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ELASTIC FULL WAVEFORM INVERSION OF NEAR-SURFACE SEISMIC DATA INCORPORATING TOPOGRAPHY

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„A Scout smiles and whistles under all circumstances“

Lord Robert Smith Baden-Powell (1857-1941)
Elastic full waveform inversion (FWI) is an imaging tool that can yield subsurface models of seismic velocities and density at sub-wavelength resolution. For near-surface applications (tens to hundreds of metres depth penetration), FWI is particularly valuable, because it requires no separation of different seismic phases, such as direct waves, reflections and surface waves, which is a difficult task at this scale. In contrast to conventional methods of seismic data analysis, FWI utilises and interprets the full wavefield. However, real data applications are still scarce. This is due to (i) the non-linearity of the inversion problem, (ii) the high computational costs and (iii) systematic errors that are not taken care of by the FWI algorithm. Although considerable progress has been made during the past few years, there are still a number of issues that remain to be resolved. In my thesis I have tackled three of these problems.

Surface waves often dominate shallow seismic data. With their high amplitudes they dominate the misfit functional and control the model update. Due to their limited depth penetration they are mainly sensitive to shallow parts, such that model updates at greater depth are often very small. In order to balance sensitivities and to increase model updates at depth, I have introduced a novel scaling technique and I have demonstrated its efficiency on synthetic models of varying complexity. The scaling technique involves normalising the squared column sums of the Jacobian matrix prior to adding regularisation and updating the model. This leads to significantly improved velocity images at depth. Although the technique is introduced on near-surface FWI, it is rather general and can be applied to all kind of geophysical inversion problems such as the inversion of geoelectric or electromagnetic data.

Investigating unstable slopes threatened by landslides is a typical near-surface application among many others, where significant topographic undulations are present. It is inevitable to account for such topography in FWI. Through the adaption of SPECFEM2D, a well-established forward solver incorporating irregular grids, I have made it possible
to run FWI on profiles featuring arbitrary surface topography. I have demonstrated the capability to handle considerable topography in the presence of a complex subsurface model including stochastic fluctuations and several block anomalies. Furthermore, I have investigated the effects of neglecting such topography during inversion. It has turned out that topographic undulations with wavelengths or amplitudes similar to the minimum seismic wavelengths have a detrimental effect on model reconstruction.

Seismic survey setups are typically governed by the needs of reflection seismology processing, that is, high fold and dense spatial sampling are required. Using tools of experimental design I have optimised the survey setup for the needs of FWI. I have established a clear recipe consisting of the following points: (i) use horizontally directed sources; (ii) multi-component geophones clearly outperform single-component receivers; (iii) a receiver spacing in the order of the minimum seismic wavelength is sufficient; (iv) the sources employed can be reduced to a few well-selected positions. In this way the costs of a survey can be drastically reduced while the quality of the obtained subsurface images is only slightly affected.

The topics addressed in my thesis shall be a step forward towards successful and efficient FWI of real data. It is anticipated that in a foreseeable future FWI will become a standard tool for the analysis of near-surface seismic data.
Elastische Wellenfeld-Inversion (WFI) ist eine bildgebende Methode, mit welcher man eine Auflösung kleiner als die minimale seismische Wellenlänge erzielen kann. Für Anwendungen im Bereich der nahen Oberfläche (bis zu einigen hundert Metern Eindringtiefe) ist WFI besonders nützlich, weil die verschiedenen seismischen Phasen nicht separiert werden müssen, was sich auf dieser Skala schwierig gestalten würde. Im Gegensatz zu herkömmlichen Analyse-Methoden seismischer Daten verwendet und interpretiert WFI das gesamte Wellenfeld. Trotzdem gibt es bisher nur wenige Studien mit echten Daten. Die Gründe dafür liegen (i) in der Nichtlinearität des Inversionsproblems, (ii) im grossen rechnerischen Aufwand und (iii) in systematischen Abweichungen, die vom WFI Algorithmus nicht berücksichtigt werden. Obwohl in den letzten Jahren grosse Fortschritte erzielt wurden, bleiben einige Fragen offen. In meiner Doktorarbeit möchte ich drei dieser Probleme angehen.


Der Aufbau seismischer Messungen wird typischerweise an die Anforderungen der Reflexionseismik angepasst, sprich, es wird eine hohe Dichte an Geophonen aufwendet. Ich habe den Aufbau optimiert für die Anforderungen der WFI. Ich habe ein klares Rezept hergeleitet, bestehend aus folgenden Punkten: (i) horizontale Quellen sollen verwendet werden; (ii) Multi-Komponenten-Geophone liefern bedeutend bessere Resultate als Ein-Komponenten-Geophone; (iii) die Geophon-Abstände sollen ungefähr einer seismischen Wellenlänge entsprechen; (iv) es reicht, wenn Quellen nur an wenigen, ausgewählten Standorten verwendet werden. So können drastisch Kosten gespart werden, während die Qualität der erhaltenen Abbildungen des Untergrundes nur wenig beeinträchtigt wird.

Die Themen, die ich in meiner Doktorarbeit behandle, sollen ein Schritt sein in Richtung erfolgreicher und effizienter WFI echter Daten. In meinen Augen ist es absehbar, dass WFI zur Standardmethode wird für die Analyse seismischer Daten der nahen Oberfläche.
3D-to-2D Filtering

A.1 Introduction

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1 Introduction
1.1 Near Surface

The near-surface zone (tens to hundreds of metres depth) needs to be characterised for a large range of applications. Using seismic waves to this end has proven useful, such that a long list can be compiled with applications in a variety of fields:

- civil engineering site investigations
  - to determine depth to bedrock (e.g. Miller et al., 1989)
  - to characterise and monitor construction sites of large buildings, dams, bridges, tunnels, etc. (e.g. Jetschny et al., 2011)
  - to obtain important engineering parameters, e.g., Young’s and shear moduli, Poisson’s ratio, bearing capacity (e.g. Maurer et al., 1999)
  - to detect subsurface cavities (e.g. Metwaly et al., 2005)

- hydrogeological and environmental studies
  - to determine the groundwater table (e.g. Birkelo et al., 1987)
  - to delineate fracturing, rock and soil boundaries (e.g. Treadway et al., 2008)

- exploration of geological resources, such as
  - salt bodies (Hale et al., 1992)
  - construction materials, e.g., sand, gravel, clay and limestone (e.g. Lucius et al., 2006)

- natural hazard assessment
  - for permafrost and ice detection (e.g. Merz et al., 2016)
  - for measuring glacier ice thickness (e.g. Nolan et al., 1995)
  - for characterising unstable mountain slopes (e.g. Heincke et al., 2006)

- other matters of public interest
  - to detect and characterise waste and buried materials (e.g. Lanz et al., 1998)
  - for characterisation of potential sites for nuclear waste deposits (e.g. Green and Mair, 1983)
  - to monitor nuclear waste repositories (e.g. Manukyan et al., 2012)
  - to locate buried archaeological structures (e.g. Metwaly et al., 2005)
Even if the key interests are in the deeper structure, such as in oil and gas exploration studies, the near-surface zone cannot be neglected. Due to its large complexity and heterogeneity, it significantly alters the recorded wavefields. In order to identify and remove these effects, the near-surface zone needs to be precisely characterised.

1.2 Seismic Methods

Seismic methods are by far the most widely used geophysical techniques for imaging the subsurface. They find application on a variety of depth scales, from centimetres in material testing to thousands of kilometres in global (earthquake) seismology. In oil and gas exploration, seismic techniques are the principal tool for mapping the subsurface structure down to depths of several kilometres. The principles of wave propagation are the same on all depth scales. However, each scale features its particularities. For example, the finite size of seismic sensors may not be neglected in laboratory studies. On the other end of the spectrum, in global seismology, earthquakes are used as sources, whose exact location, source signature and radiation pattern are further unknowns to the data analysis. In this thesis, I will focus on the near-surface scale (< 1 km) and its particularities.

Seismic surveys can be conducted on the earth’s surface, between boreholes (cross-hole) or from borehole to surface (VSP). Surface seismic surveying is the least invasive and perhaps most cost-effective approach making it the method of choice for most near-surface investigations. The resolution and fidelity with which subsurface structure can be inferred from seismic techniques exceeds that of most available alternative geophysical methods. For engineering, hydrological and environmental investigations, as opposed to oil and gas exploration, 3D seismic surveying is often too laborious and expensive; therefore the sources and the receivers are usually placed along profiles in what is known as 2D surveying.

There are three basic variants on the seismic method that exploit different wave types. In reflection seismic exploration the phases reflected at layer interfaces (Fig. 1.1, yellow arrow) are exploited and interpreted to delineate impedance contrasts in the subsurface (e.g., Yilmaz, 2001). In refraction seismic exploration (or travel time tomography), the first arrivals due to direct, critically refracted and / or diving waves (Fig. 1.1,
blue arrow) are picked and interpreted to get the distribution of the P-wave velocity $V_p$ and to locate a few distinct discontinuities (e.g., Lanz et al., 1998). In multi-channel surface wave analysis, the amplitudes and the dispersion of Rayleigh- and Love-type surface waves (Fig. 1.1, red arrow) are used to detect variations in shear wave velocity $V_s$ and in the damping ratio, respectively (e.g., Socco and Strobbia, 2004).

Fig. 1.1: (a) Seismic survey setup. A source (yellow star) is fired at or just below the surface. Various wave types (arrows) travel through the subsurface to the receivers (blue triangles). (b) Typical seismogram obtained from a near-surface survey (from Reiser et al., 2014); events from (a) are indicated. Within the orange box, these events overlap. The green line indicates the picked first breaks.

On the oil and gas exploration scale, reflection seismology processing is the most common and most advanced technique for analysis of 2D or 3D seismic data sets. The method does not build a model based on inversion, but an extensive workflow of processing steps is applied to the data. This way, a reflectivity image of the impedance contrasts in the subsurface is obtained, related to distinct changes in geological facies, such as layer boundaries or faults. A detailed tutorial to reflection seismology processing can be found in Yilmaz (2001). Here, it shall be pointed out that one group of processing steps aims at amplifying reflections (Fig. 1.1b) while other events, such as refractions and surface waves, are filtered out. Clearly, this means a loss of information, which is accepted in reflection seismology processing.
On crustal to global scales but also in near-surface investigations, traveltime tomography plays an important role. Detailed tutorials can be found for global seismology in Dahlen and Tromp (1998) and for near-surface investigations in Schuck and Lange (2007). Focussing on the latter, the principle is shortly explained here. For source-receiver offsets beyond the so called critical distance, refracted waves arrive first at the receivers because seismic velocities typically increase with depth. With traveltime tomography, the first breaks, i.e. the traveltimes of the refracted events, are inverted in order to obtain a velocity image. As a first step, traveltimes of the first arrivals are picked from the seismogram (Fig. 1.1b, green line). The entire waveforms and their amplitudes are not interpreted. Instead, the observed traveltimes are tried to be fitted with traveltimes predicted from a subsurface velocity model. In an iterative fashion the velocity model is updated in order to minimise the misfit between observed and predicted traveltimes. The velocity model that leads to the minimal misfit is taken as the final image of traveltime tomography.

The third conventional method described here focuses on a wave type that was entirely ignored by the aforementioned techniques: the surface waves. Again, surface waves are utilised in global tomography (Dahlen & Tromp, 1998) but also in near-surface studies. A detailed tutorial for characterisation of the near-surface can be found in Socco & Strobbia (2004). Multi-channel surface wave analysis makes use of the dispersive nature of surface waves. The depth penetration of surface waves is wavelength-and therefore frequency-dependent. The fact that waves typically travel faster at greater depths leads to the dispersive nature of surface waves. In a first step, dispersion curves are extracted from the surface waves in the seismograms. Because surface waves are mainly sensitive to shear wave velocity ($V_s$), 1-D $V_s$-profiles can be found that explain the dispersion curves. The method is therefore mainly suitable for layered media. If there are variations in the second or third direction, pseudo-2D or -3D methods are applied, i.e., 1-D profiles are strung together and laterally constrained by the neighbouring profiles.

The conventional methods summarised above have in common that only a small part of the wavefield (reflected events, first arrival times or surface waves) is utilised while
the rest of the seismograms is neglected, which means a large loss of valuable information. There is no conventional method to truly interpret surface waves (plus all other events) in 2D; this is the point where full waveform inversion comes into play.

1.3 Full Waveform Inversion

In contrast to the aforementioned conventional methods of seismic data analysis, the full waveform inversion (FWI) approach seeks to exploit and interpret the full information content of the seismic records, yielding models of the subsurface at sub-wavelength resolution. The basic idea is to compare the measured seismic data with the forward modelled data and minimising a misfit functional between the two by iteratively updating the model parameters; this process is called inversion. While a single parameter type (typically P-wave velocity \(V_p\)) is sufficient in the acoustic case, a set of three parameter types (typically \(V_p\), S-wave velocity \(V_s\) and density \(\rho\)) is needed in the elastic case. The final images consist of the model parameters that best explain the measured data. If a detailed reflectivity image is desired, the final velocity image can be used for pre-stack depth migration as step of reflection seismology processing (e.g., Rønholt et al., 2014).

The FWI technique emerged in the 1980’s (Mora, 1987; Tarantola, 1984) but did not gain acceptance until recent times with the availability of sufficient computing power to make the inversion problem tractable (Buske et al., 2009; Plessix, 2008). Extensive overviews of FWI are given by Virieux and Operto (2009) and by Fichtner (2011).

Especially on the near-surface scale, FWI seem to be a very promising tool. Near-surface seismic data sets feature several particularities. The weathering layer, the underlying bed rock and the transition zone in between are characterised by large velocity contrasts and heterogeneities. This leads to multiple scattering, P- to S-wave conversions, large attenuation and further elastic effects. The free surface (often featuring large topographic variations) causes large surface wave portions and, together with the large impedance contrast at the boundary to the bedrock, reverberations and guided waves. All these features yield a highly complex wavefield, from which it is difficult to extract single events. Separating events is especially challenging if they overlay each other (Fig.
1.1b, orange box). This is often the case in near-surface seismic data sets, where the offset-range is limited.

For FWI, no separation of events is needed; as its name says, FWI is aimed at modelling and comparing the full wavefield with measured data. In near-surface data sets, surface waves play a crucial role. So far, no other true 2D method exists that interprets surface waves. In reflection seismology processing and traveltime tomography, surface waves are ignored or even filtered out. Conventional surface wave analysis is restricted to the 1-D- or pseudo-2D-case. In contrast, FWI offers a true 2D-tool; with sufficient computational resources it is even possible to solve the FWI problem in 3D (e.g., Butzer et al., 2013; Raknes et al., 2015). However, for near-surface applications, where acquisition resources are often limited, most data sets are acquired along 2D profiles. Therefore, I restrict myself to the 2D case in my thesis.

1.3.1 Forward Modelling

Each FWI routine utilises an appropriate forward solver, which calculates the wavefields and extracts the synthetic data set from a wave equation. The complexity of the considered wave equation, (visco-) acoustic or elastic, optionally including anisotropy, is problem dependent. In this thesis, I consider the elastic, isotropic 2D case. The forward modelling codes can be categorised, based on how spatial derivatives are treated, into finite-difference (FD) or finite-element (FEM) schemes and variants thereof.

Robertsson et al. (1994) as well as Bohlen (2002) presented highly efficient time-domain FD schemes, which enabled (visco-) elastic modelling of the wavefield for large 3D domains. Pratt (1990) solved the wave equation with FD in the frequency domain. This is mainly attractive for multiple sources, which are typically employed in seismic surveys. In the frequency domain, the wave equation can be formulated as a linear set of equations:

\[ S(\omega)u(\omega) = f(\omega), \quad (1.1) \]

where \( \omega \) denotes the angular frequency, \( S(\omega) \) is the impedance matrix containing the model parameters, \( u(\omega) \) is the wavefield and \( f(\omega) \) contains the source terms. Once having inverted \( S \), which is computationally the most demanding task, \( u \) can be calculated
for multiple sources by simply replacing $f$. In contrast, with time domain methods the wavefield needs to be forward propagated through the model for each source individually.

FD schemes are restricted to regular grids (in both time or frequency domain), which makes it difficult to mesh arbitrary surface topography (Bohlen and Saenger, 2006; Robertsson, 1996). Furthermore, modelling surface waves requires very fine spatial discretisation, especially in combination with considerable surface topography. In my work, I used the open source time domain FD code SOFI2D (Bohlen, 2002) and its predecessor for generating independent data sets for later inversion (Chapter 2 and Appendix A).

When it comes to modelling of surface waves (optionally on irregular grids), finite element (FEM) methods may be the option of choice because they (i) naturally contain free surface boundary conditions, and (ii) highly irregular modelling grids can be treated. FEM solvers were implemented and successfully applied in the time domain (e.g., Zhang and Verschuur, 2002) and in the frequency domain (e.g., Brossier, 2011; Min et al., 2003).

As an integral part of our FWI routine, two different forward modelling algorithms can be chosen. Latzel (2010) has implemented a frequency domain FEM solver (Fig. 1.2), in which the linear set of equations (Eq. 1.1)) is solved using the state-of-the-art matrix solver routine PARDISO (Schenk and Gärtner, 2004). The main advantage of this forward solver is its efficiency for multiple sources. Except at the top of the modelling domain, the free surface boundary conditions are replaced by perfectly matched layer (PML) boundary conditions (Basu and Chopra, 2003; Zheng and Huang, 2002), which prevent any boundary reflections.

So far, the frequency domain FEM solver does not consider irregular meshes. For this, I have chosen to employ a different forward solver: SPECFEM2D (Fig. 1.2; Komatitsch and Vilotte, 1998). SPECFEM2D is a well-established and frequently applied code, maintained and further developed by a large team. Therefore, it contains many features that may play an important role for future applications, such as attenuation, anisotropy or its 3D counterpart. Its accuracy on modelling Rayleigh waves for complex arbitrary surface
topography was proven by Komatitsch et al. (1999). This comes at the price of significantly increased runtime compared to the frequency domain solver described above. In the time domain SPECFEM2D employs the spectral element method, a special form of the FEM method, with a particular choice of basis functions and integration points. This ensures improved numerical accuracy and a diagonal mass matrix.

I have written routines that read the wavefields provided by SPECFEM2D, converts them into the format required by our inversion code and performs a fast Fourier transformation because the inversion is performed in the frequency domain (Fig. 1.2). In principle, any external forward solver can be employed if the reading routine is appropriately adjusted.

![Diagram](image)

Fig. 1.2: Forward modelling workflow. The 2D equation of motion is either solved in the frequency domain using the PARDISO matrix solver (left branch; Schenk and Gärtner, 2004) or, when considering arbitrary surface topography, in the time domain using SPECFEM2D (right branch; Komatitsch and Vilotte, 1998).

### 1.3.2 Inversion

As mentioned above, the goal of FWI is to find a subsurface model that best explains the measured data. In principle, this problem could be solved with global optimisation, which immediately yields the global minimum of the misfit functional. This requires the
model space to be densely sampled and therefore involves many forward modelling runs. This is currently computationally prohibitive, such that iterative linearised schemes are preferentially applied. Starting from an initial set of model parameters, they are successively updated until the forward modelled data optimally fit the measured data. Due to the non-linearity of the FWI problem, the initial model needs to be sufficiently close to the true model in order not to get trapped in local minima (cycle skipping). Various methods exist to tackle the non-linearity, the most common of which is to start the inversion at low frequencies and progress to higher frequencies as the model converges. At lower frequencies, the misfit functional contains fewer local minima. Consequently, it appears most elegant to perform inversion in the frequency domain (Pratt, 1999). Furthermore, it was shown that it is sufficient to perform the inversion for a few distinct frequencies only while covering the full wavenumber domain (Sirgue and Pratt, 2004) instead of fitting every time sample of a seismogram. This significantly reduces the data space and therefore saves computational resources (i.e. memory and CPU time).

