Chapter 1

Goals, motivation and setup

1.1 Motivation

The topic of simulation based optimization, inverse problems and in particular, parameter estimation with PDE constraints has become central in many fields such as geophysics, atmospheric science, medical imaging, hydrology, petroleum engineering and much more. Problems such as assimilating atmospheric data, recovering the earth's conductivity and matching flow have very similar mathematical characters. Although there are many books on inverse problems and a few on inverse problems in PDE's (for example [16, 14, 19, 10, 8, 11, 18]) there is a lack of books that discuss practical numerical implementation of algorithms that solve such problems. The goal of these lectures is to close some of the gaps between theory and practice by solving some not-so-trivial problems starting from the discretization of the PDE to the optimization discussing practical issues that arise during this process. In order to be concrete we also provide with matlab code. This code *is not intended to be the most efficient code!* In fact, many algorithms and codes can do better for a particular problem. Our goal is to have a useful starting point for students and practitioners so they can solve applied problems in different applications.

We chose two parameter identification problems as prime examples for the methods we discuss here. Although stem from linear PDE's we believe they give good intuition to the main difficulties that arise when solving PDE-optimization problems. To avoid complicated discretization issues we chose to use simple finite volume techniques. In this way we can have simple and efficient code without diving too deep into the PDE aspect of the problem which by itself can fill a whole course. We shortly discuss finite element discretization for the elliptic case and believe that this can be a basis for students who wish to extend the methodology to other problems.

Figure 1.1. *DC resistivity survey. Current is injected into the ground and potentials are measured above the ground or in boreholes. The goal is to estimate the contaminated plum.*

1.2 Model Problems

The problems discuss here are problems of the form

$$\min \quad \mathcal{J}(m,u) \tag{1.1a}$$

$$\text{s.t} \quad c(m,u) = 0 \tag{1.1b}$$

The field $u \in \mathcal{U}$ and the parameter function or the model $m \in \mathcal{M}$ are assumed to be functions in the appropriate Hilbert spaces. The constraint $c(m,u)$ is typically a partial differential equation. It is often (but not always) assumed that it is possible to solve for u given m and this is referred to as the "forward problem". In the inverse problem we choose an appropriate function $\mathcal{J}$ such that we can recover m given some information about u. We now discuss three problems with such structure. These problems evolve from different applications but have very similar mathematical structure from an optimization point of view.

1.2.1 Inverse conductivity problem

Consider the problem where direct electrical current is injected into some media and the potential field in or around the object is recorded. This is demonstrated in Figure 1.1 where a sketch of this experiment is drawn. In order to obtain better resolution many source/receiver combinations are used and many different potentials at different locations are recorded. The governing partial differential equation that describes this phenomena is a simple Poisson equation

$$\begin{aligned} &\nabla \cdot m \nabla u_i = q_i(\vec{x}) \quad i = 1, \ldots, N_s \\ &u(R \to \infty) = 0 \end{aligned} \tag{1.2}$$

Here $u_i(\vec{x})$ is the potential field due to the (assumed to be known) source $q_i(\vec{x})$ and the conductivity $m(\vec{x})$. The number of sources, N_s, varies from a few tens to a few thousands. The number of sources plays a crucial role in designing numerical techniques for the solution of the problem and we return to this point. Since geophysical experiments are done in the field the boundary conditions are typically imposed at infinity. This causes another source of difficulty when dealing with the problem in practice and we discuss this point as well.

In the forward problem, we are given the conductivity and the experimental setting and we compute the field u_j everywhere. Since we record the field only at a few places the forward modeling consists of projecting the solution from source number i to receiver j. Thus, each datum can be written as

$$d_{ij} = \mathcal{Q}_j u_i + \epsilon_{ij} \tag{1.3}$$

where $\mathcal{Q}_j$ projects the i^{th} field into the j^{th} receiver and ϵ_{ij} is the noise. There are many different noise models that can be considered and we discuss this at some length later.

Now, consider that we are given a data set d_{ij} and we would like to explain them. Since the sources are assumed to be known, we are able to estimate the conductivity of the media. This is referred to as Direct Current (DC) Resistivity in geophysics or Electrical Impedance Tomography (EIT) in medical applications. One may consider minimizing the regularized output least squares minimizing the function

$$\mathcal{J}(m) \;=\; \frac{1}{2}\sum_{ij}(d_{ij}(m) - d_{ij}^{\text{obs}})^2 + R(m)$$

where $R(m)$ is an appropriate regularization operator, subject to the PDE constraint Eq. (1.2).

While DC resistivity has a very rich history in geophysics with many current users and some sophisticated codes it has not been so successful in medical applications. Although the problem is not "trivial" it is a good candidate for a model problem for a few reasons. First, as discussed above, the problem is realistic and obtaining better solutions for it has practical value. Second, very similar problems exist in hydrology, finance, semi-conductor design and more. We thus study this problem at some length.

