathbb{R}$$

which, where we can take as many we need partial derivatives (C^∞ if needed) and $\mathcal{H}_2$ the space of vector field functions

$$\boldsymbol{G} : V \subseteq \mathbb{R}^n \to \mathbb{R}^n$$

where also we can take as many derivatives as needed. Call L the gradient operator

$$\begin{array}{rcl} L : \mathcal{H}_1 & \to & \mathcal{H}_2 \\ & & \\ f & \mapsto & L(f) = \begin{pmatrix} \partial f/\partial x_1 \\ \partial f/\partial x_2 \\ . \\ . \\ . \\ \partial f/\partial x_n \end{pmatrix} \end{array}$$

we want to find L^*. Let us take a vector field $\boldsymbol{G}$ in $\mathcal{H}_2$. Then, from the inner product definition B.44 we have:

$$\begin{aligned}\langle L(f)\,,\boldsymbol{G}\rangle &= \int_V \nabla f\cdot\boldsymbol{G}\,d\boldsymbol{x}\\ &= \int_V [\nabla\cdot(f\,\boldsymbol{G})-f\,\nabla\cdot\boldsymbol{G}\,]\,d\boldsymbol{x}\\ &= \int_\Sigma f\,\boldsymbol{G}\cdot d\Sigma-\int_V f\,\nabla\cdot\boldsymbol{G}\,d\boldsymbol{x}.\end{aligned}$$

The second equation comes from identity B.38 and the third equation comes from the divergence theorem. Here Σ is the boundary of the volume V. Assuming that the product $f\,\boldsymbol{G}$ vanishes in the boundary Σ we find

$$\langle L(f)\,,\boldsymbol{G}\rangle = -\int_V f\,\nabla\cdot\boldsymbol{G}\,d\boldsymbol{x}=\langle f\,,-\nabla\cdot\boldsymbol{G}\rangle.$$

where the second inner product is in the space of scalar functions (see B.43). That is, provided that the product $f\,\boldsymbol{G}$ vanishes in the boundary we found that

$$\langle L(f)\,,\boldsymbol{G}\rangle = \langle f\,,L^*(\boldsymbol{G})\rangle$$

with

$$\begin{aligned}L^*:\mathcal{H}_2 &\to \mathcal{H}_1\\ \boldsymbol{G} &\mapsto L^*(\boldsymbol{G})=-\nabla\cdot\boldsymbol{G}.\end{aligned}\tag{B.45}$$

We say that the adjoint of the gradient is the negative divergence. Since the adjoint operation is symmetric we can say that the adjoint of the divergence is the negative of the gradient.

B.0.0.4 Product of a scalar function and a gradient: Making the previous example a bit more general, let us assume that

$$\begin{aligned}L:\mathcal{H}_1 &\to \mathcal{H}_2\\ f &\mapsto a(\boldsymbol{x})\nabla f,\end{aligned}$$

then, given a vector field $\boldsymbol{G}$ in $\mathcal{H}_2$

$$\begin{aligned}
\langle L(f)\,,\boldsymbol{G}\rangle &= \int_V a(\boldsymbol{x})\,\nabla f\cdot\boldsymbol{G}\,d\boldsymbol{x} \\
&= \int_V \nabla f\ \cdot a(\boldsymbol{x})\,\boldsymbol{G}\,d\boldsymbol{x} \\
&= \int_V [\nabla\cdot(f a(\boldsymbol{x})\,\boldsymbol{G}) - f\ \nabla\cdot a(\boldsymbol{x})\,\boldsymbol{G}\,]\,d\boldsymbol{x} \\
&= \int_\Sigma (f\ a(\boldsymbol{x})\,\boldsymbol{G})\ \cdot d\,\Sigma - \int_V f\ \nabla\cdot(a(\boldsymbol{x})\,\boldsymbol{G})\,d\boldsymbol{x}
\end{aligned}$$