The model update can be calculated with various methods. The non-linear conjugate gradient (or back-propagated residual) method is comparably cheap because it does not require calculating sensitivities explicitly (e.g., Menke, 2012). The sensitivities are the partial derivatives of the data with respect to the model parameters, i.e., they explain how the data change if a model parameter is perturbed. At the other extreme, the full Newton method even requires second derivatives for faster convergence. The Gauss-Newton method, which we apply, offers a good compromise and only requires first derivatives. Because of the non-linearity, the sensitivities depend on the model parameters; consequently, they need to be re-calculated at each iteration. With the L-BFGS algorithm, the sensitivities could be estimated based on the sensitivities at the previous iteration and the current misfit (Nocedal and Wright, 1999). However, the sensitivities also contain useful information for experimental design; and with the formulation by Zhou and Greenhalgh (2010) we have an efficient tool at hand to calculate them explicitly.

### 1.3.3 Near-surface FWI Studies in Literature

Recently, several research groups recognised the value of FWI for near-surface investigations. Sheng et al. (2006) applied early arrival waveform tomography to marine and
to land seismic data. However, they used acoustic forward modelling and restricted their analysis to a relatively small time window around the first breaks, therefore neglecting surface waves. Similarly, Gao et al. (2007) presented an application of waveform tomography in an environmental study. With 45 2D profiles they construct a 3D image of a buried paleochannel. Smithyman et al. (2009) used waveform tomography to successfully detect three shallow targets in an artificial clay embankment. Romdhane et al. (2011) brought near-surface FWI to a next level by applying a truly elastic code to a synthetic data set stemming from a complex valley-like structure including topography. There are some parallels to our work; they work in the frequency domain and they use an FEM solver for forward modelling. A similar approach was used by Bretaudeau et al. (2013) in order to invert a laboratory data set, which they connected to a near-surface experiment by upscaling dimensions. Groos et al. (2014) investigated the role of attenuation in near-surface FWI. Besides, they demonstrated that they developed a highly capable elastic FWI code using time domain FD forward modelling, applicable to Rayleigh waves. Masoni et al. (2014) tackled the cycle-skip problem inherent in FWI of surface waves by using more robust misfit functions in alternative data domains.

Most near-surface studies so far are restricted to synthetic data sets because of some open questions that need to be resolved prior to the successful application to real data. I will address some of these issues in the framework of my thesis:

i. How can the model update be increased at depth?
ii. How big is the influence of topography on FWI results?
iii. How shall a seismic survey be designed for the needs of FWI?

1.4 Thesis Objectives and Structure

The research questions above are addressed in the framework of my thesis. Surface waves play a crucial role in near-surface seismic data sets. Due to their high amplitudes (Fig. 1.1b), they dominate the misfit functional. However, due to their limited penetration depth, the sensitivities rapidly decay with depth and the information about the deeper structure mainly stems from other events, such as reflections and refractions. In Chapter 2, I present a strategy of upscaling sensitivities at depth, such that the inversion
does not only focus on the shallow structure (addressing question i.). This work was published in the *Journal of Applied Geophysics*.

Topography significantly alters the wavefields, above all, the surface waves. The ultimate goal of my PhD thesis was to incorporate topography into our inversion code. By adapting SPECFEM2D as an external forward solver, I could reach this goal and apply the modified code to first synthetic examples including topography. In Chapter 3, I show these inversion results and I investigate the effects of neglecting topography in the inversion (question ii.). This work was published as an *Express Letter* in the *Geophysical Journal International*.

The acquisition setup for near-surface seismic data is still dictated by conventional seismic data analysis methods. It is questionable if these setups are also well-suited for FWI. Using experimental design tools, I propose a setup, optimised for near-surface FWI, in Chapter 4 (question iii.). Furthermore, computational efficiency will remain a big issue in FWI research for several years. Besides the algorithm employed, two important numbers control the computational costs of FWI: the number of model parameters and the number of data points. In Chapter 4, I focus on the latter by reducing a large data set to its essential parts. This work was submitted to the *Geophysical Journal International*.

The findings of my thesis are wrapped up in Chapter 5. There, I furthermore suggest future research directions for our group and for others working on near-surface FWI.

Appendix A critically appraises a commonly used 3D-to-2D filtering technique. A point source in 2D mathematically corresponds to a line source in 3D. However, seismic data is acquired with a 3D point source. Prior to 2D FWI, the measured data needs to be transformed to line-source data. This data transformation is based on various assumptions and introduces errors to the data. I investigated how these errors propagate to the inversion results; I contributed all inversion experiments (Appendix A.4) to the work that was published in *Geophysics*. 
Elastic full waveform inversion of high-resolution seismic data is a potentially very powerful option for imaging the shallow subsurface. Unfortunately, the success of traditional full waveform inversion applied to such problems is limited by a very uneven sensitivity distribution, which can be attributed to the uneven amplitudes of body and surface waves. As a result, very shallow structures are well resolved by fitting the large amplitude surface waves, but the imaging quality decreases rapidly with depth. To account for uneven sensitivity distributions, we present a novel scaling approach that enhances weak sensitivities in regions of interest. To this end, the column sums of the Jacobian matrix – each of them corresponding to one model parameter – are equalised prior to updating the model. The performance of this methodology is demonstrated by inverting two synthetic, but realistic, data sets. Both the P- and S-wave velocity images were improved significantly by applying the new scaling technique. Our results are particularly relevant for shallow elastic full waveform inversion problems, but we also see benefits of our technique for other surface-based geophysical methods, such as geoelectrics or electromagnetics.

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2.1 Introduction

Seismic methods are by far the most widely used and potent geophysical techniques for imaging the subsurface. They find application on a variety of depth scales, ranging from centimetres in material testing to thousands of kilometres in global seismic tomography. For exploiting the full information content of seismic data, full waveform inversion (FWI) techniques have become an increasingly popular option. Synthetic studies have demonstrated that these techniques are capable of resolving subsurface structures of the order of about half of the minimum wavelength or even less (Wu and Toksöz, 1987). Although these techniques emerged in the 1980’s (Lailly, 1983; Mora, 1987; Tarantola, 1984), they did not gain wide acceptance until recently, mainly due to the lack of sufficient computing power. Excellent overviews on current FWI technology can be found in Buske et al. (2009), Fichtner (2011), Plessix (2008) or Virieux and Operto (2009).

The literature includes a plethora of encouraging synthetic FWI studies, and an increasing number of applications to field data have started to appear. Nevertheless, the technology is still far from being established as a routine data analysis tool, because several practical problems remain. The most challenging problem is certainly imposed by the strong non-linearity of the inverse problem (e.g., Mulder and Plessix, 2008). If the starting model is not close enough to the true model, then the inversion most likely gets trapped in a local minimum of the objective (misfit) function instead of converging to the global minimum related to the true subsurface structure. A commonly employed strategy to mitigate this problem is to start the inversion at low frequencies, and to include higher frequencies as the iterations proceed (Bunks et al., 1995). This is best achieved with frequency-domain FWI (Brossier et al., 2009; Pratt, 1999).

Further challenges occur when inverting for multiple model parameters simultaneously. Typically, elastic FWI seeks to recover the P- and S-wave velocities $V_p$ and $V_s$, as well as density $\rho$. These parameters have different sensitivity (Fréchet derivative) magnitudes, that is, the effect on the waveforms, caused by small changes of individual parameters, can be quite different (Operto et al., 2013). This can lead to trade-offs between the different parameter classes and model updates in the wrong direction. This problem was
discussed, for example, by Manukyan et al. (2012), who proposed balancing the average sensitivities for each parameter class. Meles et al. (2012), in the context of radar FWI, suggested working with sub-Jacobian matrices to overcome the large magnitude difference between electrical permittivity and conductivity sensitivities.

Successful FWI studies have been reported, mainly on crustal (e.g., Kamei et al., 2013) and hydrocarbon exploration scale problems (e.g., Plessix and Perkins, 2010). For such data the individual seismic phases (direct and refracted P- and S-waves, reflections and surface waves) are mostly well separated, such that the inversion can be restricted to selected parts of the seismograms. For example, by focusing on P-waves only, the computationally attractive acoustic approximation can be applied. For near-surface applications, the situation is more complicated because the individual phases are often superimposed (Fig. 2.1). The problem is particularly acute in the short-offset data portion of the seismic record, delimited by the orange box in Fig. 2.1. Unfortunately, this is a typical offset range recorded in a variety of near-surface applications, such as civil engineering investigations, groundwater search, mineral exploration, natural hazard assessments and waste disposal site investigations. The superposition of the individual seismic phases makes reflection processing very challenging (e.g., De Iaco et al., 2003). Furthermore, near-surface structures often exhibit a high degree of lateral heterogeneity, primarily caused by weathering processes, which complicates standard surface wave analyses based on an inherent 1D assumption. Therefore, near-surface seismic data analysis is often restricted to first break refraction traveltime tomography (Lanz et al., 1998), which exploits only a small portion of the information content of the seismic data.

Fig. 2.1: Near-surface data example from a groundwater study in Botswana (Reiser et al., 2014). Various events, such as (Rayleigh-type) surface waves ($L_R$), refractions ($P_{refr}$) and reflections ($P_{refl}$) often overlap and are hard to separate (as within the orange box).
Because of the difficulty in separating the individual seismic phases, one would expect FWI to be particularly useful for near-surface seismic data imaging. Gao et al. (2007), Smithyman et al. (2009) and Sheng et al. (2006) applied (visco-) acoustic FWI, in which they focused on transmitted waves such as direct and refracted events. They removed surface waves by neglecting near-offset traces and restricting the time window of the remaining traces around the first breaks. Bleibinhaus and Rondenay (2009) investigated the validity of this approach and documented the detrimental effects of ignoring the free surface, at least if surface-related phases such as Rayleigh waves cannot be removed from the data without affecting the wavelets. Nevertheless, the above-mentioned studies demonstrated the applicability of FWI to near-surface data, and, compared to traveltime tomography, the spatial resolution was significantly improved.

To better exploit the full information content of near-surface seismic data, one must go beyond acoustic FWI and perform elastic modelling and inversion. Gélis et al. (2007) demonstrated the difficulty of fitting both body and surface waves simultaneously and introduced a strategy of including surface waves at a later stage of the inversion. Romdhane et al. (2011) combined this strategy with a discontinuous Galerkin method for accurate modelling of surface waves, even in the presence of complex surface topography. Brossier et al. (2008) presented an efficient elastic FWI strategy, which they applied successfully to a synthetic landslide model. Because of the additional non-linearity introduced by the surface waves, Perez Solano et al. (2014) and Masoni et al. (2014) investigated the use of alternative misfit functions and claimed improved robustness. Groos et al. (2014) examined the role of attenuation in FWI of (synthetic) near-surface data including Rayleigh waves. They concluded that a priori quality factors to be incorporated into forward modelling can be critical for considering the often pronounced attenuation of seismic waves in the near-surface zone. An example of FWI with observed data taken from a physical scale model experiment was provided by Bretaudié et al. (2013). Their setup was designed to obtain data that were dominated by high amplitude surface waves on which various other seismic phases with lower amplitudes were superimposed. This allowed them to scale their results to the near-surface scenario where a similar, albeit less controlled situation is expected.
The presence of surface waves in near-surface data along with body waves leads to a further problem that has not yet been fully addressed. The surface waves have relatively large amplitudes and cause large sensitivities at shallow depth. They dominate the misfit functional and are consequently fitted by updating the shallow structures. Due to their dominance in the misfit functional they preclude the weaker body waves from being well fitted. Significant depth information is often contained in these weak body waves and remains unrevealed with a conventional waveform inversion procedure due to the dominance of the surface waves.

To address this problem, we present a methodology that enforces a more even sensitivity distribution using a matrix scaling technique, which is well known in statistical regression analysis (e.g., Nocedal and Wright, 1999). After a brief discussion of the background theory, we demonstrate the usefulness of our approach using synthetic subsurface models of varying complexity.

2.2 Theory

2.2.1 Full Waveform Inversion

The aim of FWI is to find a suitable subsurface model $m$, such that the predicted wavefield $u$ (using this model $m$) fits the observed data $d$ to within a certain error tolerance. This is achieved by minimising a misfit function, which is in our case based on the $L_2$-norm. Forward modelling of $u$ and the corresponding inversions can be carried out either in the time domain or in the frequency domain. We have chosen to work in the frequency domain because of (i) the efficiency of forward modelling for multiple sources (Pratt, 1990b), and (ii) the strategy of being able to tackle the non-linearity of the inversion problem by starting at low frequencies and moving to higher frequencies as the model converges (Bunks et al., 1995).

The 2D elastic isotropic wave equation is solved with a finite element algorithm (FEM) code (Latzel, 2010; Min et al., 2003). The free-surface boundary condition is implicit in the FEM code, which is favourable for our study. At the side and bottom edges of the modelling domain perfectly matched layer (PML) boundary conditions are applied (Basu and Chopra, 2003; Zheng and Huang, 2002).
The inverse problem is solved using a regularised Gauss-Newton inversion scheme (e.g., Pratt et al., 1998), whereby the model parameters in vector $m$ include P- and S-wave velocities $V_p$ and $V_s$ as well as density $\rho$. The model update at iteration $i+1$ can be written as

$$m^{i+1} = (J^T J + \alpha^2 I + \beta^2 L^T L)^{-1} \left\{ J^T \left[ (d - y) + J m^i \right] + \alpha^2 I m^i \right\},$$

(2.1)

where $J$ is the Jacobian or sensitivity matrix, $I$ is the identity matrix and $L$ is the Laplacian smoothing operator (e.g., Manukyan et al., 2012). The scalars $\alpha$ and $\beta$ determine the weights of damping and smoothing, respectively. Both are needed to stabilise the under-determined inverse problem. Damping minimises the deviation from a reference or preferred model, which is in our case the model from the previous iteration, and smoothing minimises structural complexity. In the following, we refer to $(J^T J + \alpha^2 I + \beta^2 L^T L)$ as the (regularised) approximate Hessian matrix.

The sensitivities $J_{pq}$ in $J$ describe how a modelled datum $u_p$ changes if a model parameter $m_q$ is changed:

$$J_{pq} = \frac{\partial u_p}{\partial m_q},$$

(2.2)

with $p$ ranging from 1 to the number of data points ($= 2 \times$ number of sources $\times$ number of source directions $\times$ number of receivers $\times$ number of receiver directions $\times$ number of frequencies; the factor 2 is required for including real and imaginary parts of the complex valued frequency domain data into the real valued matrix $J$), and $q$ ranging from 1 to the number of model parameters. We calculate $J$ using explicit expressions derived by Zhou and Greenhalgh (2010), transformed from elastic Lamé parameters to $V_p$, $V_s$ and $\rho$ (Manukyan et al., 2012).

### 2.2.2 Hessian Matrix Scaling

The sensitivities contained in the Jacobian matrix $J$ play a pivotal role during the solution of the inverse problem. An important property of $J$ is given by the relative (absolute) magnitudes of the individual columns. If the sensitivities within a particular column are very small, it is to be expected that the update of the corresponding model pa-
rameter will be also very small. This can be seen from the structure of the approximate Hessian matrix in Eq. (2.1); the diagonal of $JJ^T$ contains cumulative sensitivities, i.e., the sum of squared sensitivities of all data (all sources, receivers and frequencies) for one model parameter:

$$\left(J^TJ\right)_{qq} = \sum_p \left(\frac{\partial u_p}{\partial m_q}\right)^2.$$ (2.3)

The damping term, a multiple of $I$, is added to $JJ^T$, having strong relative weights where the cumulative sensitivities are small. Consequently, the corresponding model parameters are kept close to those from the previous iteration.

In surface seismic FWI problems (and most other surface-based geophysical methods), the sensitivities of near-surface parameters are generally very high and decrease rapidly with depth, which causes shallow model parameters to be much better resolved than those of deeper structures. This has been recognised, for example, by Li and Oldenburg (1996). They introduced a depth-dependent weighting scheme to account for the rapidly decreasing sensitivities of magnetic data with depth.

Here, we follow a similar approach, which is referred to as matrix scaling (Nocedal and Wright, 1999; Smith, 1976). The idea of matrix scaling is to normalise the columns of $J$, such that the column sums of squares, each corresponding to one model parameter, are equalised. These column sums are a proxy for the model resolution (Meles et al., 2012). This can be achieved by multiplying $J$ with a diagonal scaling matrix $S$ defined as

$$S = \text{diag} \left( \frac{\max \left( \sum_p J_{pq}^2 \right)}{\sum_p J_{pq}^2 + \delta} \right).$$ (2.4)

Note that the sums equal the diagonal elements of $J^TJ$ in Eq. (2.3), which means that no extra calculation is required. The scalar $\delta$ is added to the denominator for stabilising the calculation of the scaling factors. This avoids very small sensitivities from being excessively boosted, which would lead to artefacts in the resulting waveform tomograms. The solution of the scaled inverse problem yields a solution vector $S^{-1}m$, and the sought solu-
tation vector $m$ can be determined by a multiplication with $S$. A scaled version of the Gauss-Newton solution in Eq. (2.1) can therefore be obtained by substituting $J$ by $JS$ and $m$ by $S^{-1}m$, leading to

$$S^{-1}m^{i+1} = \left( SJ^TJS + \alpha^2I + \beta^3L^TL \right)^{-1} \left\{ SJ^T \left[ (d - u) + Jm^i \right] + \alpha^2S^{-1}m^i \right\}. \quad (2.5)$$

The diagonal elements of $SJ^TJS$ are now approximately equalised such that the damping term $\alpha^2I$ has equal relative weights on them and the model update will be balanced throughout the model.

An interesting property of Eq. (2.5) can be recognised when considering the underlying scaled normal equations:

$$\left( SJ^TJS + \alpha^2I + \beta^3L^TL \right)S^{-1}m^{i+1} = SJ^T \left[ (d - u) + Jm^i \right] + \alpha^2S^{-1}m^i. \quad (2.6)$$

Applying a left side multiplication with $S^{-1}$ and rearranging terms yields

$$\left( J^TJ + \alpha^2S^{-2} + \beta^3S^{-1}L^T L S^{-1} \right)m^{i+1} = J^T \left[ (d - u) + Jm^i \right] + \alpha^2S^{-2}m^i. \quad (2.7)$$

Here, the inverse scaling matrix $S^{-1}$ acts solely on the regularisation terms. That is, similar effects can be obtained by suitably adjusting the regularisation parameters. This is indeed the concept of “active constraint balancing” proposed by Yi et al. (2003), which results in spatially variable regularisation. It has been applied to acoustic FWI by Joo et al. (2012). More recently, Asnaashari et al. (2015) applied a similar form of spatially variable regularisation for target focused time lapse inversions of acoustic waveform data.

Our approach is formally similar to active constraint balancing, but it differs in the way the scaling matrix $S$ is obtained. Furthermore, we extend the application to elastic FWI, where sensitivities are even less balanced due to the strong impact of surface waves.

### 2.3 Synthetic Examples

The performance of the Hessian matrix scaling proposed above is tested on two synthetic examples. The theory introduced above is first illustrated on a simple “layered model”, which features three layers with stochastic fluctuations and a constant Poisson's ratio of 0.26 (see Fig. 2.2a, b). The true density model is calculated from $V_p$ using Gard-
ner's relation (Gardner et al., 1974). The scaling strategy is then benchmarked with a more complex and more realistic model that exhibits spatially variable Poisson's ratios (see Fig. 2.2c, d). The model includes sharp interface topography (step or fault structure) and block insertions within the upper and lower layers. In the following, it is referred to as "block model". The density model is given by a simple gradient (see Table 2.1) in order to not influence the reconstruction of the velocity anomalies by cross-talk. We computed synthetic data for 27 evenly distributed $x$- and $z$-directed sources between $x = 16$ m and $224$ m and 52 $x$- and $z$-directed receivers in the same distance range. Both, sources and receivers were placed at a depth of $z = 0.2$ m (see Table 2.1 for further details of the simulations).