1.2.2 Inverse wave equation

The inverse wave equation is used in seismology as well as in ultrasound imaging and non-distractive testing. Since waves are non-local in their nature, they carry information about the media for a long path and this allows for incomparable

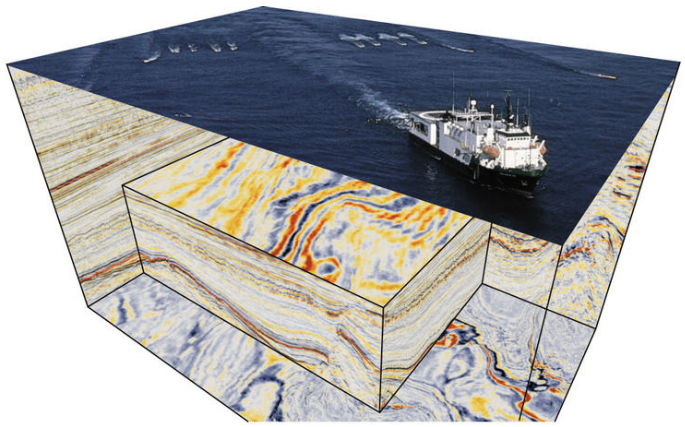

Figure 1.2. *Exploration seismology survey. A boat shoots pressure waves into the ocean measuring pressure waves behind it.*

imaging quality. However, this same nature, makes the wave equation much "less forgiving" for numerical inaccuracies. The exploration seismology setup is plotted in Figure 1.2[1]. A boat carries many receivers and transmits an acoustic wave. The wave is recorded by the receivers and the boat records all the data that is inverted to obtain the seismic velocity of the earth.

Time dependent formulation

We start by considering the wave equation in space-time written in first order form as

$$\kappa p_t = \nabla \cdot \vec{u} - \alpha p \qquad (\vec{x}, t) \in (\Omega, (0, T]) \tag{1.4a}$$
$$\rho \vec{u}_t = \nabla p - \beta \vec{u} \qquad (\vec{x}, t) \in (\Omega, (0, T]) \tag{1.4b}$$
$$p(0, \vec{x}) = p_0 \quad \vec{u}(0, \vec{x}) = 0 \tag{1.4c}$$
$$\lim_{\|\vec{x}\| \to \infty} p(t, \vec{x}) = 0 \qquad \lim_{\|\vec{x}\| \to \infty} \vec{u}(t, \vec{x}) = 0 \tag{1.4d}$$

Here p is the pressure field, $\vec{u}$ is the displacement field, $\rho > 0$ is the density, $\kappa > 0$ is the velocity and $\alpha \geq 0$ and $\beta \geq 0$ are attenuation parameters that are added to the differential equation in order to deal with the infinite boundary condition through a perfectly matched layer. Perfectly matched layer (PML) is a techniques that added absorbing layers to the domain of computation in order to avoid reflections from the boundary. The parameters α and β are anisotropic in these layers, dissipating mainly waves that reflect. Practically speaking, if a sufficiently large PML layer exist then the waves from the boundary do not significantly reflect and the boundary

[1] Image obtained from IRIS image gallary

conditions can be changed to

$$\nabla p \cdot \vec{n} = 0 \quad p \in \partial\Omega$$

This boundary condition also applied to the surface of the earth where no PML is typically set.

In seismic imaging we consider the media properties $m = (\kappa, \rho)$ to be unknown and use measurements of the fields $u = (p, \vec{u})$ in space-time to recover these properties. Since ρ changes very little in many applications, it is often assumed to be constant and the goal is to recover κ.

Similar to the discussion in the DC resistivity problem assume N_s different sources characterized by N_s different initial conditions $p_0^1, \ldots, p_0^{N_s}$. Assume further that we collect the data

$$d_{ijk} = \mathcal{Q}_{ij} p_k + \epsilon_{ijk}$$

where i is the receiver number, j is the time index and k is the source number. We see that this problem has much more information compared to the DC problem as another dimension has been added to the equations. This abandon of data helps in getting much better recovery of the seismic velocity. However, seismic data sets tend to be very large and difficult to deal with due to this reason exactly.