The second equation is the commutation of the scalar under the dot product, the third equation comes from identity B.38 and the fourth equation comes from the divergence theorem. Here Σ is the boundary of the volume V. Assuming that the product $f\,a(\boldsymbol{x})\,\boldsymbol{G}$ vanishes in Σ we find

$$\langle\, L(a(\boldsymbol{x})\,f)\,,\boldsymbol{G}\rangle \;=\; -\int_V f\,\nabla\cdot(a(\boldsymbol{x})\,\boldsymbol{G})\,d\boldsymbol{x} = \langle f\,,-\nabla\cdot(a(\boldsymbol{x})\ \boldsymbol{G})\,\rangle. \tag{B.46}$$

where the second inner product is in the space of scalar functions (see B.43). That is, provided that the product $f\,\boldsymbol{G}$ vanishes in the boundary we found that

$$\langle L(f)\,,\boldsymbol{G}\rangle \;=\; \langle f\,,L^*(\boldsymbol{G})\rangle$$

with

$$\begin{aligned}
L^*:\mathcal{H}_2 &\to \mathcal{H}_1 \\
\boldsymbol{G} &\mapsto L^*(\boldsymbol{G}) = -\nabla\cdot[a(\boldsymbol{x})\ \boldsymbol{G}].
\end{aligned}$$

In words, we say that the adjoint maps gradient scaled into scaled divergence. That is, a factor outside the gradient will be sent inside the divergence symbol under the adjoint operation.

B.0.0.5 The curl: The curl can be defined in n–dimensional spaces but here we will only use the three–dimensional space version, in order to simplify

the development and because it is the most commonly used. The definition of curl is a linear operator L from $\mathcal{H}_2$ to $\mathcal{H}_2$ [8] such that:

$$\begin{aligned} L : \mathcal{H}_2 &\rightarrow \mathcal{H}_2 \\ \boldsymbol{G} &\mapsto L(\boldsymbol{G}) = \nabla \times \boldsymbol{G} = \begin{pmatrix} \partial g_2/\partial x_3 - \partial g_3/\partial x_2 \\ \partial g_3/\partial x_1 - \partial g_1/\partial x_3 \\ \partial g_1/\partial x_2 - \partial g_2/\partial x_1 \end{pmatrix} \end{aligned}$$

provided that all partial derivatives exist.

We now find the adjoint of the curl. Using the inner product definition B.44 we have that for any vector field function $\boldsymbol{F}$ in $\mathcal{H}_2$

$$\begin{aligned} \langle\, L\,\boldsymbol{G}\,, \boldsymbol{F}\rangle &= \int_V (\nabla \times \boldsymbol{G}) \cdot \boldsymbol{F}\; d\boldsymbol{x} \\ &= \int_V -\nabla \cdot (\boldsymbol{F} \times \boldsymbol{G}) + G \cdot (\nabla \times \boldsymbol{F}) d\boldsymbol{x} \\ &= -\int_\Sigma (\boldsymbol{F} \times \boldsymbol{G})\; d\,\Sigma + \int_V \boldsymbol{G} \cdot (\nabla \times \boldsymbol{F}) d\boldsymbol{x} \\ &= -\int_\Sigma (\boldsymbol{F} \times \boldsymbol{G})\; d\,\Sigma + \langle\, \boldsymbol{G}\,, L(\boldsymbol{F})\,\rangle. \end{aligned}$$

Here in the second step we used the identity B.39 and in the third step the divergence theorem. So, provided the boundary condition $\boldsymbol{F} \times \boldsymbol{G} = 0$ on Σ, we have that the curl operator is self–adjoint.