First, we demonstrate the dominance of the surface waves using the layered model shown in Fig. 2.2(a, b). A time-domain wavefield snapshot of the vertical ground displacement $u_{zz}$ at $t = 0.1$ s caused by a vertically directed source at $x = 16$ m is shown in Fig. 2.3(a). It is calculated with the SOFI2D modelling software (Bohlen, 2002). It can be clearly seen that the amplitudes of the (Rayleigh-type) surface waves are much larger than those of the refracted P-waves, which have penetrated to greater depths. Since we perform FWI in the frequency domain, we are interested in the equivalent of the time-domain snapshot, that is, the frequency-domain Green's functions. In Fig. 2.3(b), their real parts are shown, again for a vertical source at $x = 16$ m, and a frequency $f = 40$ Hz (the corresponding image for the imaginary parts is similar and therefore not shown). As in the time-domain snapshots, the high amplitudes are concentrated near the surface. In Fig. 2.3(c), the sensitivities of $V_s$ are shown for the same source and frequency and a vertical component receiver at $x = 222$ m. As expected, the sensitivities are also concentrated along the surface, even for this large offset and relatively low frequency of about half the central frequency (Table 2.1). The cumulative sensitivities of $V_s$ (Eq. (2.3)) for all sources and source directions, all receivers and receiver directions and all frequencies considered during the inversions (Table 2.2) are shown in Fig. 2.3(d): They are largest in the shallowest part of the model, thereby indicating that the model update will be focused in this region.
Fig. 2.2: True models used in the modelling study: (a) $V_p$ of simple layered model with stochastic fluctuations and (b) constant Poisson’s ratio of 0.26; (c) more complex model with a dipping structure, block insert anomalies and spatially varying Poisson’s ratio (d). The source (×) and receiver (●) positions are indicated above the model but they are located at 0.2 m depth.

<table>
<thead>
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<th>Table 2.1: Forward modelling parameters</th>
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<tr>
<td>Sources</td>
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<tr>
<td>receivers</td>
</tr>
<tr>
<td>source signature</td>
</tr>
<tr>
<td>forward modelling cell size</td>
</tr>
<tr>
<td>$V_p$</td>
</tr>
<tr>
<td>$V_s$</td>
</tr>
<tr>
<td>Poisson’s ratio</td>
</tr>
<tr>
<td>Density</td>
</tr>
<tr>
<td>$\lambda_{\text{min}} = V_{s,\text{min}} / f_{\text{max}}$</td>
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In order to obtain the initial model for waveform inversion, “true” traveltimes calculated with a finite difference Eikonal solver (Podvin and Lecomte, 1991), were inverted for $V_p$ using a strategy similar to Lanz et al. (1998). A simple gradient model ($V_p = 1648$-$3225$ m/s) acted as initial model for the traveltime inversion. The resulting traveltime tomogram for the layered model is shown in Fig. 2.4(a). Although the traveltime RMS misfit could be reduced to 10.3% of the initial RMS (see Table 2.3), there is still a poor match between the true and the recovered models. This can be best recognised in the velocity-depth function extracted from the tomogram at $x = 180$ m (orange line in Fig. 2.4d).
Fig. 2.4: Resulting $V_p$-images from inversion of data modelled on the layered model (Fig. 2.2); (a) initial model obtained from traveltime inversion; (b) unscaled WFI result; (c) scaled WFI result; and (d) comparison of a profile at $x = 180$ m (indicated in (a-c) with the dashed line).

Table 2.3: RMS misfits before and after each step of the inversion procedure.

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<th>layer model</th>
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<th>block model</th>
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<tr>
<td></td>
<td>traveltime RMS</td>
<td>waveform RMS</td>
<td>traveltime RMS</td>
<td>waveform RMS</td>
</tr>
<tr>
<td>initial model</td>
<td>100%</td>
<td>n/a</td>
<td>100.0%</td>
<td>n/a</td>
</tr>
<tr>
<td>traveltime tomography</td>
<td>10.3%</td>
<td>100%</td>
<td>7.7%</td>
<td>100%</td>
</tr>
<tr>
<td>unscaled FWI</td>
<td>n/a</td>
<td>31.0%</td>
<td>n/a</td>
<td>15.1%</td>
</tr>
<tr>
<td>scaled FWI</td>
<td>n/a</td>
<td>18.1%</td>
<td>n/a</td>
<td>6.4%</td>
</tr>
</tbody>
</table>
In the following, FWI results from the conventional unscaled inversion and the newly introduced scaled inversion will be compared. The real and imaginary parts of the frequency domain waveform data were inverted for \( V_p \), \( V_s \) and density. To make Gauss-Newton inversion tractable, we merged the forward modelling cells to larger inversion cells of 5.0 m width and 2.0 m depth. Such a parameterization is adequate for the spatial resolution expected from elastic FWI in the order of half a wavelength (Wu and Toksöz, 1987).

The traveltime tomogram (Fig. 2.4a; orange line in Fig. 2.4d) served as an initial \( V_p \)-model, and the initial \( V_s \)-model (Fig. 2.5a; orange line in Fig. 2.5d) was obtained from the traveltime tomogram by assuming a constant Poisson’s ratio of 0.29. The initial density model was obtained using Gardner’s relation (Gardner et al., 1974). Reconstruction of density proved to be difficult, as previously described by others (Virieux and Operto, 2009). Therefore we will restrict our analysis to \( V_p \) and \( V_s \).

Following Sirgue and Pratt (2004), we have chosen seven inversion frequencies in the range from 20 to 150 Hz. They were subdivided into three partly overlapping groups (Table 2.2). In order to reduce cycle skipping effects, the lowest frequency group was considered initially, and then it was moved to higher frequencies in the course of the iterations.

The source signature was treated as unknown and it was estimated using the approach of Maurer et al. (2012). Regularisation was supplied in form of damping. The damping weight (factor \( \alpha \) in Eq. (2.1)) was determined using a local line search algorithm (Brent, 1973). The application of smoothing was removed in order to retain sharp interfaces in the inversion results (i.e., \( \beta = 0 \) in Eq. (2.1)). The inversion was run until convergence, i.e., until the RMS only decreased marginally per iteration, which was usually the case after 12 iterations per frequency group.
Fig. 2.5: Resulting $V_s$-images from inversion of data modelled on the layered model (Fig. 2.2); (a) initial model obtained by multiplying the traveltime inversion result for $V_p$ with a constant factor of 0.54 (corresponding to a Poisson’s ratio of 0.29); (b) unscaled WFI result; (c) scaled WFI result; and (d) comparison of a profile at $x = 180$ m (indicated in (a-c) with the dashed line).

The results of the unscaled inversion are shown for $V_p$ in Fig. 2.4(b, d) and for $V_s$ in Fig. 2.5(b, d). Compared to the traveltime tomograms, the spatial resolution is much improved, especially in the upper part of the model, where the shallow layer interface is imaged clearly. The waveform misfit could be reduced to 31.0% with respect to the initial model (Table 2.3). The deeper interface and the deepest layer are still less resolved. Considering the sensitivity distribution (Fig. 2.3c) this had to be expected. Minor artefacts emerged at the right edge of the model around $(x, z) = (238$ m, $6$ m), when adding
the highest frequency group to the inversion. However, they are outside of the source spread, where no interpretable results can be expected.

![Fig. 2.6: Scaling factors calculated at the first iteration of each frequency group (see annotation at the left) during the inversion for the layered model. Note the different ranges of values for $V_p$ (left column; a,c,e) and $V_s$ (right column; b,d,f).](image-url)

Finally, a scaled inversion was performed using Eq. (2.5), again starting from the traveltime inversion result. The initial scaling factors for each frequency group were calculated according to Eq. (2.4) and are shown in Fig. 2.6. As expected, the scaling factors generally increase with depth, more rapidly towards the edges of the model. The increase is more pronounced for higher frequencies, which comes from the sensitivities at depth being smaller for higher frequencies. The range of scaling factors for $V_p$ is larger than for $V_s$, which means that the corresponding cumulative sensitivities are smaller. This makes sense, since the surface waves are predominantly sensitive to changes in $V_s$. The different ranges of scaling factors automatically address the problem of individual magnitudes of various parameter classes and makes further balancing unnecessary. The scaled inversion further improved the images of $V_p$ (Fig. 2.4c, d) and $V_s$ (Fig. 2.5c, d). In
particular, the deeper parts of the model below $z = 40$ m are better resolved, which can mainly be seen from the profile. The misfit could be further reduced to 18.1% (Table 2.3). After illustrating the benefits of Hessian matrix scaling on a relatively simple model, we next investigate if similarly good results can be achieved with the more complex model shown in Fig. 2.2(c, d). This model exhibits steeply dipping structures and two small-scale block anomalies, as well as more realistic and spatially variable Poisson’s ratios. Particularly the reconstruction of the deep low-velocity structure is expected to be challenging. Due to the increased lateral heterogeneity of this model, the size of the inversion cells was adjusted to $4.0 \times 2.0$ m. The remaining inversion parameters were identical to those in the previous example.

Not surprisingly, the traveltime tomography (Fig. 2.7a, d) yields only a poor image of the complex structures. The shallowest interface is partly imaged, but at greater depth, the model remains close to the initial model. The poor performance is caused primarily by the limited depth penetration of the seismic rays due to lacking large offsets.

With the unscaled FWI the shallow high-velocity anomaly can be better imaged (Fig. 2.7b, Fig. 2.8b) and the deeper anomaly can be identified, although it appears rather blurred. Below $z = 60$ m the model is barely updated, which is the result of the small waveform sensitivities associated with this region. Around the sources and receivers there are artefacts emerging in $V_p$. This is due to the poor initial model; because of the uneven sensitivity distribution the data are tried to be fitted by updating the uppermost layers only, which is not a successful strategy for fitting the body waves. The scaled inversion results (Fig. 2.7c, d, Fig. 2.8c, d) offer a significant improvement compared with the unscaled inversions. In particular, the $V_s$-image reconstructs most of the true model accurately. The spatial resolution is inferior in the $V_p$-tomogram than in the $V_s$-result due to the longer wavelengths of P-waves, and artefacts related to the right edge of the model have a stronger impact. Moreover, the sensitivities are generally larger in $V_s$ and, consequently, larger scaling factors are required for $V_p$ (see Fig. 2.6). This bears the risk of (over-) boosting small sensitivities, which leads to increased artefacts, mainly in $V_p$. This was prevented by introducing $\delta$ in Eq. (2.4). It is important that $\delta$ is chosen small enough, such that scaling factors still have considerable weights.
Fig. 2.7: Resulting $V_p$-images from inversion of data modelled on the block model (Fig. 2.2c,d); (a) initial model obtained by traveltime inversion; (b) unscaled WFI result; (c) scaled WFI result; and (d) comparison of a profile at $x = 150$ m (indicated in (a-c) with the dashed line).

Nevertheless, the $V_p$-result from the scaled inversion is much superior to the one from the unscaled version; the artefacts around the sources and receivers could be avoided by focussing the model update at depth rather than at the shallow subsurface. The models are poorly reconstructed at $x > 200$ m. As for the simple model (Fig. 2.4, Fig. 2.5), this can be attributed to the fact that this region is poorly illuminated by the source-receiver geometry employed. Comparable effects are expected at the left edge of the model, but here the artefacts are less pronounced because the initial model is closer to the true model in this region.
Fig. 2.8: Resulting $V_s$-images from inversion of data modelled on the layered model (Fig. 2.2); (a) initial model obtained by multiplying the traveltime inversion result for $V_p$ with a constant factor of 0.54 (corresponding to a Poisson’s ratio of 0.29); (b) unscaled WFI result; (c) scaled WFI result; and (d) comparison of a profile at $x = 180$ m (indicated in (a-c) with the dashed line).

Fig. 2.9 shows the time-domain data misfit between observed and computed seismograms for the final inverted model for a $z$-directed source at $x = 16$ m and all $z$-directed receivers. Overall, the unscaled and the scaled inversions yield models that explain the data very well (Fig. 2.9a). In particular, the high amplitude surface waves (Fig. 2.9c) with their strong influence on the misfit function are well fitted, already after the unscaled inversion. This was expected since they dominate the misfit functional and they are consequently fitted first. This reduces the waveform RMS to 15.1% of the initial value (Table 2.3). In contrast, the small amplitude body waves (Fig. 2.9b) are only well fitted after the
scaled inversion, which reduces the waveform RMS to 6.4%. During the unscaled inversions, these low amplitude waves were overwhelmed by the high amplitude surface waves and did not contribute much to the tomographic images. The better balanced sensitivities of the scaled inversion increased the importance of the body waves, which was key for the improvements.

Fig. 2.9: Time-domain data misfit for a vertical source at $x = 16$ m and all vertical receivers, equally distributed with 4 m spacing at $x = 16$-224 m in the block model. In the (a) full section, the model responses from the unscaled inversion (green) and the scaled inversion (red) can hardly be distinguished from the true data (black). This also holds for the zoom on the surface waves (c). The difference becomes obvious when zooming in on diffracted waves (b), which is best fitted by the model response of the scaled inversion.
2.4 Discussion

We have demonstrated one possible option for choosing the scaling factors based on cumulative sensitivities. For that purpose, we had to introduce a stabilisation parameter $\delta$ (Eq. (2.4)), which added some subjectivity to the inversion process. A proper choice of $\delta$ is critical; choosing $\delta = 0$ would perfectly equalise the diagonal elements of $\mathbf{S}^T \mathbf{J} \mathbf{S}$. However, following such a strategy would inevitably lead to instability due to exaggerated boosting of very small sensitivities. Extensive numerical tests have shown that the inversion results for the layered model are rather insensitive to varying $\delta$ even over three orders of magnitudes. The inversion results for the more complex block model were more sensitive to the choice of $\delta$; choosing it too small resulted in increased artefacts mainly in the recovered $V_p$-model whereas choosing it too large resulted in the model update being too much focused on the $V_p$-model because of the stronger relative weight of $\delta$ on the smaller sensitivities in $V_p$. However, choosing $\delta$ slightly smaller than the median of the cumulative sensitivities for $V_p$ yielded stable results in all considered cases and seems to be an appropriate recipe.

In principle, the choice of the scaling factors is arbitrary and can be adapted to the inversion problem. A possible option includes choosing $\delta = 0$ and mapping the scaling factors logarithmically onto a predefined interval, similar to the strategy by Joo et al. (2012). This yielded similar inversion results to the ones shown in this study, but with increased artefacts in $V_p$. Another possibility is to set again $\delta = 0$ and defining an upper threshold of the scaling factors. Various tests were performed with different thresholds. Best results were obtained by limiting the largest 30% of the scaling factors to the maximum of the remaining 70%. Again, this resulted in increased artefacts in $V_p$. Besides these rather general options, it is also possible to choose the scaling factors such that updates in specific regions are enforced. This can be useful when changes over time are expected in a restricted region only (Asnaashari et al., 2015).

Another method of balancing the model update includes adjusting the inversion cell size to the sensitivities (e.g., Plattner et al., 2012). This would cause an increased size of the inversion cells with depth. A beneficial feature of this approach is that it further reduces the number of inversion parameters. Therefore, this is common practise in vari-
ous geophysical disciplines, such as geoelectrics (e.g., Rücker et al., 2006) or surface-NMR (e.g., Hertrich et al., 2010), but its applications to FWI are rare. We have performed tests with variable cell sizes, but we found it difficult to adjust the grid such that it equilibrates the sensitivities while maintaining the desired spatial resolution.

2.5 Conclusions

We have demonstrated that a novel scaling approach of the approximate Hessian matrix in Gauss-Newton-type FWI problems can improve inversion results considerably. Our scaling strategy enhances weak sensitivities and thus the model updates in the corresponding regions that would otherwise remain unresolved. This is generally beneficial for surface-based geophysical measurements that exhibit typically large sensitivities near the surface and then decrease rapidly with depth. For elastic FWI problems this is particularly acute because of the dominance of surface waves, which are only sensitive to shallow depth region. Additionally, we also see benefits for many other geophysical techniques, such as geoelectrics and electromagnetics.

In our approach the scaling factors were calculated based on cumulative sensitivities, which were directly taken from the approximate Hessian matrix. This strategy has proven to be useful on two synthetic examples from elastic FWI, where the quality of the tomograms could be improved markedly at greater depths. It should be quite trivial to generalise this concept of scaling to address specific objectives of a geophysical inversion. For example, it is possible to force inversions to perform updates in regions that are of special interest.
The effects of neglecting ground surface topography variations in elastic full waveform inversion are investigated using two classes of synthetic example. The first type of example shows that failing to account for even small amplitude fluctuations in topography introduces velocity artefacts in the near-surface part of the tomogram as well as degrades significantly the spatial resolution of features at greater depths. The disturbances are particularly severe when the topographic fluctuations have wavelengths comparable to the minimum seismic wavelength. The second type of synthetic example considers long wavelength topography variations of various amplitudes. It is found that neglecting topography with an amplitude fluctuation greater than half the minimum seismic wavelength leads to appreciable inversion image artefacts. Therefore, the incorporation of surface topography, even if it appears minor, is essential for successful elastic full waveform inversion of land seismic data.

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3.1 Introduction

Full waveform inversion (FWI) of seismic data is a very powerful tool, capable of yielding subsurface images at sub-wavelength resolution (Wu & Toksöz, 1987). Especially for near-surface applications (investigation depth < 200 m), FWI is a favoured option because there is no need to separate different wave types (P- and S-waves, reflections, surface waves, etc.) prior to performing the data analysis. Despite the early theoretical formulations (Tarantola, 1984; Mora, 1987), convincing FWI studies have emerged only recently and developments are still ongoing. Comprehensive reviews on FWI can be found in Virieux & Operto (2009) and Fichtner (2011).

The Earth’s free surface has a first-order imprint on seismic waveforms obtained from surface-based experiments. Therefore, topographic undulations are expected to have a significant impact on FWI. A simple approach to account for these variations is to apply static corrections prior to FWI (Smithyman & Clowes, 2012). However, this only accounts for the mis-positioning of the sources and receivers and time fluctuations due to the topography but it does not consider the wavefield dynamics (amplitudes) and the additionally introduced wave scattering / mode conversion. Brenders (2011) and Smithyman et al. (2009) sought to handle the topography by introducing an additional air layer into the modelling domain, but they restricted themselves to the visco-acoustic case. Bleibinhaus & Rondenay (2009) investigated ground surface topography effects on visco-acoustic FWI. They concluded that ignoring topographic variations causes some artefacts in the tomograms, but the results were still satisfactory. The robustness of (visco-) acoustic FWI towards topographic variations can be explained by the fact that such inversions consider only small time windows starting from the first breaks. In contrast, elastic FWI incorporates larger portions of the seismograms including shear waves and surface waves. Due to their high amplitudes, the surface waves have a substantial influence on elastic FWI, particularly for near-surface problems (Nuber et al., 2015). Consequently, topographic effects are expected to have a major influence on elastic FWI.

To the best of our knowledge only scant attention in the literature has been paid to surface topography in near-surface or exploration-scale elastic FWI studies. This is partly due to the computational complexity of the problem. Finite-difference modelling of
Rayleigh waves (especially with topography involved) requires a very fine spatial discretisation (Robertsson, 1996), which is often prohibitive for realistic subsurface models (Bohlen & Saenger, 2006). In addition, the regular grids used for finite-difference modelling allow only limited possibilities for considering irregular topography. Finite and spectral element methods inherently include the free surface as a natural boundary condition, therefore accurate modelling of Rayleigh (and body) waves can be performed at no extra costs (Komatitsch & Vilotte, 1998). This has been recognised by Yuan et al. (2015), who used spectral elements for performing successful FWI of Rayleigh and body wave data, but they considered only a flat topography. The only elastic FWI study that we are aware of which includes surface topography was that of Romdhane et al. (2011) who used a frequency domain finite element forward solver.