Frequency domain formulation

To deal with the curse of dimensionality and decouple space-time it is possible to work in the frequency domain. Taking the Fourier transform in time we obtain

$$i\omega\kappa p = \nabla \cdot \vec{u} - \alpha p + i\omega s \qquad \vec{x} \in \Omega \tag{1.5a}$$

$$i\omega\rho\vec{u} = \nabla p - \beta\vec{u} \qquad \vec{x} \in \Omega \tag{1.5b}$$

$$\lim_{\|\vec{x}\| \to \infty} p(\vec{x}) = 0 \qquad \lim_{\|\vec{x}\| \to \infty} \vec{u}(\vec{x}) = 0 \tag{1.5c}$$

where s is the source and with some abused of notation we do not change the variables in the Fourier domain. This equation can be further reduced to eliminate $\vec{u}$

$$\vec{u} = (i\omega\rho + \beta)^{-1} \nabla p$$

Obtaining that

$$i\omega\kappa p = \nabla \cdot (i\omega\rho + \beta)^{-1} \nabla p - \alpha p + i\omega s$$

Reorganizing and multiplying by $i\omega$ we obtain

$$\nabla \cdot (\rho + \frac{\beta}{i\omega})^{-1} \nabla p + (\omega^2 \kappa - i\omega\alpha) p = \omega^2 s \tag{1.6}$$

This is a complex Helmholtz equation that can be solved for different frequencies.

For the inverse problem, once again we consider the data

$$d_{ijk} = \mathcal{Q}_{ij} u_k + \epsilon_{ijk}$$

where i is the receiver number, j is the frequency index and k is the source number. The advantage of the frequency domain formulation is that it decouples space-time computation. Its greatest disadvantage is that it requires the solution of the Helmholtz equation for many high frequencies. This solution is not trivial to obtain, especially in 3D.

1.3 Regularization and Optimization

We now unify the discussion about the problems above into a general framework. In the previous section we explored some basic model problems where a PDE is given with some unknown parameters. The goal is to recover the parameters based on observation. The first question one may ask is, can we actually recover the parameter given the (noisy) data? That is, are the parameters identifiable given the data?

The answer for this question is not simple and needs to be studied for each problem in depth. However, in practice, the parameters are **never** fully identifiable without making some very limiting assumptions! This point is crucial to understand (and we will dwell on it later in the course) as one should realize the limitation of our techniques. Maybe one of the obvious reasons is that the number of data is finite and noisy, while the parameters we wish to recover live in a functional space. This begs the question, but what if we have many measurements with excellent accuracy? In this case one needs to look a bit more carefully into each problem. It turns out that for some of the problems discussed here, even infinite data with high accuracy will not result in an stable identifiable parameter.

In order to obtain unique and stable solutions it is therefore common to reformulate the problem as an optimization problem of minimizing a data fitting term and a regularization term, that is, out of all the models that fit the data to some extent we want the one that have a "well behaved" character. Such character is defined as having a small value for a functional $R(m)$. For example, we may want to have a smooth model thus picking $R(m) = \int_\Omega |\nabla m|^2 d\vec{x}$. Balancing the data fitting and the regularization term we arrive to the following optimization problem

$$\min \ \ \mathcal{J}(m,u) = \frac{1}{2}\|\mathcal{Q}u - d\|^2 + \alpha R(m) \tag{1.7a}$$

$$\text{s.t} \ \ c(m,u) = 0 \tag{1.7b}$$

The regularization parameter α determines how well should the data be fitted. For a small parameter, α we have good data fit (assuming low noise).

In the above discussion we arrive the optimization problem Eq. (1.7) from the need to overcome the non-uniqueness in the solution and obtain a "reasonable" model. It is possible to obtain the same formulation from statistical considerations and in particular, from a Bayesian approach [12]. Here we do not discuss Bayesian methods in depth but will point to some of the results when needed.

1.3.1 Discretization and Optimization

The optimization problems we presented above are continuous optimization problems, where the variables "live" in some Hilbert space. There are two different approaches for the solution of such problems. The first refers to as optimize and discretize and the second is refers to as discretize and only then optimize. In the first approach we discretize the optimization problem directly, obtaining and solving a discrete optimization problem. In the second approach "optimize-discretize" we first write the necessary conditions for the continuous optimization problem and only then discretize the problem. In some cases the process of optimize-discretize commute but, by in large, it does not. It is therefore important to understand the different frameworks when deciding about a particular path.

Generally speaking there are pros and cons for each of these methods. In the Discretize then Optimize (DO) we may need to differentiate computational facilitators such as mesh generation routines. This can become rather complicated (and may not be differentiable). On the other hand, the Optimize and Discretize (OD) approach we discretize the necessary conditions (the derivatives of the Lagrangian). The discretized necessary conditions may not be a true gradient of any objective function and thus, if the mesh is not sufficiently fine, can lead to the wrong descent direction. This feature is particularly disadvantageous if a multilevel method is used.

The general rule of thumb we take here that we prefer to use the Discretize then Optimize almost always. We will see that for most applications that are derived from elliptic and parabolic equations this approach is superior. It allows for the use of "standard" optimization techniques and can benefit directly from advances in numerical optimization.