B.0.0.6 Product of a scalar function and a curl: In the previous problem let us multiply the curl by scalar field a; that is

$$\begin{aligned} L : \mathcal{H}_2 &\rightarrow \mathcal{H}_2 \\ \boldsymbol{G} &\mapsto L(\boldsymbol{G}) = a(\boldsymbol{x})\; \nabla \times \boldsymbol{G}. \end{aligned}$$

[8] Strictly speaking this should be from $\mathcal{H}_2$ to a less smooth space $\mathcal{H}_3$, since those functions with derivatives up to an order n, get reduced to spaces with derivatives up to an order $n-1$ when the curl is operated on them. However due to symmetry theorem of adjoint operators, the adjoint of the adjoint is the original operator, so we need the range to be in $\mathcal{H}_2$. That is, strictly speaking the space of functions for these operators should be C^∞. We will ignore this mathematical detail through the rest of the document because this is irrelevant for the purposes here.

Give any vector field $\boldsymbol{F}$ in $\mathcal{H}_2$ we find:

$$\begin{aligned}
\langle\, L\,\boldsymbol{G}\,,\boldsymbol{F}\rangle &= \int_V (a(\boldsymbol{x})\,\nabla\times\boldsymbol{G})\cdot\boldsymbol{F}\;d\boldsymbol{x}\\
&= \int_V (\nabla\times\boldsymbol{G})\cdot(a(\boldsymbol{x})\,\boldsymbol{F})\;d\boldsymbol{x}\\
&= \int_V \nabla\cdot(a(\boldsymbol{x})\,\boldsymbol{F}\times\boldsymbol{G}) + \boldsymbol{G}\cdot(\nabla\times(a(\boldsymbol{x})\,\boldsymbol{F}))\\
&= \int_\Sigma (a(\boldsymbol{x})\,\boldsymbol{F}\times\boldsymbol{G})\;d\,\Sigma + \int_V \boldsymbol{G}\cdot(\nabla\times(a(\boldsymbol{x})\,\boldsymbol{F}))\\
&= \int_\Sigma ((a(\boldsymbol{x})\,\boldsymbol{F})\times\boldsymbol{G})\;d\,\Sigma + \langle\,\boldsymbol{G}\,,L^*(\boldsymbol{F})\,\rangle.
\end{aligned}$$

with

$$\begin{aligned}
L^*:\mathcal{H}_2 &\rightarrow \mathcal{H}_2\\
\boldsymbol{F} &\mapsto L(\boldsymbol{F}) = \nabla\times(a(\boldsymbol{x})\boldsymbol{F}).
\end{aligned}$$

So, provided the boundary condition $(a(\boldsymbol{x})\,\boldsymbol{F})\times\boldsymbol{G} = 0$ in Σ we have that the adjoint of the product of a scalar field and a curl is the curl of the product of the scalar field and its vector field argument.

B.0.0.7 The Laplacian: is a linear operator L from $\mathcal{H}_1$ to $\mathcal{H}_1$ such that:

$$\begin{aligned}
L:\mathcal{H}_1 &\rightarrow \mathcal{H}_1\\
f &\mapsto L(f) = \nabla^2 f = \sum_{i=1}^{n}\frac{\partial^2 f}{\partial x^2}.
\end{aligned}$$

provided that all partial derivatives exist.

We want to find the adjoint of the Laplacian. We use the results found above. That is, since, from B.40 $L(f) = \nabla^2 f = \nabla\cdot\nabla f$, we can write Laplacian as the cascade of two operators:

$$\boldsymbol{S}(f) = \nabla f \qquad \text{and} \qquad T(\boldsymbol{S}) = \nabla\cdot\boldsymbol{S}$$

so,

$$\begin{aligned}
\langle L(f)\,, g\rangle &= \langle TSf\,, g\rangle \\
&= \langle Sf\,, T^{*}g\rangle \qquad \text{definition of adjoint} \\
&= \langle Sf\,, -\nabla g\rangle \qquad \text{see comment after B.45} \\
&= \langle f\,, -S^{*}\,\nabla g\rangle \quad \text{definition of adjoint} \\
&= \langle f\,, \nabla\cdot\,\nabla g\rangle \quad \text{property B.45} \\
&= \langle f\,, \nabla^{2} g\rangle \\
&= \langle f\,, Lg\rangle.
\end{aligned}$$