In view of the difficulties to implement efficient forward solvers that consider topographic effects accurately, it is important to know when topographic undulations can be ignored, and when they have a significant impact on elastic FWI results and must be included. In this study we investigate this issue in more detail. We first introduce our FWI algorithm and the associated forward solver. Then we demonstrate the effects of ignoring topographic variations using a range of synthetic models.

3.2 The FWI Algorithm

The idea of FWI is to minimise the misfit between observed data $d$ and forward modelled data $u$ by updating the model parameters $m$, in our case the P- and S-wave velocities $V_p$ and $V_s$ as well as the density $\rho$. Therefore, every inversion code consists of a forward modelling engine and an inverse solver.

We have adapted the SPECFEM2D forward solver (Komatitch & Vilotte, 1998) in our FWI code because it naturally contains free surface boundary conditions and it can handle arbitrary surface topography. Its accuracy and efficiency in modelling Rayleigh waves for complex topographic models was demonstrated by Komatitsch et al. (1999), and by our own comparisons with an in-house finite element code (Latzel, 2010).

SPECFEM2D operates in the time domain, but we have chosen to perform the inversion in the frequency domain (e.g., Pratt et al., 1998), where the $L_2$-misfit between ob-
served and calculated spectral data is minimised. This requires the modelled wavefields to be Fourier transformed. Working in the frequency domain reduces the data space significantly by inverting for a few distinct frequencies whilst retaining the full wave-number coverage (Sirgue & Pratt, 2004). The non-linearity and local minimum trapping problem is tackled by starting at low frequencies and successively moving to larger frequencies as the model converges. We employ a Gauss-Newton approach to calculate the updated model parameters $m^{i+1}$:

$$m^{i+1} = \left( J^T J + \alpha^2 I + \beta^2 L^T L \right)^{-1} \left\{ J^T \left[ (d - u) + Jm^i \right] + \alpha^2 I m^i \right\},$$  

(3.1)

where the matrix $J$ contains the sensitivities, $I$ is the identity matrix, $L$ is the Laplacian smoothing operator, $i$ is the iteration index and the scalars $\alpha$ and $\beta$ specify the relative weights of the regularisation terms in the form of damping and smoothing. The sensitivities contained in $J$ are calculated using explicit expressions derived by Zhou & Greenhalgh (2010). Furthermore, at every iteration, source coupling factors are estimated using the strategy given by Maurer et al. (2012).

### 3.3 Effects of Neglecting Surface Topography

To study the effect of ground topography on FWI we have setup a synthetic but realistic 2D model (Fig. 3.1a) consisting of a background medium having a linear velocity gradient ($V_p = 1139-3445$ m/s, $V_s = 649-1964$ m/s), upon which stochastic fluctuations are superimposed. Embedded in the model are various deterministic high- and low-velocity block anomalies of different sizes and at different depths. The velocity contrasts and the $V_p/V_s$-ratios are also varied. The density model includes a gradient background ($\rho = 1798-2371$ kg/m$^3$) with stochastic fluctuations but without embedded anomalies. Synthetic data sets are computed for 27 equidistant sources at the positions $x = 16, 24, ..., 224$ m and 52 equidistant receivers at the positions $18, 22, ..., 222$ m. Sources and receivers are both $x$- and $z$-directed and buried at 0.5 m depth.

For all our inversions we have chosen simple $V_p$ and $V_s$ initial models with a linear gradient. The reconstruction of $\rho$ is a challenging problem (Virieux & Operto, 2009). To avoid such complications and to focus on the topography problem we employ the true density model as the initial model, but we keep $\rho$ as a free parameter during the inver-
sions. We consider frequencies between 10 and 150 Hz. The P-wavelengths range thus from 10 m to 350 m, whereas the S-wavelengths range from 5 m to 180 m. Initially, we consider only the lowest three frequencies and successively add higher frequencies in the course of the iterations. We do not apply any smoothing (i.e. $\beta = 0$ in Eq. (3.1)) in order to retain sharp boundaries in the model. The damping weight $\alpha$ is chosen in each inversion such that the RMS is efficiently minimised and possible artefacts can be kept under control. For each frequency group, $\alpha$ is decreased with increasing iterations. It is further adjusted in accordance with the relative weights of the sensitivities for each parameter type, that is, different values are used for $V_p$, $V_s$ and $\rho$ (Manukyan et al., 2012a) in order to balance the model updates of the different parameter types. Convergence is typically achieved after about 12 iterations per frequency group.

![Fig. 3.1: Left column: true $V_s$-models featuring ground topographies with minimum wavelengths of (a) 60 m, (d) 36 m, (g) 12 m. Middle column (b, e, h): corresponding inversion results when incorporating topography into the inversion process. Right column (c, f, i): corresponding inversion results when neglecting topography in the inversion process.](image)

The goal of the first simulations, the models for which are depicted in Fig. 3.1(a, d, g), is to investigate the effects of topographic roughness. For that purpose, we add small random amplitude fluctuations of up to $\pm 2$ m to an initial flat ground surface, whereby the minimum wavelengths of the fluctuations vary from 60 m (Fig. 3.1a) to 12 m (Fig.
The latter is similar to the minimum seismic wavelength. Such variations must be expected in many near-surface seismic surveys.

Before we discuss the influence of topographic undulations on inversion results, it is instructive to analyse their effects on seismic data. In order to clearly identify the effect of the anomalies and the topography, we consider noise-free data and discuss the effect of random noise later. Fig. 3.2 shows three example shot gathers that stem from the subsurface model shown in Fig. 3.1(g) and some modification thereof. The shot gather, shown in Fig. 3.2(a), is computed with flat topography and without the anomalous bodies. The expected events, refracted P- and S-wave as well as the dispersive Rayleigh waves ($L_R$) are clearly visible. The shot gather obtained in the presence of the deterministic anomalies but still with flat topography is displayed in Fig. 3.2(b). The aforementioned seismic phases are slightly altered. Furthermore, the anomalous block inserts clearly introduce new features to the data. The most prominent ones ($L_{R,sc}$) are travelling at the same speed as the direct Rayleigh waves ($L_R$), and we conclude that they are scattered at the shallow anomalies around $x = 58$ m and around $x = 143$ m. Typically, FWI is employed to image deterministic anomalies as shown in Fig. 3.1(g). Therefore, the difference between Fig. 3.2(a, b) represents the signal of interest. Finally, seismograms computed with the model as shown in Fig. 3.1(g) (i.e., with topography and with anomalies present) are depicted in Fig. 3.2(c). The topography leads to a general loss of coherency and it also introduces considerable scattering, e.g. of the Rayleigh waves ($L_{R,sc}$). A comparison of the three shot gathers clearly shows that topography has a substantial effect on the data, and its imprint on the waveforms is considerably larger than that of the deterministic anomalies, which are the target objects of such an investigation. Therefore, it must be expected that the resulting tomograms will be adversely affected by ignoring the topography.
Fig. 3.2 Vertical component displacement seismograms originating from a vertical source at $x = 16$ m for variations of the model shown in Fig. 3.1(g). (a) Without anomalies present, with flat topography; (b) with anomalies present, with flat topography; (c) with anomalies present, with rough topography. The labelled events are the refracted P-, S- and direct or scattered Rayleigh waves ($L_R$, $L_{R,sc}$).

All models shown in Fig. 3.1(a, d, g) can be very well reconstructed when the actual topography is considered during the inversions (Fig. 3.1b, e, h). We only show the $V_s$ tomograms, but the same conclusions can be drawn from the $V_p$ tomograms. Neglecting the surface topographic variations leads to significant distortions in the tomographic images. In the presence of long wavelength variations, particularly deep seated anomalies are poorly resolved (Fig. 3.1c). Furthermore, chequerboard-like artefacts arise just below the surface around $x = 112$ m, where the (neglected) topography has a peak. In order to keep the artefacts under control, increased regularisation is needed, which in turn precludes proper model reconstruction, mainly at depth. The reconstruction quality is similar in Fig. 3.1(f), where intermediate wavelength topography is neglected. Topographic fluctuations having dominant wavelengths comparable to the smallest seismic wavelength give rise to more intense artefacts (Fig. 3.1i). Only the shallowest anomalies can be reasonably resolved. We conclude that neglecting the distinct peaks in the topography causes problems in the model reconstruction which become particularly acute when the variations are of the order of the smallest seismic wavelength.
In a second set of simulated data inversions we study the influence of the amplitude of topographic variations. Here, we have chosen a model with long wavelength topography variations that lies well within the range of the seismic wavelengths employed. The peak amplitudes in the models, shown in Fig. 3.3(a, d, g), are ±1, ±2 and ±8 m, the latter being similar to the minimum seismic wavelength. Again, the original models can be very well reconstructed provided that the topography is properly incorporated into the FWI process (Fig. 3.3b, e, h). Neglecting the topography with the smallest amplitude fluctuation does not introduce serious distortions (Fig. 3.3c). Only minor chequerboard-like artefacts can be observed, e.g. around (x, z) = (84 m, 10 m). Furthermore, the velocities of the deepest and the rightmost anomalous block inserts are slightly underestimated, whereas the velocities of the lengthy anomaly around (x, z) = (94 m, 30 m) are slightly overestimated. Ignoring topography with an amplitude of 2 m already leads to clear deficiencies in the model reconstruction (Fig. 3.3f). The low-velocity anomalies can still be well resolved down to intermediate depth, but the deepest anomaly is blurred. The high-velocity anomalies are blurred even at intermediate depths. Neglecting topography vari-
atations with amplitude 8 m (around the minimum seismic wavelength) causes the inversion to fail (Fig. 3.3i). Only the large shallow low velocity anomaly at x = 60 m is visible, with artefacts prevailing.

Fig. 3.4: RMS reduction relative to the initial RMS for the inversions shown in Fig. 3.3. The continuous lines correspond to the inversions incorporating topography, the dashed lines to the ones neglecting topography. The amplitudes of the topographic variations are labelled in the legend. The inversion frequency ranges are given at the top.

When the topography is neglected the data (which carries the influence of topography) cannot be fitted equally well by the model (which fails to account for such effects). As long as topography is incorporated in the inversion, the RMS (root-mean-square data misfit) reduces to very small values (Fig. 3.4). The values of interest are the RMS reductions per frequency group, i.e., the relative change between a peak and the next trough in the RMS curve. After every twelfth iteration new frequencies are introduced; this explains the discontinuities in the RMS curves of Fig. 3.4. For the models shown in Fig. 3.3, the RMS typically reduces to 10% of the initial RMS per frequency group, provided to-
Topography is incorporated (Fig. 3.4, continuous lines). When neglecting the topography, the RMS reduction follows the quality of the model reconstruction (Fig. 3.4, dashed lines). For the smallest topography amplitude (Fig. 3.3c), the RMS still reduces to around 15% because the model can still be reasonably reconstructed. However, when neglecting the largest amplitude topography, the RMS only reduces to values as large as 50%, which corresponds to a poor model reconstruction (Fig. 3.3i). Even for the lowest frequency group (10, 15 and 20 Hz), it is not possible to fit the data within the same range as when incorporating topography (even when iterating until convergence). This shows that also the low frequencies are rather sensitive to topographic fluctuations.

3.4 Concluding Remarks

We have demonstrated through simulated data inversion experiments that even minor topographic variations have a surprisingly large effect on elastic FWI, when they are not considered properly. The distortions seem to be particularly severe when the wavelengths of the topographic undulations and/or their amplitudes are comparable to the minimum seismic wavelengths employed. Presumably this relates to most favourable conditions for surface wave scattering. Paradoxically, the artefacts, introduced by neglecting the topography predominantly appear at greater depths and not, as one might expect, near the surface.

The detrimental effects of ignoring topography can be compared with other possible distortions in FWI. We have run an additional inversion experiment, in which we have contaminated the data with a realistic amount of random noise. The results indicate that the distortions introduced by random noise are considerably smaller than those caused by neglecting the topography. Another source of errors concerns the 3D-to-2D transform required for 2D FWI. Auer et al. (2013) investigated the effects of inadequacies in the asymptotic filters used in transforming the field data from 3D to 2D. Also these errors seem insignificant compared to the effects of topography. Groos et al. (2014) focused on effects of attenuation; they found that the estimation of the source wavelet during the inversion can partly account for an erroneous quality factor or even neglected attenuation in the model. Likewise, one might expect that the source coupling factor estimation applied in our study could at least partially correct for the phase shift fluctua-
tions due to mis-positioning of the sources and receivers, when neglecting topography. However, short wavelength topographic undulations introduce wave scattering, for which coupling factors cannot accommodate. Ignoring anisotropy where it is present can also lead to false velocity estimations or to misplacements of deep structure (Prieux et al., 2011), but the distortions are much less severe compared with topography effects. Butzer et al. (2013) compared 2D FWI results using 3D models with and without structural variations occurring perpendicular to the 2D profiles. These structural variations out of the inversion plane cause significant alterations of the wavefield and lead to problems for FWI similar to those we have observed, that is, artefacts and loss of spatial resolution. It must be therefore expected that the 2D assumption may also cause problems in the presence of significant 3D topography. Further studies are required for quantifying such effects. If minor topographic variations perpendicular to the 2D profiles cause similarly large problems as those along the profile lines, the validity of elastic 2D FWI in presence of 3D topography must be critically assessed.
Full waveform inversion (FWI) is an increasingly popular tool for analysing seismic data. Current practise is to record seismic data sets that are suitable for reflection processing, that is, a very dense spatial sampling and a high fold are required. Using tools from optimised experimental design (ED) we demonstrate that such a dense sampling is not necessary for FWI purposes. With a simple noise-free acoustic example we show that only a few suitably selected source positions are required for computing high-quality images. A second, more extensive study includes elastic FWI with noise-contaminated data and free surface boundary conditions on a typical near-surface setup, where surface waves play a crucial role. The study reveals that it is sufficient to employ a receiver spacing in the order of the minimum shear wavelength expected. Furthermore, we show that horizontally oriented sources and multi-component receivers are the preferred option for 2D elastic FWI, and we found that with a small amount of carefully selected source positions, similarly good results can be achieved, as if as many sources as receivers would have been employed. For the sake of simplicity, we assume in our simulations that the full data information content is available, but data pre-processing and the presence of coloured noise may impose restrictions. Our ED procedure requires an a priori subsurface model as input, but tests indicate that a relatively crude approximation to the true model is adequate. A further prerequisite of our ED algorithm is that a suitable inversion strategy exists that accounts for the non-linearity of the FWI problem. Here, we assume that such a strategy is available. For the sake of simplicity we consider only 2D FWI experiments in this study, but our ED algorithm is sufficiently general and flexible, such that it can be adapted to other configurations, such as crosshole, VSP or 3D surface setups, also including larger scale exploration experiments. It also offers interesting possibilities for analysing existing large-scale data sets that are too large to be inverted. With our methodology it is possible to extract a small (and thus invertible) subset that offers similar information content as the full data set.
4.1 Introduction

Seismic full waveform inversion (FWI) is a very promising tool for obtaining high-resolution images of the subsurface. The expected resolution is in the order of half the minimum wavelength (Wu and Toksöz, 1987). The theory behind FWI was already developed in the 1980s (Lailly, 1983; Mora, 1987; Tarantola, 1984), but the method only became popular recently due to the enormous computational expenses. Comprehensive FWI overviews can be found in Plessix (2008), Buske et al. (2009), Virieux and Operto (2009) and Fichtner (2011). The method is nowadays applied to a broad range of scales, ranging from laboratory investigations in the sub-meter range (e.g. Bretaudeau et al., 2013; Pratt, 1999), engineering and environmental applications (a few tens to a few hundreds of meters, e.g. Romdhane et al., 2011; Smithyman et al., 2009), exploration problems (a few kilometres, e.g. Bleibinhaus and Hilberg, 2012; Jaiswal et al., 2009; Raknes et al., 2015), active source wide-angle surveys (a few tens of kilometres, e.g., Malinowski et al., 2011; Operto et al., 2004), crustal-scale passive seismic investigations (a few tens of kilometres, e.g. Fichtner et al., 2013) to whole Earth studies (a few hundreds to a few thousands of kilometres, e.g. French and Romanowicz, 2014).

The FWI methodology applied to all these scales is similar, but the specific goals and constraints impose different challenges and require different experimental setups. For example, laboratory experiments may need to consider the finite size of the sensors; whereas whole Earth studies are restricted by logistical constraints for placing sensors (e.g., it is challenging to obtain a station density in oceanic areas that is comparable to regions on land). The survey design of active seismic experiments at exploration scales are typically governed by the requirements of reflection seismics, where it has to be ensured that the spacing satisfies the Nyquist-Shannon sampling criterion for avoiding aliasing effects. Here, FWI is employed primarily for determining velocity models that are later used for pre-stack depth migration or reverse time imaging (e.g., Rønholt et al., 2014).
In near-surface seismic data sets it is challenging to isolate reflections from other wave types, such as surface waves and guided waves (e.g., Schmelzbach et al., 2005). FWI is expected to be particularly beneficial at such scales, because it requires no wave type separation, and high resolution images can be obtained. The data sets to be acquired for FWI may not necessarily have to meet the criteria dictated by seismic reflection processing methodology.

Experimental design (ED) tools offer suitable means to set up an optimal survey or to choose an optimal subset of an existing dense data set (e.g. Maurer et al., 2010). The methodology has successfully been applied to electromagnetic problems (e.g., Maurer and Boerner, 1998), geoelectrics (e.g. Stummer et al., 2004; Wilkinson et al., 2006), earthquake network design (e.g., Hardt and Scherbaum, 1994) and seismic crosshole applications (e.g. Curtis, 1999a). So far, optimised ED techniques have gained only little attention in the field of FWI. Djikpesse et al. (2012) formulated an efficient Bayesian ED methodology in order to optimise resolution in FWI and applied it to a crosshole example. Other attempts to optimise the survey design of FWI include the work of Romdhane et al. (2011) who directly compare inversion results from \(x\)- and \(z\)-directed receivers and decimate the number of sources employed while keeping a regular spacing. Brenders and Pratt (2007) investigated the influence of the minimum frequency used and of spatial subsampling. Sirgue and Pratt (2004) designed optimal frequency selection schemes. Likewise, Maurer et al. (2009) developed efficient frequency and spatial sampling strategies for acoustic crosshole FWI. Manukyan et al. (2012) investigated the information content offered by multi-component recordings for elastic crosshole FWI problems. Similar investigations by Vigh et al. (2014) also highlighted the importance of multi-component recordings for elastic marine applications.

An important question that remains to be answered is if it is really necessary for near-surface seismic FWI purposes to acquire high fold data sets, as required for reflection processing, or if much sparser data sets are sufficient. Initial investigations for crosshole surveys indicated that a dense spatial sampling is not required for FWI problems (Maurer et al., 2009), but it is unclear if this conclusion can be transferred to surface-based surveys in a straightforward manner. Here, sources and receivers are only
located at or just below the surface, which yields a less constrained one-sided inversion problem. More importantly, the free surface plays a very important role, because high-amplitude surface waves are superimposing reflected phases. In order to model surface waves, the acoustic approximation is insufficient, and elastic FWI is mandatory.

In this paper, we provide an in-depth study on how to design shallow seismic surveys, optimised for elastic FWI incorporating surface waves. After introducing the theoretical background of our FWI implementation, we present the basics of optimised ED and our specific algorithm, whose performance is illustrated with a simple acoustic example. This example is used for examining the dependency of ED on the underlying subsurface model. Then, we discuss the more realistic elastic case including noise, for which we inspect the importance of numerous recording parameters, such as receiver spacing, the choice of source and receiver types and optimal placement of sources. Based on our results, we ultimately offer specific guidelines for shallow seismic survey designs. Furthermore, we highlight potential problems associated with the assumptions made in our simulations.

### 4.2 Theory

#### 4.2.1 Full Waveform Inversion

The aim of full waveform inversion (FWI) is to find a realistic subsurface model, for which forward modelled data $u$ can be computed that match the observed data $d$ within the data error bounds. This is typically achieved through a linearised inversion procedure, in which the model parameters $m$ are updated successively, until the root-mean-square ($RMS$) misfit between $u$ and $d$ is minimised, that is, until convergence is achieved (e.g., Tarantola, 2005). Due to the dominance of surface waves in shallow seismic data, the acoustic approximation is not justified but elastic FWI is required. We parameterise our subsurface models with P- and S-wave speeds $V_p$ and $V_s$ and density $\rho$ (i.e., $m = [V_p, V_s, \rho]$), which are discretised on a regular 2D grid. For the sake of simplicity, we do not consider anisotropy and anelastic effects, but it is conceptually possible to extend $m$, such that these effects can be included.
In principle, any forward solver that predicts $u(m)$ can be employed for an FWI algorithm. Here, we consider a frequency-domain finite element approach (Latzel, 2010; Min et al., 2003). As outlined by Pratt (1999), frequency domain modelling is very efficient for multiple sources, and typically the response for only a few distinct frequencies needs to be computed. In finite element modelling, the free surface is the natural boundary condition, such that accurate modelling of surface waves is possible at no extra costs. At the top of the modelling domain, the free surface is maintained, while at the other edges of the domain it is replaced by perfectly matched layer boundary conditions (Basu and Chopra, 2003; Zheng and Huang, 2002).

For the solution of the inverse problem, also carried out in the frequency domain, we follow a Gauss-Newton approach (Pratt et al., 1998) using

$$m^{i+1} = \left( J^T J + \alpha^2 I + \beta^2 L^T L \right)^{-1} \left( J^T \left( d - u \right) + Jm^i \right) + \alpha^2 Im^i. \quad (4.1)$$

The matrix $J$ contains all sensitivities, $I$ is the $N \times N$ identity matrix with $N$ being the number of model parameters contained in $m$, $L$ is the Laplacian smoothing operator and $i$ is the iteration index ($m^i = 0$ is the initial model). The scalars $\alpha$ and $\beta$ determine the weights of regularisation in form of damping and smoothing, which stabilise the inversion. These weights are adjusted to the various parameter classes ($V_p$, $V_s$ and $\rho$) in order to balance the corresponding sensitivities and model updates (Manukyan et al., 2012a). Damping is supposed to keep the model parameters close to a given reference model. We have chosen the model parameters of the previous iteration as a reference; therefore, damping essentially controls the step length in our formalism. Prior to each model update step, source functions are estimated using the approach described in Maurer et al. (2012).

For large-scale inversion problems it can be challenging to compute and store the approximate Hessian matrix $J^T J$. Therefore, alternative options, such as non-linear conjugate gradients or L-BFGS methods (e.g., Nocedal and Wright, 1999) have to be considered. However, for our subsequently described ED procedure the explicit computation of $J^T J$ is required. Since this matrix has to be established anyway, we employ the Gauss-Newton algorithm in this study. We use the expressions by Zhou and Greenhalgh (2010) for calculating the sensitivities.
4.2.2 Experimental Design

The goal of experimental design (ED) is to set up a survey or choose data from a large data set, such that benefit is optimised while acquisition and/or computational costs are minimised. For that purpose, we first need to specify the terms “benefit” and “cost”. The costs of a seismic survey depend on several factors, such as accessibility, manpower and many more. We assume that the costs linearly scale with the number of sources employed. We restrict our definition of costs to be a function of the number of sources only, although placing receivers can be challenging too (e.g. three-component receivers or ocean bottom sensors). It is important to note that the methodology is sufficiently general, such that receivers could be included into the design process too.

The survey benefit can be defined via the information content offered by the data set. This can be quantified by means of measures from linear inverse theory. As discussed by Curtis (1999a), a variety of options exists to quantify the goodness of a particular data set. Here, we consider measures that are based on the approximate Hessian matrix $J^TJ$. The reliability of the model reconstruction depends on the ability to invert $J^TJ$ (Maurer et al., 2010). Without the regularisation terms ($\alpha = \beta = 0$), this matrix is usually singular. The regularisation terms are therefore essential, but the “goodness” of $J^TJ$ shall be maximised, such that the contribution of regularisation will be minimised. The sensitivities, contained in the Jacobian matrix $J$, are governed primarily by the survey design. We can therefore maximise the “goodness” of $J^TJ$ by choosing appropriate source-receiver configurations. As a consequence of the non-linearity of the FWI problem, it is important to note that the sensitivities contained in $J$ depend on the model parameters. As further discussed in the sequel of the paper, this needs to be considered when setting up ED.

A conceptual example is shown in Fig. 4.1. We assume that we have $M$ sources available in total, from which we would like to choose a useful subset of source positions (while keeping all the receivers active). Based on an a priori subsurface model we compute the sensitivities for all possible source-receiver configurations. A data set that includes all possible source-receiver configurations will be subsequently referred as a comprehensive data set $\Omega_M$. For displaying the “goodness” of the comprehensive matrix $J^TJ$, we show its eigenvalue spectrum (eigenvalues sorted by their magnitude and nor-
malised by the maximum eigenvalue; solid line in Fig. 4.1a). In theory, the “goodness” is proportional to the number of non-zero eigenvalues. Due to finite numerical precision, the eigenvalues rarely equal zero. We therefore introduce a threshold, below which an eigenvalue is considered insignificant. Here, and throughout the paper, we define this threshold to be $10^{-10}$ times the largest eigenvalue. As shown in Fig. 4.1a, the intersection of the comprehensive eigenvalue spectrum with the threshold level is at about 45% of the eigenvalues. Maurer et al. (2009) defined this intersection to be the “relative eigenvalue range ($RER$)”. It is a measure of the resolved portion of the model space. The choice of the threshold value is not critical; it only scales the $RER$ values. We have repeated our experiments with a range of threshold values and the results were essentially identical.

![Fig. 4.1: (a) Logarithmic eigenvalue spectra and $RER$ values for a survey when using either 10% or all (100%) sources. (b) Benefit-cost curve for a seismic experiment. Costs are defined by the normalised number of sources (1 = all sources), and benefit is defined as normalised $RER$ ($nRER$) (1 = benefit from all sources). The vertical double-arrows specify the benefit-cost pairs related to the eigenvalue spectra in (a).](image)

For obtaining an optimised survey layout we employ a greedy algorithm (e.g. Coles et al., 2015). Initially, we compute eigenvalue spectra and the corresponding $RER$ values for subsets including data from only one source at a time. The data from the source as-
sociated with the largest $RER$ will be chosen to form $\Omega_1$. Then, the next source is chosen using

$$\max_{\text{sources in } \Omega_2 \setminus \Omega_1} RER_{k+1} \quad (k = 1\ldots M - 1)$$

(4.2)

with $k+1$ being the index of the next selected source. For displaying the performance of the algorithm, we construct benefit-cost curves as shown in Fig. 4.1b. The horizontal cost axis ranges from 0 (no source) to 1 (all sources). The benefit, indicated on the vertical axis, is displayed by means of a normalised $RER$ ($nRER$), which is defined as $RER_{k\text{t}/RER_{M}}$. In this example, 80% ($nRER = 0.8$) of the maximally resolvable portion of the model space can be resolved using only 10% of all sources.

Our ED algorithm requires a large number of eigenvalue spectra to be computed. This can be computationally prohibitive for realistically sized FWI problems. Therefore, we have additionally considered an alternative goodness function. The diagonal elements of $J^TJ$ include the squared column sums of $J$. Meles et al. (2010) showed that the (absolute) column sums of $J$ are a good proxy for the diagonal elements of the model resolution matrix (e.g. Menke, 2012), which is also a measure of the “goodness” of a particular survey layout. Therefore we can define a new measure $g_k$ that offers similar information as the $RER$, but is much cheaper to compute:

$$g_k = \sum_{i=1}^{N} \frac{D^\Omega_i}{D^\Omega_i + \delta},$$

(4.3)

with $D^\Omega = \text{diag}(J^TJ)$. The parameter $\delta$ is a small positive number that stabilises the procedure in the presence of very small $D^\Omega_i$ values. Consequently, we can substitute Eq. (4.2) by

$$\min_{\text{shots in } \Omega \setminus \Omega_1} g_{k+1}. $$

(4.4)

We have benchmarked the approximate measure in Eq. (4.4) against the term in Eq. (4.2) using a small data set, and found that the design results were quite similar for both measures. Therefore, we have employed Eq. (4.4) within the optimisation procedure, but we still use the corresponding $nRER$ values for displaying the final benefit-cost...
curves because it is a measure for the resolved model space (only a few eigenvalue decompositions need to be performed for that purpose).

4.3 Numerical Examples

With a series of numerical examples we aim to find configurations for acquiring near-surface seismic data optimised for FWI. After introducing the general setup, we start with a simple noise-free acoustic example to investigate the model dependency of our ED results. We then move on to more realistic elastic investigations including noise, with which we seek (i) a suitable receiver spacing, (ii) optimised combinations of x- and z-directed sources and receivers, and (iii) the minimal number of sources employed and their appropriate positions. Finally, we test the robustness of our findings on a different subsurface model.

4.3.1 Experimental setup

Fig. 4.2 shows the true and the initial models employed for the synthetic experiments; for the elastic case, $V_s$ is obtained from $V_p$ by applying a constant Poisson’s ratio of 0.29, density $\rho$ is obtained from $V_p$ using Gardner’s relation (Gardner et al., 1974). A 24 Hz Ricker wavelet was used for producing the synthetic data set. Seven inversion frequencies are considered accordingly: 6.4, 9.6, 12.8, 19.2, 25.6, 36.8 and 48.0 Hz, in order to cover the full wavenumber domain (Sirgue and Pratt, 2004). The amplitude spectrum of the Ricker wavelet further determines the weight, with which the frequencies contribute to ED and FWI. This is favourable, because in observed data, frequencies towards both ends of the spectrum are expected to exhibit low signal-to-noise ratios. The maximum frequency $f_{\text{max}}$ governs the minimum wavelength $\lambda_{\text{min}}$:

$$\lambda_{\text{min}} = \frac{V_{s,\text{min}}}{f_{\text{max}}} = \frac{734 \text{ m/s}}{48 \text{ Hz}} = 15.3 \text{ m}. \quad (4.5)$$

In order to obtain good numerical accuracy, the size of the forward modelling cells is set to 1 m. The expected spatial resolution of FWI is in the order of half the minimum wavelength. Therefore, 25 forward modelling cells are merged into one inversion cell of size $5\times5$ m, which is still below the expected spatial resolution.
For the inversions, the frequencies are gathered into three partly-overlapping groups: (i) 6.4, 9.6, 12.8 Hz; (ii) 12.8, 19.2, 25.6 Hz and (iii) 25.6, 36.8, 48.0 Hz. Each inversion is started with the lowest frequency group and progressed to larger frequencies as the model converges, in order to prevent cycle skipping. In our case, only six iterations per frequency group are needed until convergence is achieved, that is, until the root mean square deviation between $d$ and $u$ did not change anymore by more than 3%. For consistency, all inversions are run with the same frequency schedule and the same parameters, leaving the choice of the regularisation weight to a line search algorithm, which ensures that the RMS is efficiently minimised (after Nocedal and Wright, 1999). Two additional constraints are given: (i) the weight of damping is four times higher than the weight of smoothing ($\alpha = 2\beta$ in equation reference goes here), and (ii) damping of the model update in $\rho$ is five times higher than damping in $V_p$ and $V_s$, because it was observed that large model updates in $\rho$ can make the inversion unstable. All the inversion runs converged to a comparable RMS level.
Fig. 4.2: Models considered in the synthetic studies. $V_s$ is obtained from $V_p$ by applying a fixed Poisson’s ratio of 0.29. Density $\rho$ is obtained from $V_p$ with Gardner’s relation. (a) True model A; (b) true model B; (c) initial model.

4.3.2 Experimental Design for Acoustic FWI

We consider noise-free acoustic data modelled for 61 pressure receivers located at $x = 60, 70, \ldots, 660$ m at 1 m depth and 62 potential source locations placed at $x = 55, 65, \ldots, 665$ m at 1 m depth, such that they do not coincide with the receivers.

For determining an optimal experimental layout we need to specify a subsurface model, with which the sensitivities, contained in $JTJ$, can be computed. Ideally, one would employ the true model. However, the true model is unknown prior to the seismic survey. Typically, all the a priori information available is included in the initial model. Often, the initial model is obtained from traveltime tomography, which ensures that it is sufficiently close to the true model (e.g., Malinowski et al., 2011). The initial model is therefore an
obvious choice for ED. However, it is unclear, if the discrepancies between using the initial or the true model could affect the design process in a negative way (due to the high non-linearity of the FWI problem). Therefore, we repeat our ED procedure, using either the initial or the true model, and compare the results.

We have mimicked the initial model with the vertical gradient model shown in Fig. 4.2c. Such a gradient model is relatively easy to obtain, because it is characterised by three parameters only – $V_p$ at the surface, the velocity gradient and a fixed Poisson’s ratio. In fact, it can still be obtained from the sparse datasets acquired with optimised measurement geometry. If the traveltime tomography result shall be used as initial model, the measurement geometry shall additionally fulfil the corresponding needs. Using tools of ED, we have found that mainly the far offsets are important in this case.

The benefit-cost curves for these two scenarios are shown in Fig. 4.3. Both curves show a rapid increase, when only a few source positions are included. At about 12 sources they both start to flatten out and they reach the area of diminishing returns, that is, it becomes very expensive to increase the information content of the data set. Between 12 and 30 sources the two benefit-cost curves show some discrepancies, but overall they match very well. With both designs it is possible to get about 50% of the full information content with a mere 3 out of 62 sources, and 80% of the information can be obtained with only 12 sources.

![Fig. 4.3: Benefit-cost curves for the acoustic experiment.](image)

Fig. 4.3: Benefit-cost curves for the acoustic experiment. With 3 and 12 sources an $nRER$ value of 0.5 and 0.8 could be achieved respectively. Open dots indicate data sets for which inversion was carried out. The corresponding images are shown in the figures indicated besides the open dots.
It is noteworthy that the maximum $RER$ reached with the true model ($RER_{\text{max}} = 0.25$) is 14% larger than the maximum $RER$ reached with the initial model ($RER_{\text{max}} = 0.22$). This can be explained by the fact that the stochastic fluctuations in the true model lead to a better illumination of the subsurface, because the waves are scattered at the heterogeneities and illuminate the subsurface structures from different angles. However, the normalised curves $nRER$ vs. costs, as shown in Fig. 4.3, are comparable. For the crosshole case, the effect of scattering was further illustrated by Maurer et al. (2009), who plot sensitivities and the spatial distribution of the diagonal elements of the model resolution matrix for two models with various roughness.

To verify that the designs with the initial and true models are indeed similar, we compare the images from FWI of the subsets obtained from the source selections based on either the true or the initial model. Inversions are performed for the comprehensive data set including all 62 sources (Fig. 4.4a) and for subsets with 12 or 3 sources, chosen with ED based on either the initial (Fig. 4.4b-c) or the true model (Fig. 4.4d-e). For the comprehensive data set (Fig. 4.4a) all the important features are well reproduced, such as the shallow high-velocity anomaly around $(x, z) = (480 \text{ m}, 20 \text{ m})$ and the deep fault-like structure around $(x, z) = (450 \text{ m}, 200 \text{ m})$. With 12 sources (80% benefit), the model can be resolved equally well, regardless whether the sources are chosen based on the initial model (Fig. 4.4b) or based on the true model (Fig. 4.4d). Even with 3 sources only (50% benefit), the main features are still well recognisable, although slightly blurred (Fig. 4.4c, e). Besides visual comparison of the inversion results, we have quantified the tomogram quality by the RMS deviations between the true model and the inversion results. We have also tested the cross-correlation measure as applied by Reiser et al. (2017), which led to the same conclusions. For this first acoustic example, all model RMS values lie within a very narrow window of about 3%, indicating that all setups yield reasonable inversion results.
Fig. 4.4: Acoustic FWI experiment with model A (Fig. 4.2a); images from inverting data sets including all 62 sources (a), 12 sources selected with the initial model (b) and the true model (d), and for 3 sources selected with the initial model (c) and the true model (e). The open dots above the images indicate the pressure source positions employed. The RMS deviations to the true model are indicated in the bottom right corners.

The source patterns are indicated with open dots above the subsurface images in Fig. 4.4. For the initial model, the selection follows the symmetry of the model, such that the patterns of selected sources are symmetric. First, a few sources around the centre of the model are selected (Fig. 4.4c), but soon the sources at the edges of the spread are added in (Fig. 4.4b), which ensures a regular illumination of the model. The symmetry disappears when selecting the sources based on the true model. Here, the source position selection is guided by the pattern of the stochastic fluctuations in the model; the sources are preferably located above the shallow high-velocity anomaly around \( x = 480 \) m (Fig. 4.4d).

From this first acoustic simulation we can already derive a few interesting conclusions. Most importantly, it is found that only a few sources are required for constraining the \( V_p \) model very well. Secondly, ED based on the initial model does yield a highly optimised source selection, as long as the initial model is sufficiently close to the true model (which is further a prerequisite for FWI). Although the source patterns for the two design models are different, the benefit-cost curves and the resulting images are similar.

4.3.3 Experimental Design for Elastic FWI

The acoustic example described above offered interesting insights, but for designing realistic near-surface surveys, we move on to the elastic case with free surface boundary
conditions at the top of the modelling and inversion domain. Incorporating surface waves is crucial in near-surface FWI. Furthermore, we try to make our simulations more realistic by adding considerable noise to the waveform data. In the time domain, the standard deviation of the seismograms was calculated and 30% white noise relative to it was added. Finally, we also include the receiver spacing into our ED considerations. We invert for $V_p$, $V_s$ and density, but we restrict the images shown here to the wave speeds. It has been previously shown that it is difficult to recover meaningful density images due to parameter trade-offs (e.g. Operto et al., 2013). Therefore, we have artificially damped the model update in density, such that the corresponding images stay close to the initial model.

The full data space includes the same 62 source and 61 receiver positions as already employed for the acoustic simulations. Instead of pressure sources and receivers we consider $x$- and $z$-directed source and receiver components. For the sake of simplicity and computational efficiency, we restrict ourselves to pure 2D problems. Therefore, no source and receiver components perpendicular to the tomographic planes are modelled. In real data applications, out-of-plane heterogeneity will also play an important role on the quality of the model reconstruction. This aspect was studied by Butzer et al. (2013) and placing sensors out-of-plane could be part of ED, but this would be beyond the scope of this study.

In the following, we denote a particular source-receiver configuration as "src_type-rec_type", where src_type and rec_type can be either $x$, $z$ or $xz$. For example, $z$-directed sources and multi-component receivers with $x$- and $z$-components are denoted as "$z$-xz". It is important to note that for the source type $xz$ not necessarily both components at a particular position must be activated. Instead, $x$- and $z$-source directions can be chosen individually.

In principle, pressure (explosion) sources could also be included in the design process. In this case, since pressure sources do not produce primary shear waves, shear wave energy only stems from P-to-S converted waves (e.g., at the surface). We have experimented with pressure sources, and we found that the resulting images are often prone to artefacts because S-wave speeds are less constrained. We conclude that elastic
near-surface FWI surveys should be performed preferably with directed sources, which produce primary shear waves; and we have thus not considered pressure sources in our elastic simulations.

With the acoustic example we have demonstrated that the choice of the design model is not overly critical. We have performed similar tests for the elastic case, and we found that this conclusion remains valid for elastic data as well. Therefore, we base our elastic experiments on the a priori known initial model shown in Fig. 4.2c.