This is an interesting way to prove that the Laplacian is a self–adjoint operator, however it does not explicitly show the boundary conditions for this to happen. Therefore I will try this again using the (already familiar) methodology (integration by parts) used on this document.

$$\begin{aligned}
\langle L(g)\,, f\rangle &= \int_{V} f\,\nabla^{2} g\; d\boldsymbol{x} \\
&= \int_{V} \nabla\cdot(f\nabla g) - \nabla f\cdot\nabla g\; d\boldsymbol{x} \qquad \text{see equation B.41} \\
&= \int_{\Sigma} f\;\nabla g\cdot d\Sigma - \int_{V}\nabla f\cdot\nabla g\; d\boldsymbol{x} \quad \text{divergence theorem} \\
&= \int_{\Sigma} f\;\nabla g\cdot d\Sigma - \int_{V}\left[\nabla\cdot(g\nabla f) - g\nabla^{2} f\right] d\boldsymbol{x} \quad \text{B.41 again but} \\
&\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad \text{change } f \text{ by } g \\
&= \int_{\Sigma}(f\;\nabla g - g\;\nabla f)\cdot d\Sigma + \int_{V} g\nabla^{2} f\; d\boldsymbol{x} \quad \text{divergence theorem} \\
&= \int_{\Sigma}(f\;\nabla g - g\;\nabla f)\cdot d\Sigma + \langle g\,, L(f)\rangle.
\end{aligned}$$

So we showed again that the adjoint of the Laplacian operator is itself (the Laplacian operator is self–adjoint) and exposed the boundary condition. We require

$$f\,\nabla g - g\;\nabla f = 0 \tag{B.47}$$

in the boundary Σ. This proof could have been written in a couple of lines by using the second Green's identity. Actually we proved the second Green's

identity

$$\int_V (f\,\nabla^2 g - g\,\nabla^2 f)\,d\boldsymbol{x} = \int_\Sigma (f\nabla g - g\,\nabla f)\cdot d\Sigma. \tag{B.48}$$

B.0.0.8 Product of a scalar function and a Laplacian: Let assume that the operator L is such that

$$\begin{aligned} L : \mathcal{H}_1 &\rightarrow \mathcal{H}_1 \\ f &\mapsto L(f) = a(\boldsymbol{x})\nabla^2 f. \end{aligned}$$

As usual we write, for any given scalar field g in $\mathcal{H}_1$

$$\begin{aligned} \langle L(f)\,, g\rangle &= \int_V a\,\nabla^2 f\; g\; d\,\boldsymbol{x} \\ &= \int_V a\; g\;(\nabla^2 f)\, d\,\boldsymbol{x} \\ &= \int_V f\,[\nabla^2\,(a\,g)] + \int_\Sigma [f\,\nabla(a\,g) - (a\,g)\,\nabla f]\cdot d\Sigma. \\ &= \langle f, L^*(g)\rangle + \int_\Sigma [f\,\nabla(a\,g) - (a\,g)\,\nabla f]\cdot d\Sigma. \end{aligned}$$

In the third line we used the second Green's identity B.48. So provided the boundary condition:

$$f\,\nabla(a\,g) - (a\,g)\,\nabla f = 0$$

in Σ, we find that the adjoint of L is:

$$\begin{aligned} L^* : \mathcal{H}_1 &\rightarrow \mathcal{H}_1 \\ g &\mapsto L^*(g) = \nabla^2(a\; f). \end{aligned}$$

B.0.0.9 Observation We found that in all cases of product of scalars with operators ($\nabla, \nabla\cdot, \nabla\times$ and ∇^2), the scalar switches to the inside if it is outside, and vice–versa when finding the adjoint.