### 4.3.4 Suitable Receiver Spacing

Due to the design of receiver cables and other logistical constraints, it seems unpractical to design receiver layouts with an irregular spacing (although wireless receivers become available; e.g., Savazzi and Spagnolin, 2009). Instead, we compare three receiver deployments with regular spacings. Shannon’s sampling criterion dictates spatial sampling of half the minimum wavelength, which corresponds to $\Delta_{\text{samp}} = 28.7$ m for the first frequency group (up to 12.8 Hz). However, Brenders and Pratt (2007) obtain satisfactory waveform tomography images with source spacings well beyond Shannon’s criterion. We therefore test three different receiver spacings: $\Delta r_1 = 10$ m $= 0.35 \times \Delta_{\text{samp}}$ (61 receivers), $\Delta r_2 = 20$ m $= 0.70 \times \Delta_{\text{samp}}$ (31 receivers) and $\Delta r_3 = 40$ m $= 1.40 \times \Delta_{\text{samp}}$ (16 receivers).

For the experimental procedure, we consider $xz-xz$ configurations, which include 124 possible sources (62 $x$-directed and 62 $z$-directed sources). The resulting benefit-cost curves are shown in Fig. 4.5. The curves for 10 and 20 m spacing are relatively close to each other, thereby indicating that doubling the number of receivers offers only marginal benefits (only 3% for the full cost experiment including 124 sources). Using a very coarse receiver spacing of 40 m still produces good results, but the loss of information is significantly larger (8% at the full cost level and up to 21% in the critical zone, where the curves enter into the area of diminishing returns (around 31 sources). From these observations we conclude that a receiver spacing of 20 m offers a reasonable compromise between acquisition efforts and survey benefits, and we have included only 31 receivers into our comprehensive data set used for the subsequent simulations. This receiver spacing furthermore conforms Shannon’s sampling criterion, which is desirable when
later minimising the number of sources used. In an acoustic waveform tomography study, Brenders and Pratt (2007) have found that the image quality is satisfactory until the receiver spacing approaches $\Delta_{\text{samp}}$, while using twice as large source spacing.

![Graph showing benefit-cost curves for different source spacing]

**4.3.5 Suitable Source-Receiver Configurations**

Obviously, most subsurface information can be retrieved, when considering $xz$-$xz$ configurations, but such a survey may be labour intense and costly. Therefore, the majority of near-surface surveys are acquired with $z$-$z$ configurations using hammer, weight-drop or vibrator sources. With our ED computations we make an attempt to quantify the value of the options available, and we check whether other configurations can produce similarly good results as the $xz$-$xz$ configuration. Fig. 4.6 shows the benefit-cost curves for selected configurations. The data set $xz$-$xz$, serving as a reference, is indicated by the black line. In Fig. 4.6, the $nRER$ for all curves is obtained by normalising all $RER$ values by the maximum $RER$ value from the comprehensive data set (i.e., all sources from the $xz$-$xz$ configurations). This allows cross-comparison of various configurations.

As expected, best results are obtained for the comprehensive $xz$-$xz$ data set (Fig. 4.7a-b). The level of detail in $V_s$ is eye-catching, and the spatial resolution is excellent; the model RMS deviation to the true model accounts for 2.5% only. Due to the larger P-
wavelengths, \( V_p \) is less well resolved, therefore, the RMS deviation is slightly larger (3.2%).

We continue our analysis by omitting more and more components. First, we omit one of the source directions (x-xz and z-xz configurations). The resulting benefit-cost curves almost coincide with those of the xz-xz configurations (Fig. 4.6). Although, x-xz and z-xz configurations include only 62 sources, a maximum nRER of 0.94 can be achieved. From a practical view, vertical sources (e.g. hammer blow or drop weight) are more common, because it is more difficult to design horizontal sources that transmit sufficient energy into the ground (e.g., Knödel et al., 2004). Therefore, z-xz seems to be a very favourable configuration. However, it is interesting to note that the full-cost x-xz images (Fig. 4.7c-d) are slightly better than the corresponding z-xz images (Fig. 4.7e-f), although the model RMS deviations are equal. Minor artefacts are visible in the \( V_p \) image of the latter configuration. The x-xz images can hardly be distinguished from the inversion of the comprehensive data set (Fig. 4.7a-b), but the model RMS deviations are slightly larger (3.7% and 2.8% for \( V_p \) and \( V_s \) respectively).

Fig. 4.6: Benefit-cost curves for selected source-receiver combinations. Open dots refer to the figures with the corresponding FWI images (colour coding according to the legend in the bottom right corner).
If the survey shall be restricted to one component on both the source and the receiver side, the benefit-cost curves in Fig. 4.6 indicate that it is most beneficial to use the $x$-$z$ configuration (or the reciprocal configuration $z$-$x$). They reach a $nRER$ of 0.84 when using all $x$-directed sources and $z$-directed receivers. In contrast, the $x$-$x$ configurations achieve only a maximum $nRER$ of 0.78 and the $z$-$z$ configurations provide the lowest value (0.72). These results are partially confirmed by the corresponding FWI images. For the $x$-$z$ case, a high-quality image for $V_s$ can be obtained, but the inversion is prone to artefacts, again mainly in $V_p$ (Fig. 4.7g). FWI of $x$-$x$ components still yields a satisfactory image for $V_s$ but the spatial resolution in $V_p$ at greater depths is poor (Fig. 4.7i-j). The opposite is the case for $z$-$z$ (Fig. 4.7k-l): A relatively good image for $V_p$ can be obtained, but the $V_s$ image appears rather blurred, mainly at greater depths. The comparison of the model RMS deviations shows that $z$-$z$ yields the best image for $V_p$ while $x$-$z$ yields the best image for $V_s$ in case of using one source and one receiver component.
Fig. 4.7: Model A: FWI images (left: $V_p$, right: $V_s$) for selected source-receiver combinations (see labels at the left). All source positions were considered for computing the images. The RMS deviations to the true model are indicated in the bottom right corners.
4.3.6 Optimising the Number of Sources

First, we consider the most commonly (and cheapest) employed configurations z-z. For that purpose, we extract data sets offering 80% and 50% of the information relative to the corresponding full cost experiments (Fig. 4.6).

For the z-z case, 28 sources (45%) are required to reach the 80% benefit level and 11 sources (18%) to reach the 50% benefit level (Fig. 4.6), respectively. The FWI images at the 80% level (Fig. 4.8e-f) are only slightly degraded compared with the z-z full-cost experiment (Fig. 4.8c-d). At the 50% level, the corresponding images are degraded significantly (Fig. 4.8g-h), which also manifests itself in a strong increase of the RMS values.

Next, we repeat the analysis with our preferred x-xz configuration. Only 20 sources (32%) are needed for obtaining 80% benefit (Fig. 4.6). This reduction affects the reconstruction of $V_p$ but the image obtained for $V_s$ is still good (Fig. 4.9e-f). With only 8 sources (13%) the 50% benefit can be reached and the quality of the $V_s$ image is still good (Fig. 4.9g-h). The image for $V_p$ is somewhat blurred, especially at greater depths.

The source patterns are displayed on top of the corresponding images in Fig. 4.8 and Fig. 4.9. For all simulations the algorithm initially selects more or less regularly distributed source locations, but at a later stage the sources start clustering in the central parts of the profile. It is noteworthy that the outermost source positions do not seem to be of particularly high importance, and they are not selected for reaching the 50% benefit (Fig. 4.8g-h and Fig. 4.9g-h). Interestingly, the opposite is observed, when similar ED computations are performed for refraction travel time tomography experiments. In that case, the algorithm picks preferably source locations towards both ends of the profile for obtaining sufficient depth penetration.

The source patterns selected with ED are irregular. Nevertheless, a regularly spaced source deployment may offer logistical advantages. We have tested this option, and it turned out that 50% benefit can be reached with the same number of regular spaced sources as with the sources selected by the ED algorithm. This indicates that the ED problem includes ambiguities, that is, there may exist several source configurations that lead to similar benefits. Choosing 11 (z-z case) or 8 (x-xz case) regularly distributed sources at once seems as optimal (in terms of benefit) as subsequently selecting them.
with the greedy algorithm. We have repeated the simulations, shown in Fig. 4.8g-h and Fig. 4.9g-h, with regular source spacing. In the $z$-$z$ case, choosing regular source spacing slightly decreases the RMS values but the images are still prone to artefacts (Fig. 4.8i-j). In the $x$-$xz$ case, the RMS and the artefacts are slightly increased for regular source spacing, indicating that the source selection from ED is superior to the regular spacing.

Fig. 4.8: Model A: FWI images (left: $V_p$, right: $V_s$) for optimised $z$-$z$ configurations. On the left side the number of sources employed and the corresponding percentage of the full-cost experiment are displayed (see also Fig. 4.6). Selected $z$-directed sources are indicated above the images with downward pointing triangles. The uppermost panels (a-b) show inversion results of the comprehensive dataset ($xz$-$xz$) as a reference. The lowermost panels (i-j) display the tomographic results obtained with the same number of sources as in (g-h) but with regular spacing. The RMS deviations to the true model are indicated in the bottom right corners.
Fig. 4.9: Model A: FWI images (left: $V_p$; right: $V_s$) for optimised $x$-$xz$ configurations. On the left side the number of sources employed and the corresponding percentage of the full-cost experiment are displayed (see also Fig. 4.6). Selected $x$-directed source positions are indicated above the images with triangles pointing to the right. The uppermost panels (a-b) show inversion results of the comprehensive dataset ($xz$-$xz$) as a reference. The lowermost panels (i-j) display the tomographic results obtained with the same number of sources as in (g-h) but with regular spacing. The RMS deviations to the true model are indicated in the bottom right corners.
Fig. 4.10: Model B: FWI images (left: $V_p$; right: $V_s$) for optimised $x$-$xz$ configurations. On the left side the number of sources employed and the corresponding percentage of the full-cost experiment are displayed (see also Fig. 4.6). Selected $x$-directed sources positions are indicated above the images with triangles pointing to the right. The uppermost panels (a-b) show inversion results of the comprehensive dataset ($xz$-$xz$) as a reference. The lowermost panels (i-j) display the tomographic results obtained with the same number of sources as in (g-h) but with regular spacing. The RMS deviations to the true model are indicated in the bottom right corners.
4.3.7 Checking the Model Dependency

Since our ED is based on the initial model, the results should be valid for the inversion of any other models, for which this initial model is appropriate. We test this hypothesis by repeating the inversions experiments, shown in Fig. 4.9, with model B (Fig. 4.2b).

The images obtained with the comprehensive data set (Fig. 4.10a-b) and the increased RMS values indicate that model B is more challenging to recover. We observe a few artefacts around the source positions, mainly visible in $V_p$. Results obtained with the x-xz configurations (Fig. 4.10c-d) are, however, very comparable to those in Fig. 4.10a-b, just like it is the case for model A. With 20 sources (80% benefit; Fig. 4.10e-f), the model for $V_p$ appears rather blurred and it is difficult to distinguish artefacts from structure. The reconstruction of $V_s$ is still very good; it only degrades significantly, when employing not more than 8 sources (50% benefit; Fig. 4.10g-h). The decrease of image quality when omitting sources, are comparable to model A; thereby indicating a fairly general validity of our findings. Likewise, the source patterns are comparable to those observed in Fig. 4.8 and Fig. 4.9, and the conclusions with regard to optimised vs. regular source patterns also apply to model B (panels (g-j) in Fig. 4.8-Fig. 4.10).

4.4 Discussion

The simulations presented above demonstrated the usefulness of our ED approach, but we also would like to emphasise a few challenges related to the approach. Probably the most severe issue of the FWI method in general, is its strong non-linearity. This problem is not alleviated by our approach. We make the assumption that the choice of the initial model, the frequency schedule and the regularisation scheme allow a full exploitation of the data information content, that is, convergence to the global minimum can be achieved. This is often, but not always the case. For example, there are artefacts observed in some FWI images that were computed with data sets exhibiting a relatively high $nRER$ value (e.g., results for z-xz configurations in Fig. 4.7e-f). The results for these inversions may be improved by fine-tuning the regularisation parameters. However, for the sake of consistency we kept the inversion strategy unchanged throughout all inversions, and we left the choice of the regularisation weight to our line search algorithm. Addressing the non-linearity is an issue that must be always considered in FWI prob-
lems. Our ED approach does not contribute directly to the solution of this problem, but it offers improved subsurface information, when the non-linearity problem has been addressed adequately. A possible option to address the problem is non-linear ED, where an optimised experimental setup is determined that is suitable for a range of likely subsurface models (Maurer et al, 2010).

A potential limitation of our ED algorithm is imposed by the simplified goodness function (Eq. (4.3)). This is demonstrated in Fig. 4.6 by means of the rarely used $xz$-$x$ configuration (grey curve). In order to minimise the alternative goodness functional (Eq. (4.3)), it seems beneficial to select all $x$-directed sources (i.e., overlap with the $x$-$x$ curve until source 62) prior to selecting the first $z$-directed source. The kink and the sudden increase of the slope in the $xz$-$x$ curve beyond source 62 indicate that it would likely be beneficial to select $z$-directed sources at an earlier stage for maximising the $RER$. This problem is caused by the generally larger magnitudes of the sensitivities of $x$-directed sources compared with $z$-directed sources. The simplified goodness function in Eq. (4.3) is more strongly governed by the sensitivity magnitudes than the eigenvalues related with the $RER$ measure. Interestingly, this problem does not seem to affect the $xz$-$xz$ curve, and it is of course not an issue when only a single source component is available.

Further limitations can be imposed by data pre-processing that may be necessary for obtaining stable inversion results. Pre-processing typically includes frequency filtering and/or extracting selected portions of the seismograms. Both options will affect the information content offered by the comprehensive data set and may thus have an impact on the experimental design results.

Frequency filtering is related to an optimal choice of frequencies for FWI experiments. This topic has been discussed by Sirgue and Pratt (2004) and Maurer et al. (2009). Likewise, selecting suitable time windows can be also a topic of ED, and first attempts have been presented by . In this contribution we have assumed a prescribed frequency range computed with the full seismograms. It will be a topic of future research to combine the identification of optimized source-receiver combinations with the choice of suitable frequencies and/or time windows.
Besides a greedy algorithm, which chooses sources one after another, a global algorithm, which chooses the desired number of sources at once, could yield superior sources distributions. This is most obvious when looking at the extreme case of using two sources only. The greedy algorithm chooses the first source preferably around the middle of the profile and the second source such that it complements the first source. In contrast, we expect a global algorithm to choose two sources that are distributed more regularly. However, global algorithms are still prohibitively expensive for such studies, even when using simplified goodness functions.

Goodness measures that are based on eigenvalue spectra, such as the RER, are a valuable option, because they allow straightforward quantification of the resolved model space and the null space. A potential problem is that such measures provide no information on particular model parameters. This is, for example, visible in Fig. 4.7: The $V_p$ image obtained with z-z configurations is superior to most other $V_p$ images computed with data sets related with larger $nRER$ values. The poor $nRER$ score of the z-z configuration is caused by its inability to produce good $V_s$ images (Fig. 4.7l).

A possible extension of our current methodology is to include goodness functions that maximise the resolution of a particular parameter type ($V_p$, $V_s$ or $\rho$). One could even focus on certain subsurface regions that are of special interest. This is the topic of focussed experimental design, and can be achieved with benefit measures that are based on the model resolution matrix (e.g. Curtis, 1999b; Wagner et al., 2015). In fact, our simplified goodness function, defined in Eq. (4.3), could also be employed for that purpose by summing over the sensitivities with respect to the model parameters of interest only.

The benefit-cost curves in Figs. 4.3, 4.5 and 4.6 exhibit a relatively smooth transition into the area of diminishing returns, and it is difficult to identify a clear kink in the curves, where the benefit-cost ratio is optimal. Therefore, we discuss the choice of a suitable data set using the percentages relative to the full cost experiments. The noise-free acoustic example indicates that choosing only a small number of sources, that is, 50% of the full cost experiment or even fewer sources, still leads to very good results. We have also experimented with noise-free elastic data and came to similar conclusions. However, the results obtained with noise-contaminated elastic data indicate that acquir-
ing data sets at a level of at least 80% of the corresponding full cost experiments is advisable, depending on the extent of the full cost experiment.

For the sake of simplicity we have considered only white noise in our simulations, but in a realistic scenario the presence of colored noise must be expected. This survey-specific problem may be partially alleviated with an increased data redundancy. Therefore, it seems advisable to acquire slightly more data than indicated by the ED procedure.

Our results will be most beneficial for designing shallow seismic experiments, where the tomograms constitute the final product. Seismic surveys performed on hydrocarbon exploration scales are typically designed such that the data sets produce optimal pre-stack depth migration or reverse-time migration images. Therefore, one may conclude that our ED strategy is of lesser importance for such surveys. However, it is nowadays standard practice that FWI is employed for establishing velocity models that serve as input for the subsequently applied migration algorithms. Even with substantial computing resources, it is still challenging to apply FWI to large and densely sampled data sets. Therefore, strategies have been developed for alleviating the computational costs. For example, source encoding techniques were devised, with which several sources can be simulated simultaneously (e.g., Krebs et al., 2009). Alternatively, posteriori ED could be applied, that is, our ED strategy could be employed for selecting a small subset out of a large data volume for performing FWI.

4.5 Conclusions

We have employed optimised experimental design techniques for delineating useful source-receiver configurations that are amenable for acoustic and elastic FWI. It was found that it is not necessary to employ a dense spatial sampling and to achieve a high fold, as it is dictated by Shannon’s sampling criterion and required for seismic reflection processing techniques. Instead, a relatively coarse spatial sampling is sufficient for obtaining detailed FWI images. More specifically, we suggest designing shallow seismic surveys on the basis of the following considerations:
1. We recommend horizontal $x$-directed sources. In combination with multi-component receivers they offer similar information content as multi-component sources (i.e., $x$- and $z$-directed sources). Using only $z$-directed sources (which may be easier to implement in practise) is another reasonable strategy.

2. For obtaining high resolution $V_s$-images, multi-component geophones clearly outperform single-component receivers. Although the former are more expensive, we recommend using such devices, whenever possible.

3. When only single-component sources and receivers are available, it is recommended to use $z$-directed sources and $x$-directed receivers or vice versa.

4. A receiver spacing of the order of the minimum shear wavelength is judged to be sufficient.

5. The optimal number of sources and receivers and their locations can be determined with benefit-cost curves, as shown in Figs. 4.3, 4.5 and 4.6. The resulting source patterns generally exhibit a denser spacing in the central parts of the profile, but regularly spaced sources offer similarly good results.

The number of sources used can be optimised with our ED algorithm. However, for real data one should not overly tweak the number of sources. With high levels of correlated and uncorrelated noise and / or unexpected earth features, additional sources can increase the stability of the inversion. Likewise, all the other limitations of our ED algorithm, mentioned in the discussion section, must be considered during the ED process.

Our ED methodology is sufficiently general, such that it can be adapted to any type of seismic survey (large-scale seismic surveys, crosshole applications, VSP, anisotropy etc.). For example, for including anisotropy it will be necessary to consider more subsurface parameters compared with isotropic problems, and it has to be made sure that all the parameters can be resolved independently. The corresponding survey layouts will likely differ from those derived for isotropic cases, but the eigenvalue and RER analysis, described in this paper, will be essentially identical. Methodological FWI developments are progressing rapidly, but so far, only little efforts have been made to establish opti-
mised input data sets. Our approach can fill this gap, and make FWI attractive to a broader range of applications.
5.1 Conclusions

The expectations placed on full waveform inversion (FWI) were quite high; this technique aims at retrieving images at sub-wavelength resolution. The inversion results shown in Chapters 2-4 proved that this expectation can be met. Especially the results for $V_s$ are intriguing, because the wavelengths in $V_s$ are smaller than in $V_p$ due to the smaller velocities.

The $V_s$-structure remained largely unresolved with conventional methods. This is unfortunate, because engineers are often interested in the shear modulus, which can be obtained from $V_s$ and $\rho$. Multi-channel surface wave analysis yields $V_s$-profiles, but the method fails to resolve strong variations in 2D and therefore yields rather poor lateral resolution. In principle, it is possible to obtain images for $V_s$ from reflection seismology processing, but it relies on isolating shear wave reflections from the seismogram, which is often difficult or impossible. Similarly, traveltime tomography can be performed with S-wave traveltimes only if picking is possible. But again, the expected spatial resolution is rather poor. In contrast, I have obtained very sharp $V_s$-images with FWI, even for complex subsurface heterogeneities below considerable topography (Chapter 3). For this purpose, only small data sets are required, which are relatively cheap to acquire (Chapter 4).