The dot product of a vector function and a gradient. The general first order linear differential operator: We can write a general first order linear differential operator acting on a scalar field $f \in \mathcal{H}_1$ as

$$Lf = \sum_i b_i(\boldsymbol{x}) \frac{\partial f}{\partial x_i} + (c\, f)(\boldsymbol{x}) = \boldsymbol{B} \cdot \nabla f + (c\, f)(\boldsymbol{x}), \tag{B.49}$$

for scalar fields $b_i(\boldsymbol{x})$ and $c(\boldsymbol{x})$ all in $\mathcal{H}_1$. Here $\boldsymbol{B}$ is a vector with components $b_i(\boldsymbol{x})$.

The last term (a factor of a scalar field by f) is obviously self–adjoint and non–interesting. We are after the adjoint of the first term, which is the dot product of the vectors $\boldsymbol{B}$ and ∇f and we call L_B.

As usual, let us pick an arbitrary scalar function $g \in \mathcal{H}_1$. Then,

$$\begin{aligned}
\langle L_B(f)\,, g\rangle &= \int_V (\boldsymbol{B} \cdot \nabla f)\; g\, d\boldsymbol{x} \\
&= \int_V (g\, \boldsymbol{B}) \cdot \nabla f\, d\boldsymbol{x} \\
&= \int_V \nabla \cdot (g\, f \cdot \boldsymbol{B}) - f\, \nabla \cdot g\, \boldsymbol{B}\, d\boldsymbol{x} \\
&= \int_\Sigma f\, g\, \boldsymbol{B} \cdot d\Sigma - \int_V f\, \nabla \cdot g\boldsymbol{B}\, d\boldsymbol{x} \\
&= \int_\Sigma f\, g\, \boldsymbol{B} \cdot d\,\Sigma - \langle f\,, L^* g\rangle.
\end{aligned}$$

Second line is commutation, third line is due to identity B.38 , and fourth line is due to the divergence theorem. Given the boundary condition

$$f\, g\, \boldsymbol{B} = 0,$$

in Σ, the adjoint operator L^* is given by:

$$\begin{aligned}
L_B^* : \mathcal{H}_1 &\rightarrow \mathcal{H}_1 \\
g &\mapsto L^* g = -\nabla \cdot (g\; \boldsymbol{B}).
\end{aligned}$$

So the adjoint of the second order operator L is given by

$$\begin{aligned}
L^*(g) &= L_B^*(g) + c\, g(\boldsymbol{x}) \\
&= -\nabla \cdot g\boldsymbol{B} + c\, g(\boldsymbol{x}) \\
&= -\sum_{i=1}^{n} \frac{\partial\; g b_i(\boldsymbol{x})}{\partial x_i} + (c\, g)(\boldsymbol{x}).
\end{aligned} \tag{B.50}$$

with the boundary condition:

$$(f\, g\, b_i)(\boldsymbol{x}) = 0,$$

for any $\boldsymbol{x}$ in Σ.

It is common on wave equations to find the operator defined by

$$L\, u(\boldsymbol{x}) = \nabla \cdot (a(\boldsymbol{x}) \nabla u(\boldsymbol{x}))\,.$$

By the rules of differentiation of the divergence we see that

$$L\, u(\boldsymbol{x}) = \nabla a(\boldsymbol{x}) \cdot \nabla u(\boldsymbol{x}) + a(\boldsymbol{x}) \nabla^2 u(\boldsymbol{x}).$$

and from the previous derivation with $\boldsymbol{B} = \nabla a(\boldsymbol{x})$ and the adjoint of the product of a scalar function and a Laplacian we have

$$\begin{aligned} L^*(g) &= -\nabla \cdot [g \nabla a] + \nabla^2 (a\; g) \\ &= -\nabla a \cdot \nabla g - g \nabla^2 a + \nabla^2 (a\; g) \\ &= \cancel{-\nabla a \cdot \nabla g} \cancel{- g \nabla^2 a} + (a \nabla^2 g + \cancel{2 \nabla a \cdot \nabla g} + \cancel{g \nabla^2 a}) \\ &= \nabla a \cdot \nabla g + a \nabla^2 g \\ &= \nabla . (a\, \nabla g) \end{aligned}$$

So $L = L^*$ and L is self–adjoint.

In particular Tarantola's [1] example on the acoustic wave equation.

$$Lu = \left[\frac{1}{K(\boldsymbol{x})} \frac{\partial^2}{\partial t^2} - \nabla . \left(\frac{1}{\rho(\boldsymbol{x})} \nabla \right) \right] u(\boldsymbol{x}, t) = s(\boldsymbol{x}, t). \tag{B.51}$$

is self–adjoint since $K(\boldsymbol{x})$ is time independent.

Table 1 shows a summary of the results obtained so far, assuming the proper boundary conditions are chosen so that the surface integral contribution is zero.

A general linear second order differential operator: A general linear second order differentiator operator in $\mathcal{H}_1$ can be written as

$$\begin{aligned} L : \mathcal{H}_1 &\rightarrow \mathcal{H}_1 \\ f &\mapsto L(f) = \sum_{i=1}^{n} \sum_{j=1}^{n} a_{ij} \frac{\partial^2 f}{\partial x_i \partial x_j} + \sum_{i=1}^{n} b_i \frac{\partial f}{\partial x_i} + c\, f. \end{aligned} \tag{B.52}$$

Table 1: Some common operators and its adjoint pairs

Gradient/Divergence	$a(\boldsymbol{x})\nabla u(\boldsymbol{x})$	$-\nabla\cdot[a(\boldsymbol{x})\boldsymbol{G}(\boldsymbol{x})]$
Curl	$a(\boldsymbol{x})\,\nabla\times\boldsymbol{F}(\boldsymbol{x})$	$\nabla\times[a(\boldsymbol{x})\boldsymbol{F}(\boldsymbol{x})]$
Laplacian	$a(\boldsymbol{x})\nabla^2 u(\boldsymbol{x})$	$\nabla^2[a(\boldsymbol{x})g(\boldsymbol{x})]$
Mixed	$\nabla\cdot a(\boldsymbol{x})\nabla u(\boldsymbol{x})$	$\nabla\cdot a(\boldsymbol{x})\nabla g(\boldsymbol{x})$

Let us find the adjoint L^*. The first and zero order differentials are trivial an considered in previous examples. Let us focus in the first double sum. That is, let us define

$$\begin{aligned} L_A : \mathcal{H}_1 &\to \mathcal{H}_1 \\ f &\mapsto L_A(f) = \sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\frac{\partial^2 f}{\partial x_i \partial x_j} + \end{aligned}$$

We are tempted to start applying the definition of inner product and integration by parts to get L_A^*. However I do not know about any integration by parts that will take care of the whole matrix (of a_{ij}) to matrix (of second order partial derivatives) inner product [9]. Based on the observation in the observation B.0.0.9 above, I guess how L^* should look like and then verify that it is indeed the adjoint we are looking for.

I claim that

$$\begin{aligned} L_A^* : \mathcal{H}_1 &\to \mathcal{H}_1 \\ g &\mapsto L_A^*(g) = \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2 (a_{ij}\, g)}{\partial x_i \partial x_j} + \end{aligned} \tag{B.53}$$

Then I compute

$$\langle L_A f\,, g\rangle - \langle L_A^* g\,, f\rangle$$

[9] Actually A is a tensor operator and in Einstein's notation, $a_{ij}\partial_i\partial_j f$ is a zero rank contracted tensor. This belongs to the field of differential forms under the mathematical branch of differential geometry.

and show that it is an exact differential, which after applying the divergence theorem produces the condition in the boundary Σ. We see that:

$$\langle L_A f\,, g\rangle - \langle L_A^* g\,, f\rangle \;=\; \int_V \sum_{i=1}^{n}\sum_{j=1}^{n}\left(a_{ij}\,g\frac{\partial^2 f}{\partial x_i \partial x_j} - f\,\frac{\partial^2 (a_{ij}\,g)}{\partial x_i \partial x_j}\right) d\boldsymbol{x}$$