Although I could not invert field data in the framework of my thesis, I have made significant contributions towards FWI being applied to real data. In the introduction I have illustrated the value of FWI for the application on near-surface seismic data sets. High-amplitude surface waves often dominate near-surface seismic data sets and overlay other events, such as reflections and refractions. For FWI, events do not need to be separated but the full information content is interpreted. Currently, it is the most accurate 2D method for interpreting surface waves, and it yields models at sub-wavelength resolution. This is conceptually appealing, but it turned out to be a non-trivial task to establish a suitable and versatile FWI workflow.

The high-amplitude surface waves, which dominate near-surface seismic data sets, contribute most to the misfit functional between modelled and observed data. Due to their limited penetration depth, they only illuminate the shallowest part of the
investigated area. Consequently, sensitivities are largest at shallow depth. In Chapter 2, I presented a novel scaling approach in order to boost sensitivities and the corresponding model update at depth. To this end, the approximate Hessian matrix is scaled by the inverse of the cumulative sensitivities squared, in order to balance its column sums. With this strategy, the model update at depth is significantly increased. The success of the method was demonstrated with two synthetic examples of various complexities. The resulting tomograms offer a much better data fit, particularly the body waves are significantly better fitted. The theory behind the new scaling technique was formulated for the FWI problem, but in principle it could be applied to any kind of Gauss-Newton inversion problem, e.g. in electrical resistivity tomography.

The main part of my work included the incorporation of topography into our FWI code. I have decided to adapt SPECFEM2D due to several reasons. First, and most importantly, its accuracy was thoroughly proven by the developers and further reviewed by comparison with our in-house finite element code. Second, it was an investment in future applications because it contains many useful features, such as visco-elasticity and anisotropy and there is even a 3D equivalent of the code. I have written routines to read the wavefields, to convert them into the required format and to transform them to the frequency domain, in which the inversion is performed. In principle, any forward solver (e.g. our in-house finite difference time domain code “Matterhorn”) can now be adapted by simply adjusting the reading routine.

The performance of our FWI code incorporating surface was proven in Chapter 3 by applying it to synthetic modelling examples featuring various degrees of surface topography. The inversions fail when neglecting even small topography undulations, but the new version of our code is able to handle arbitrary surface topography. The effects of neglecting topography were investigated for two types of topographic undulations. The first set of experiments focused on the roughness of surface topography, varying the wavelength of topographic undulations. The second set of experiments focused on the amplitude of long-wavelength topographic variations. It turned out that deteriorations become particularly severe, when either the wavelength or the amplitude of topography is in the order of the minimum shear wavelength of the seismic data. The effects of
neglecting surface topography were compared to other error sources that are often faced in FWI, such as 3D-to-2D filtering errors, neglecting attenuation, anisotropy or 3D out of plane structure. Only the latter yielded comparable deteriorations, which brings me to the conclusion that 2D FWI shall only be applied where the subsurface and the topography are sufficiently invariant in the third direction.

The setup of seismic acquisition is still governed by the needs of conventional data analysis tools, namely, reflection seismology processing, traveltime tomography and multi-channel surface wave analysis. In Chapter 4, I have made an attempt to optimise experimental layouts for shallow seismic experiments. I established a recipe including the following important points: (i) the use of pressure and vertical sources can be omitted without substitution; (ii) multi-component receivers are highly recommended; (iii) the receiver spacing should correspond to the minimum wavelength expected; and (iv) a few well-selected horizontal sources are sufficient to properly resolve the subsurface. These recommendations are based on the analysis of benefit-cost curves and inversion results. The costs of a survey were defined by the number of sources employed. The benefit was defined by the relative eigenvalue range ($RER$). Because the $RER$ relies on the eigenvalue spectrum of the approximate Hessian matrix, which is expensive to compute, the selection of the optimal source positions was based on an alternative, cheaper, goodness function. The results reminded on the Pareto principle (or 80/20-rule), which states that 80% of the benefit can be obtained with 20% of the costs. Even when having a dense data set at hand, the data to be fed into the FWI algorithm should be properly chosen. Often, by selecting, say, 20% of the data, large redundancy can be prevented and still, most of the information content remains. In typical exploration type applications, huge data sets are available, and FWI is only run for obtaining a suitable migration velocity model. This is a typical case in which it is sufficient to run FWI on a considerably reduced subset of the data.

5.2 Future Research

In my view, every effort should be made in order to apply FWI on real data. First attempts with our FWI code yielded promising results, but it also turned out that a sophisticated pre-processing strategy is required for successful inversions. The pre-
Future Research

processing steps can roughly be categorised into data selection (Section 5.2.1) and amplitude correction (Section 5.2.2). Pre-processing is certainly an important topic of future research, but I also suggest a number of other methodological improvements that shall further contribute to the success of near-surface seismic FWI.

Over the past years, our group has acquired a plethora of near-surface seismic data sets with various complexities. This offers possibilities of testing our code under more and more challenging circumstances. Furthermore, we are currently building a hybrid wave laboratory in which physical and numerical models can be closely coupled. The possibility of controlling the physical model yields a perfect environment for testing new features. In my view, these tests on laboratory and field data should guide the development of our FWI code.

5.2.1 Data Selection

Although FWI aims at modelling the full wavefield, some data selection is required prior to the inversion. Clearly, the inversion of real data starts with quality control; “bad traces” need to be removed immediately. After Fourier transformation, the available frequency content shall be identified and the inversion frequencies are chosen accordingly. Often, correlated noise occurs within distinct frequency windows which should be avoided.

More sophisticated data selection includes automated schemes, with which data are gradually introduced to the inversion. For instance, the inversion can be started with focusing on body waves. To this end, the near-offset traces dominated by surface waves are removed from the data set. Furthermore, the traces can be multiplied with exponentially decaying functions, starting at the first breaks. During the inversion, the exponential damping can be reduced in order to gradually introduce surface wave energy to the inversion.

Based on the actual model and inversion frequencies, traces that are prone to cycle skipping can be identified and automatically removed from the actual data sets. They can be re-introduced, once the inversion converges.
5.2.2 3D effects

Due to the large efforts required for 3D seismic data acquisition, I judge that most seismic surveys for near-surface studies will be carried out along 2D profiles for several years to come. However, the earth exhibits 3D structures and seismic waves are affected by these 3D structures; this has several implications. In 2D FWI it is inherently assumed that the investigated medium does not change in the third direction. The near-surface zone is very heterogeneous, such that this assumption is often violated.

Even if it is not violated, there is a difference between wave propagation in 3D and 2D. A point source in 2D corresponds to a line source in 3D which spreads its energy over the surface of a cylinder. However, seismic data is acquired with 3D point sources which spread their energy over the surface of a sphere. Due to the different spreading characteristics, 3D data needs to be filtered prior to FWI in 2D (see Appendix A). The theoretical derivation of the filter that we employed so far, assumes straight rays and a homogeneous velocity model and it is formulated for the far-field only. In Appendix A, we investigated the errors resulting from these violated assumptions. We found that besides some artefacts, the resulting FWI tomograms were still satisfying. However, we limited our analysis to the crosshole case and a simple acoustic reflection type experiment, resembling an exploration type application. I expect the performance of the filter to be rather poor when applying it to surface waves, leading to faulty amplitudes and consequently degraded FWI images.

Forbriger et al. (2014) introduced a “hybrid data transformation” applicable to body and surface waves and demonstrated its performance in a numerical study (Schäfer et al., 2014). Our data sets could be filtered using this improved strategy in order to reduce filtering errors.

Another approach to overcome the 3D-to-2D issue is to use a 3D forward modelling engine although sources and receivers are placed along a 2D profile, therefore rendering the additional filter unnecessary. This does not increase the number of inversion parameters, if the assumption is still made that the model is invariant in the third direction (which is an inherent assumption of pure 2D inversion). However, it does increase the number of forward modelling parameters. With efficient boundary
conditions, it should be possible to restrict forward modelling to a relatively small stripe around the profile. With optimised parallelisation and increasing computer power, this forward modelling problem should be tractable. With SPEFCEM3D, there is a 3D equivalent to the currently used 2D forward solver, which could be utilised as an external forward solver.

The presence of 3D heterogeneities represents a more serious problem. A possible option could be to identify and remove the corresponding events from the data. I judge this to be very difficult because corresponding events overlay with other, in-plane, events. As shown by Butzer et al. (2013), neglected out-of-plane structures can severely degrade the images obtained with 2D FWI. If there are significant topographical variations outside the profile, I expect similar degradations. For treating out-of-plane features it seems unavoidable to me to introduce a 3D model parameterisation (also for the inversion). I propose to treat a domain being twice as wide (perpendicular to the profile) as deep, such that all out-of-plane reflections can be considered. Within this area, distinctive topography needs to be surveyed and incorporated into the modelling and inversion grids. The inversion grid may be coarser in the third direction than in the two principle directions (elongated inversion cells). For existing 2D data sets, the additional out-of-plane model parameters shall help explaining 3D effects in the data. In future investigations, it may be useful to complement the 2D acquisition profile for this “pseudo-3D” inversion with a few well-selected shots or receivers outside the profile. The optimal positions of these additional shots and receivers can be determined with tools of experimental design.

5.2.3 Model Parameterisation

Throughout my thesis I have restricted myself to rather regular grids, i.e., the size of the inversion cells was well balanced, even when treating topography. This is unfortunate, because the sensitivities are not balanced at all. I have made first attempts of adapting the size of the inversion cells to the magnitudes of the sensitivities, that is, I used an inversion grid that was expanding with depth. The first results were promising; the model update could be increased at depth while I could save two thirds of the model parameters. However, the cells must be chosen such that they still meet the expected
spatial resolution. In order to further optimise the inversion grid used and to minimise the number of inversion parameters, one could think of an alternative model parameterisation. Plattner et al. (2012) have applied an adaptive wavelet parameterisation to electrical resistivity tomography. Due to the potential computational savings, such an approach seems promising also for the FWI problem, especially for the pseudo-3D case described above.

5.2.4 Attenuation

Throughout my thesis I have not considered anelastic attenuation although the near-surface zone is often highly attenuating. Groos et al. (2014) investigated the effects of ignoring attenuation and demonstrated the detrimental effects. They have shown that inverting for additional source coupling effects partly accounts for missing attenuation in the forward modelling; this is our actual strategy. However, Groos et al. (2014) have furthermore shown that incorporating a fixed attenuation model into forward modelling significantly improves the results (even if the attenuation model is not entirely correct). Since SPECFEM2D is capable of treating the visco-elastic case, this strategy may be a valuable option for our FWI experiments. The attenuation model can be obtained from the analysis of the amplitude vs. offset behaviour in the seismograms.

A more thorough approach is to add the quality factors to the inversion problem as additional parameters. This might be necessary due to the large heterogeneities that occur in the attenuation as well as in the elastic parameters in the near-surface zone. One option is to simply make $V_p$ and $V_s$ complex-valued. This option was implemented in our code for the acoustic case by Vasmel (2012) who successfully recovered blocky attenuation anomalies in a crosshole configuration. However, inversion for attenuation still needs to be implemented for the elastic case. Personally, I am critical when it comes to this implementation because of the complexity of the problem. Introducing the quality factors $Q_p$ and $Q_s$ to the inversion problem significantly increases the number of model parameters (and therefore computational costs), leading to additional parameter trade-offs. This means that one parameter type may be less resolved at the cost of better resolving another parameter type. Furthermore, trade-offs between attenuation and source or receiver coupling factors must be expected, such that possible attenuation
models should be interpreted with care. Finally, the fundamental question about which attenuation mechanism found in literature (e.g. Aki and Richards, 2002; Kjartansson, 1979) works best for FWI still needs to be answered.

Groos et al. (2014) have nicely demonstrated that in some cases incorporating attenuation into forward modelling suffices. This is substantially easier than inverting for attenuation and should therefore be considered as a valuable option.
Seismic full waveform inversion is often based on forward modelling in the computationally attractive 2D domain. This implies the assumption of a line source extended in the out-of-plane medium invariant direction, with far-field amplitudes decaying inversely with the square root of distance. Realistic point sources, however, generate amplitudes that decay approximately with the inverse of distance. Conventionally, practitioners correct for this amplitude difference and the associated phase shift by transforming the recorded 3D field data to the approximate 2D equivalent by using simplistic asymptotic filter algorithms. Such filters assume straight ray paths, a constant velocity medium and far-field recordings. Here, we assess the validity of 3D-to-2D data transformation in the context of cross-hole seismic full waveform tomography by propagating 3D and 2D wavefields through 2D media and comparing 2D reference synthetics with their filtered 3D equivalent. The filter performs well in simple situations, which confirms the general applicability of the conventional asymptotic approach. However, we observe substantial errors in more complex elastic models, associated with overlapping arrivals and strongly curved raypaths. To test if this error translates into deficient model reconstruction in full waveform inversion, we performed complementary inversion experiments using a frequency-domain algorithm. Purely acoustic waveform inversions of 3D-to-2D filtered data are only weakly affected, but in the case of elastic full waveform inversion, where S-wave influence is present, adverse effects increase substantially. Two-dimensional full waveform inversion in combination with filtering seems to be an acceptable strategy, as long as (i) the model is two-dimensional, (ii) the recording geometry is straight and perpendicular to strike, and (iii) only slight S-wave energy is contained in the data. The latter two conditions are generally met in exploration type marine seismic surveys at short offsets and in some cross-well applications employing explosive sources and non-directional pressure receivers.

A.1 Introduction

Full waveform inversion (FWI) is a powerful means of subsurface imaging. It emerged in the 1980s but was not fully exploited at that time because of limited computational resources (Mora, 1987; Tarantola, 1986). As opposed to ray-based travel time tomographic methods, which use only first arrival time information, the entire seismogram information is used in the waveform inversion process, allowing the reconstruction of realistic earth models at sub-wavelength resolution (Fichtner, 2011). The first successful applications of the theory were achieved using acoustic time-domain inversion schemes (Lailly, 1983; Tarantola, 1984), but later, frequency-domain approaches were introduced which offered certain computational advantages (Pratt, 1999; Zhou and Greenhalgh, 2003).

Full waveform inversion is mostly performed in the computationally attractive 2D domain (Brossier et al., 2009; Mulder et al., 2010) since solving the 3D forward elastic problem is still a rather challenging task. Only a few examples of true 3D full waveform inversions have been published (Ben-Hadj-Ali et al., 2008; Sirgue et al., 2011; Vigh and Starr, 2008; Warner et al., 2013). Generally, it is the solution of the forward problem, which must be repeated many times for each model update that contributes most to the total computational expense of full waveform inversion. In time-domain modelling, the limiting factor is total run-time, as each source position requires a new forward computation. In frequency-domain modelling, which is often preferred in exploration type FWI, multiple sources add little to the computational costs, but when considering full 3D treatment, the system matrices can become extremely large and often exceed the available memory resources.

Even though the 3D acoustic problem is tractable nowadays (e.g. Sirgue et al., 2011), 2D recording geometries (and the usage of geometrical spreading corrections) will most likely remain prevalent – at least in engineering, environmental and cross-hole type
applications. The 2D assumption is acceptable in terms of information content, provided
the medium properties only change in two dimensions (e.g. the \(xz\)-plane) and no out-of-
plane arrivals are present in the data. However, one always has to take care of the fact
that any numerical or analytical solution of the 2D wave equation inherently carries the
assumption of a line source being infinitely extended in the out-of-plane (strike)
direction (e.g. Cervený, 2005). In a 3D homogeneous, constant-velocity medium, any
realistic seismic point source (explosive, sparker, airgun) generates a spherical
wavefront, whereas the line-source wavefront is cylindrical. The associated amplitude
and phase differences between the recorded 3D and the modeled 2D data have to be
accounted for prior to the inversion. Mostly, this is accomplished using the popular
preprocessing step of 3D-to-2D data transformation of the field data, often termed
gEometrical spreading correction, although phase differences are involved as well
(Bleibinhaus et al., 2009; Mulder et al., 2010).

The potential shortcomings of this preprocessing step have so far received little
attention and to the best of our knowledge there exist no studies in the literature that
give an extensive quantitative appraisal of the accuracy of 3D-to-2D data transformation –
 at least in the context of full waveform inversion. Ernst et al. (2007) allude to a
thorough testing of their frequency-domain approach and observe good performance in
far-field regimes. Pica et al. (1990) mention that they tested filter performance and claim
sufficient accuracy, but show neither data examples nor quantitative errors. Igel et al.
(1993) show a numerical example for a 1D acoustic layered model to illustrate the poor
performance of the filter, but the authors provide no quantitative error values.
Wapenaar et al. (1992) demonstrate how filtered point source amplitudes of first and
second events in a two-layer model deteriorate from line-source amplitudes, but they
didn’t examine phase errors. Miksat et al. (2008) present a comparison of the straight-
ray approximation and filtering combined with raytracing. They tested filters on
homogeneous, layered and lens-type structural models, but only considered single,
isolated transmission events, where they found maximum relative amplitude errors up
to 20%. Finally, Williamson and Pratt (1995) warn of errors up to \(~35\%) for a linear
gradient region in which velocity changes by a factor of two. However, they did not
present results nor did they analyse the error numerically. Consequently, it is important to investigate the errors associated with the 3D-to-2D data transformation process and how they manifest themselves in the inversion results.

After providing the theoretical background of the differences between 3D and 2D wave propagation and the nature of the asymptotic correction filters, we present an extensive numerical modelling study aimed at quantifying the seismogram differences between true 2D and 3D-to-2D corrected data for a variety of situations. Finally, we demonstrate to what extent these errors propagate to discrepancies in the inverted models.

A.2 Theoretical Background

A.2.1 Approaches to the 2.5D Problem

There are various approaches to generate synthetic seismograms that are quantitatively comparable to recorded field data, without having to deal with true 3D modelling. Techniques to solve the 3D-to-2D problem can roughly be classified into three major categories (Roberts, 2005): (i) Reformulating the problem in (quasi-)cylindrical coordinates (Igel et al., 1993; Takenaka et al., 2003) and synthesizing line source data by integrating over many point-sources along the experimental axis in CMP (common midpoint) sorted data (Wapenaar et al., 1992); (ii) Asymptotic 2.5D filtering procedures (Bleistein, 1986; Deregowski and Brown, 1983; Esmersoy and Oristaglio, 1988; Miksat et al., 2008; Vidale et al., 1985; Williamson and Pratt, 1995; Yedlin et al., 2012) to convert the 3D (point source) data to 2D (line source) data; (iii) True 2.5D modelling by Fourier transforming the governing partial differential equation along the \( y \)-axis to the \((\omega, k_y, x, z)\)- or \((t, k_y, x, z)\)-domain and solving the resulting 2D problem for many \( k_y \)-components (Novais and Santos, 2005; Sinclair et al., 2012; Song et al., 1995; Zhou et al., 2012; Zhou and Greenhalgh, 1998), which yields approximate 3D wavefields.

2.5D techniques (ii and iii) directly exploit symmetries of the so called 2.5D configuration. A typical 2.5D problem consists of a 3D point source situated inside a 2D medium (i.e., a 3D medium with material properties being invariant in the strike (or \( y \)-coordinate) direction; Cao and Greenhalgh, 1997). It is common practice in 2D seismic
experimental design to acknowledge the benefits of 2.5D symmetry by placing sources and receivers in a plane perpendicular to the strike axis. This obviates any out-of-plane arrivals and leads to problems that are essentially 2D (Williamson and Pratt, 1995).