The expression in the parenthesis can be written as

$$\begin{aligned} a_{ij}\,g\frac{\partial^2 f}{\partial x_i \partial x_j} - f\,\frac{\partial^2 (a_{ij}\,g)}{\partial x_i \partial x_j} &= a_{ij}\,g\frac{\partial^2 f}{\partial x_i \partial x_j} + \frac{\partial (a_{ij}\,g)}{\partial x_i \partial x_j}\frac{\partial f}{\partial x_j} \\ &\quad -\frac{\partial (a_{ij}\,g)}{\partial x_i \partial x_j}\frac{\partial f}{\partial x_j} - f\,\frac{\partial^2 (a_{ij}\,g)}{\partial x_i \partial x_j} \\ &= \frac{\partial}{\partial x_i}\left(a_{ij} g\frac{\partial f}{\partial x_j}\right) - \frac{\partial}{\partial x_j}\left(f\frac{\partial (a_{ij} g)}{\partial x_i}\right). \end{aligned}$$

Now, since

$$\sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial}{\partial x_j}\left(f\frac{\partial (a_{ij} g)}{\partial x_i}\right) \;=\; \sum_{i=1}^{n}\sum_{j=1}^{n}\frac{\partial}{\partial x_i}\left(f\frac{\partial (a_{ji} g)}{\partial x_j}\right),$$

we find that

$$\sum_{i=1}^{n}\sum_{j=1}^{n} a_{ij}\,g\frac{\partial^2 f}{\partial x_i \partial x_j} - f\,\frac{\partial^2 (a_{ij}\,g)}{\partial x_i \partial x_j} \;=\; \sum_{i=1}^{n}\frac{\partial}{\partial x_i}\left[\sum_{j=1}^{n} a_{ij} g\frac{\partial f}{\partial x_j} - f\frac{\partial (a_{ji} g)}{\partial x_j}\right].$$

and so

$$\begin{aligned} \langle L_A f\,, g\rangle - \langle L_A^* g\,, f\rangle &= \int_V \sum_{i=1}^{n}\frac{\partial}{\partial x_i}\left[\sum_{j=1}^{n} a_{ij} g\frac{\partial f}{\partial x_j} - f\frac{\partial (a_{ji} g)}{\partial x_j}\right]. \\ &= \int_V \nabla \cdot p_i d\boldsymbol{x} \end{aligned}$$

Is an exact differential with

$$p_i = \sum_{j=1}^{n} a_{ij} g\frac{\partial f}{\partial x_j} - f\frac{\partial (a_{ji} g)}{\partial x_j},$$

and we can apply the divergence theorem to finally get

$$\langle L_A f\,, g\rangle - \langle L_A^* g\,, f\rangle \;\; = \;\; \int_\Sigma p_i \cdot d\Sigma.$$

So provided that $p_i = 0$ in the boundary Σ, the adjoint of L_A exists and it is given in equation B.53. Combining this result with the adjoint of the general linear first order differential operator in equation B.50 we find that the adjoint of the general linear second order partial differential operator B.52 is

$$\begin{aligned} L^* : \mathcal{H}_1 &\rightarrow \mathcal{H}_1 \\ g &\mapsto L(g) = \sum_{i=1}^{n}\sum_{j=1}^{n} \frac{\partial^2(a_{ij}g)}{\partial x_i \partial x_j} - \sum_{i=1}^{n} \frac{\partial\,(b_i\,g)}{\partial x_i} + c\,g. \end{aligned} \qquad \text{(B.54)}$$

with the boundary condition

$$p_i = \sum_{j=1}^{n} a_{ij} g \frac{\partial f}{\partial x_j} - f\frac{\partial(a_{ji}g)}{\partial x_j} + b_i f\, g = 0$$

for all $\boldsymbol{x}$ in Σ.

With this adjoint we cover all second order linear partial differential equations including all wave equations.

We use the results on this section to derive the adjoints of the wave equation operators in the examples for this document.