3D-to-2D data transformation using an asymptotic filter (ii) is by far the most widespread approach adopted by researchers and practitioners. It has the advantage of simple implementation and negligible computational cost. In almost all field data applications of full waveform inversion reported in the literature, authors rely on very simple straight-ray approximations of these transformations (Belina et al., 2009; Bleibinhaus et al., 2009; Crase et al., 1990; Hicks and Pratt, 2001; Mulder et al., 2010; Pica et al., 1990; Reiter and Rodi, 1996; Shipp, 2001). Some investigators even completely neglect the phase correction and apply only amplitude corrections by multiplying the recorded field data with a square-root-of-time dependent gain function.

True 2.5D modelling (iii) allows converting the 3D problem to multiple 2D problems that have to be solved for the various wavenumber components. Each 2D problem can be solved in either the frequency domain (\(\omega-k_y\)) or the time domain (\(t-k_y\)) and the final result is then obtained by taking the inverse Fourier transformation with respect to \(k_y\). This reduces to a simple summation of the wavenumber spectra if computations are restricted to the central plane (\(y=0\)) with \(k_y=0\) corresponding to the simple 2D problem. Compared to the filtering approach, 2.5D modelling is computationally more involved, but has a wider range of applicability as it can be applied in case of irregular recording geometries (crooked lines).

### A.2.2 Differences between 2D and 3D Wave Propagation

The frequency-domain solution (Fourier-transformed Green's function) to the wave equation for an omni-directional (pressure) 3D point source in an unbounded, acoustic, homogeneous medium is given by (Aki and Richards, 2002):

\[
\tilde{G}^{3D}(r, \omega) = \frac{1}{4\pi r} \exp \left( \frac{i\omega r}{c} \right),
\]

where \(\omega\) is the angular frequency, \(r\) is distance and \(c\) is acoustic wavespeed. The corresponding time-domain expression is
The frequency-domain 2D Green’s function solution for an unbounded, acoustic, constant density fullspace is given by (Abramowitz and Stegun, 1964):

\[ G^{2D}(r,t) = \frac{1}{4\pi r} \delta \left( t - \frac{r}{c} \right). \]  \hspace{1cm} (A.2)

where \( H_0 \) is the Hankel function of the first kind and zero order. Using the large-argument approximation of the Hankel function (Morse and Feshbach, 1953), valid when the distance \( r \) is large relative to the wavelength \( \lambda \approx c/\omega \), one obtains the asymptotic 2D acoustic Green’s function in the frequency domain shown on the right-hand-side of Eq. (A.3). By Fourier transforming Eq. (A.3) the time domain acoustic 2D Green’s function is obtained (Bleistein, 1984; Morse and Feshbach, 1953):

\[ G^{2D}(r,t) = \frac{1}{2\pi} U \left( t - t_0 - \frac{r}{c} \right) \left( t - t_0 \right)^2 - \frac{r^2}{c^2} \right)^{\frac{1}{2}}, \]  \hspace{1cm} (A.4)

where \( U(t) \) is the unit step function. The most obvious difference between 3D and 2D wave propagation is their different amplitude decay with distance or time. In the case of a 3D point source in a homogeneous medium, energy spreads over the surface of a sphere, thus amplitudes scale with \( 1/r \). In the 2D case energy spreads over the surface of an expanding cylinder and amplitudes scale with \( 1/\sqrt{r} \). Contrary to the time domain 3D Green’s function (Eq. (A.2)), which is characterised by a delta function that immediately goes to zero after passing a receiver, the 2D Green’s function includes later arriving energy from an increasingly distant continuum of point sources along the \( y \)-axis. This results in the so called ”long-tail” or ”\( t \)-tail”, which mathematically originates from the square-root term in Eq. (A.4) and causes an asymmetric shape of the 2D receiver wavelet. A comparison of the 3D and the corresponding 2D Ricker wavelet propagated through a homogenous model is shown in Fig. A.1. In the frequency domain, the 3D Green’s function (Eq. (A.1)) shows regularly oscillating behavior, whereas the 2D Green’s function (Eq.(A.3)) is scaled by \( 1/\sqrt{\omega} \), which results in smaller amplitudes at
larger angular frequencies (not shown). The $\pi/4$ phase shift between the 3D and 2D solutions can be understood from the multiplication with $\exp(i\pi/4)$ in the asymptotic 2D Green’s function on the right-hand-side of Eq. (A.3). The dominance of lower frequencies in the 2D Green’s function can physically be explained by an increasingly destructive interference pattern of point sources along the $y$-axis for higher frequencies.

A.2.3 Asymptotic Point-Source to Line-Source Filters

Asymptotic point-source to line-source conversion filters have been presented by various authors in different contexts (Bleistein, 1986; Deregowski and Brown, 1983; Esmersoy and Oristaglio, 1988; Miksat et al., 2008; Vidale et al., 1985; Williamson and Pratt, 1995; Yedlin et al., 2012), with (Bleistein, 1986) being the most cited for his Asymptotic Ray Theory (ART) derivation. A simpler derivation of the filter function is based on forming the ratio of the acoustic 3D frequency-domain Green’s function (Eq. (A.1)) and the asymptotic approximation of the acoustic 2D frequency-domain Green’s function (see Eq. (A.3), far right). This yields the asymptotic filter transfer function (often referred to as the Bleistein filter) for a homogeneous full-space acoustic medium.
\[ \tilde{G}^{2D}(\omega) = \tilde{G}^{3D}(\omega) \exp \left( \frac{i\pi}{4} \sqrt{\frac{2\pi\sigma}{|\omega|}} \right), \]  

(A.5)

where the quantity \( \sigma \) is defined as \( \sigma = cr \). For general inhomogeneous media it is given as the line integral of the velocity with respect to the arclength \( s \) of the ray trajectory (Miksat et al., 2008). In 1D layered media \( \sigma \) can be written as

\[ \sigma = \int c(s) ds = \left( \frac{s_{\text{tot}}}{\sqrt{t}} \right)^2 = \left( \frac{s_1 + s_2 + \ldots + s_n}{\sqrt{t}} \right)^2, \]  

(A.6)

with \( s_{\text{tot}} \) being the total arclength and \( s_i \) being the individual arc segments in each layer (Miksat et al., 2008). It is important to note that the general form of \( \sigma \) for inhomogeneous media involves both the traveltime \( t \) and the length of the associated raypath \( s \) and consequently the amplitude is scaled by both of them in combination.

Applying an inverse Fourier transform to Eq. (A.5) yields the filter function in the time domain (Aki and Richards, 2002):

\[ G^{2D}(t) = \sqrt{2\pi\sigma} \left[ \frac{U(t)}{\sqrt{t}} * G^{3D}(t) \right]. \]  

(A.7)

Some authors in the field of georadar full waveform inversion use frequency-domain 3D-to-2D filter implementations that rely on picking first break arrival times and taking an average to estimate the quantity \( \sigma \) in Eq. (A.5). Consequently, they only adequately correct amplitudes of the picked arrival but fail for later phases (Ernst et al., 2007; Klotzsche et al., 2010). However, the most common approach for seismic purposes is a very crude approximation of the time-domain expression (Eq. (A.7)), which consists of a multiplication of each time-domain trace with the function \( \sqrt{t} \) on a sample-by-sample basis to correct amplitudes, followed by a time-domain convolution with the function \( 1/\sqrt{t} \) to adjust phases. Real data examples of this approach are given by Bleibinhaus et al. (2009), Crase et al. (1990), Hicks and Pratt (2001), Mulder et al. (2010), Pica et al. (1990), Reiter and Rodi (1996) and Shipp (2001). There exist more accurate ways to implement Eq. (A.7), allowing for individual treatment of each arrival with its own amplitude scaling factor \( \sigma \) (e.g. Miksat et al., 2008), which have certain applications in
earthquake seismology. However, such approaches require well separated events in time and a velocity model that is known beforehand. This is not generally of practical relevance in active (controlled source) source seismology.

A.2.4 Limitations of the Asymptotic Filter Approach

Filtering errors can be significant for highly heterogeneous media (Miksat et al., 2008; Williamson and Pratt, 1995). Both the frequency-domain and the time-domain expressions (Eq. (A.5) and (A.7), respectively) require the high frequency ray approximation to hold. The validity of the asymptotic approximation is violated when the argument $\omega/r = kr = r/\lambda$ in Eq. (A.6) gets small, i.e., when the wavelength $\lambda$ is large or the distance $r$ is small (i.e., in the near-field). In seismic exploration, the ray (high frequency) approximation is regularly violated (Kravtsov and Orlov, 1990). Examples in which wave theory is required include overlapping events (multiples, caustics, bow ties), or free surface and interbed multiples interfering with primary reflections. Further problems arise when elastic mode conversions (P-to-S and S-to-P) and interference between P- and S-waves occur. Whenever earlier or later arrivals or P- and S-modes start to overlap and interfere with each other, the phase difference between 3D and 2D wave propagation can no longer be taken as $\pi/4$.

A.3 Synthetic Modelling Study

In this study, we assess the validity of Bleistein’s asymptotic filter in non-uniform media involving more complex wave propagation effects commonly observed in acoustic and elastic cross-hole type seismic surveys. Additionally, we present one acoustic reflection-type synthetic experiment, representative of a shallow marine seismic survey. We judge that the results for the cross-hole examples are similarly applicable to surface recording geometries and can be up- or downscaled to larger and smaller dimensions given a comparable distance-to-wavelength ratio.

A.3.1 Methodology

A 2D time-domain staggered-grid visco-elastic finite-difference (FDTD) code and its 3D equivalent (Bohlen, 2002) were employed to compute 2D reference synthetic seismograms and their 3D counterparts, representing the observed seismic “field data”.
3D models were set up by extending the 2D models in the third direction ($y$-direction). We established a suite of 2.5D (i.e., invariant in $y$-direction) and 2D transmission and reflection type models of increasing degree of complexity and computed their 2D and 3D synthetic responses. In our analysis we ignored the free surface, source or receiver ghosts, attenuation and restricted ourselves to Ricker type source time functions. Acoustic and elastic seismograms were generated with the same visco-elastic code, but for acoustic modelling, the density $\rho$ was set to a constant value of 2600 kg/m$^3$ and the shear wave velocity was set to a very small value of 10 m/s (van Vossen et al., 2002). This approach was followed to avoid any bias due to interchanging the numerical method. Visco-elastic dissipation was neglected by setting the quality factor $Q$ to a very high value of $2 \times 10^5$. Amplitudes shown for acoustic experiments correspond to scalar pressure recordings, whereas amplitudes in the elastic experiments correspond to particle velocities in the $x$- (horizontal) or $z$-direction (depth). We used 10 or more grid points per minimum wavelength, but the reflection-type model required a finer discretization to avoid numerical grid dispersion. We used absorbing boundaries (Bohlen, 2002) with a size of 50 grid points and a damping exponent of 1.6. In transmission-type experiments we kept a minimum offset to the boundaries of 50 grid points for the sources and 30 grid points for the receivers. For the reflection-type model, minimum separation of sources and receivers from the boundaries was 100 grid points. The active modelling domain dimensions were 150 m $\times$ 150 m for transmission- and 300 m $\times$ 200 m for reflection-type experiments, respectively. In all modelling and inversion experiments presented below, we used a Ricker-type source wavelet with a central frequency of 100 Hz. Table A.1 and Table A.2 list the essential characteristics, the corresponding recording geometries and the individual FDTD parameterizations for each model. In the reflection-type experiment we muted the first event, as is common practice in marine seismics, before we computed the normalised root-mean-square deviation ($NRMSD$) between the seismic traces of the filtered 3D and the reference 2D synthetic gathers. This misfit measure is defined as
$$NRMSD[\%] = \frac{\sqrt{\sum_{i=1}^{n} (x_{2D,i} - x_{3D,i})^2}}{\sqrt{\sum_{i=1}^{n} x_{2D,i}^2}}. \quad (4.6)$$

with $n$ being the number of time samples and $x_{2D/3D,i}$ being the $i$-th time sample of the reference 2D and filtered 3D trace, respectively. Note that in the case of seismogram comparisons, $NRMSD$ values represent the misfit between directly modeled 2D synthetics and filtered 3D synthetics, whereas in the case of inversion results, $NRMSD$ values correspond to the normalised RMS deviation between the true velocity model and the model obtained from "2D-2D" inversions (i.e., inverting 2D synthetics with a 2D algorithm) or "3D-2D" inversions (i.e., inverting filtered 3D synthetics with a 2D algorithm).

Table A.1: Overview of finite-difference parameterization of investigated models. $GP/\lambda_{min}$: Gridpoints per minimum wavelength, $N_{dt}$: Number of time steps, $dt$: time step, $dh$: grid spacing, $BC/exp.$: Boundary thickness and exponential damping factor.

| Model type       | $dh$ [m] | $dt$ [s] | $N_{dt}$ | $GP/\lambda_{min}$ | $f_c$ [Hz] | $x/z/y$ [m] | $BC$ [m] / exp. |
|------------------|----------|----------|----------|---------------------|------------|-------------|----------------|-----------------|
| Reflection       | 0.25     | $4 \times 10^{-5}$ | 7000     | 20                  | 100        | 400 x 300 x 200 | 50 / 1.6        |
| Cross-hole       | 0.5      | $5 \times 10^{-5}$ | 4000     | $\sim 10$          | 100        | 250 x 250 x 250 | 50 / 1.6        |

Table A.2: Summarised description of the geometry and characteristics of the investigated models. Types: Transmission- or Reflection-type geometry.

<table>
<thead>
<tr>
<th>Model ID</th>
<th>Type</th>
<th>$V_r$ [km/s]</th>
<th>$V_s$ [km/s]</th>
<th>$\rho$ [t/m$^3$]</th>
<th>Source</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>GAR</td>
<td>R</td>
<td>1.0 – 3.0</td>
<td>0.01</td>
<td>2.6</td>
<td>explosive</td>
<td>1-D, gradient</td>
</tr>
<tr>
<td>SAT</td>
<td>T</td>
<td>$\sim 1.05$ – $1.38$</td>
<td>0.01</td>
<td>2.6</td>
<td>explosive</td>
<td>stochastic model</td>
</tr>
<tr>
<td>BAT</td>
<td>T</td>
<td>1.0 – 2.0</td>
<td>0.01</td>
<td>2.6</td>
<td>explosive</td>
<td>block anomalies</td>
</tr>
<tr>
<td>SET</td>
<td>T</td>
<td>$\sim 1.78$ – $2.35$</td>
<td>$\sim 1.05$ – $1.38$</td>
<td>$\sim 2.10$ – $2.75$</td>
<td>-E: explosive</td>
<td>elastic version of SAT</td>
</tr>
<tr>
<td>BET</td>
<td>T</td>
<td>1.7 – 3.4</td>
<td>1.0 – 2.0</td>
<td>2.0 – 4.0</td>
<td>-E: explosive</td>
<td>elastic version of BAT</td>
</tr>
</tbody>
</table>
A.3.2 Results

Acoustic Crosshole Case

Fig. A.2: Acoustic stochastic model SAT. (a) Model geometry and transmission-type source-receiver setup. The model shows stochastic fluctuations with acoustic wave-speed that varies between \( \sim 1.05 \) and \( 1.38 \) km/s. Density is set to a constant value of 2600 kg/m\(^3\) (b) 2D acoustic FDTD synthetic seismic gather obtained using a 100 Hz dominant-frequency Ricker-type explosion source. Various later phases of relatively low amplitude arrive after the first break. (c) Sample trace at a depth of 74 m (indicated by the red line in diagram (b)) in the time domain. 2D data is shown in red and filtered 3D data is shown in black. There is a relatively good fit between 2D and filtered 3D traces. (d) Normalised amplitude spectrum of the same trace. Amplitude spectra and phase spectra (not shown) of 2D and filtered 3D compare very well. Stochastic heterogeneity seems to straighten the effective ray paths.
**Stochastic model (stochastic, acoustic, transmission-type: SAT).** – First, we analyse an acoustic constant density fullspace model including stochastic fluctuations of 15% around a median P-wave velocity of 1250 m/s based on a Karman power law distribution with a Hurst (or roughness) coefficient of 0.75, a horizontal correlation length of 23 m and a vertical correlation length of 5 m. (for definitions of these statistical measures, see for example, Holliger and Levander (1992). The recording geometry is of the cross-hole type with a single buried source and a vertical array of 60 receivers distributed over the depth range 16 - 134 m. There is a high velocity zone at the level of the shallow receivers and a low velocity zone enclosing the deeper receivers (Fig. A.2a). The source is located within an intermediate velocity zone. A significant amount of scattered energy of relatively low amplitude arrives shortly after the first onset (Fig. A.2b). Interestingly, the SAT model seems to be surprisingly forgiving with regard to filtering errors. 2D and filtered 3D data fit each other very well with an average NRMSD of ~3.8%. This is comparable to the errors that we observe in a homogeneous fullspace model (3.4%) and well within the expected range of precision of the numerical algorithm. The example trace at a depth of 74 m illustrates the very good fit between 2D and filtered 3D data in the time and in the frequency domain (see Fig. A.2c, d).

**Block model (blocky, acoustic, transmission-type: BAT).** – The next model comprises two anomalous blocks with high and low velocities embedded in a constant velocity background medium and is ought to mimic engineered structures (e.g., artificial cavities, tunnels or foundations; Fig. A.3a). The source-receiver geometry is equivalent to the one of the stochastic model SAT. The simulated wavefield is fairly complex, involving several overlapping arrivals (Fig. A.3b), but the filter performance is quite acceptable, with an average NRMSD of ~8.6%, which is approximately twice the error found for the stochastic model SAT.
Acoustic block-anomaly model BAT. (a) Model geometry and transmission-type source-receiver setup. One block is of low velocity, the other of high velocity and both are embedded in a constant velocity background. Density is set to a constant value of 2600 kg/m³. (b) 2D acoustic FDTD synthetic seismic gather obtained using a 100 Hz dominant-frequency Ricker-type explosion source. In the lower half of the gather, moderate interference occurs between earlier and later phases. (c) Sample trace at a depth of 104 m (indicated by the red line in diagram (b) shown in the time domain. 2D data are shown in red and filtered 3D data are shown in black. Fit between 2D and filtered 3D is not as good as for model SAT but still satisfactory. (d) Amplitude spectra of the same trace, showing some minor differences.

Elastic Crosshole Case

Next, we consider full elastic wavefields propagated through modified versions of the acoustic block model BAT and the acoustic stochastic model SAT. We introduced elasticity in the models by setting the S-wave velocities (which had been previously fixed at an unphysical value of 10 m/s for all acoustic experiments) to the original P-
wave velocities and setting the new P-wave velocities to the original values multiplied by a factor of 1.7, which is a typical $V_P/V_S$ ratio for crustal rocks (corresponding to a Poisson’s ratio of ~0.25). This up-scaling was necessary to avoid shorter wavelengths (for the S-phases) and the associated smaller spatial grid interval, which would have significantly increased the computational requirements. Unlike all the acoustic examples, which entailed computations of scalar pressure, the elastic simulations were in terms of vectorial particle velocity in the $x$, $z$- and $y$-directions (only $x$ and $z$ in the 2D case). Thus, the wavefield and seismogram examples shown below generally display particle velocities. Since the straight-ray approximate time-domain filter works purely on a sample-by-sample basis, no modifications had to be made to apply it to the particle velocity seismograms. Elastic experiments were performed both with an omni-directional explosion source (denoted by “-E”, attached to the model acronym) and an $x$-directed point force (denoted by “-X”).

It is important to note that increasing the P-wave velocity by itself will exacerbate the conversion error, because the dominant wavelength is increased. Thus we performed additional acoustic experiments where we solely increased the P-wave velocity by a factor of 1.7 (while $V_S$ was kept at 10 m/s). Average $NRMSE$ increased from 3.8% to 4.8% and 8.6% to 9.7% for models SAT and BAT, respectively. We infer that the much more significant increase in error in the elastic case is not primarily due to the higher dominant wavelength but can mostly be attributed to elastic effects (presence of shear waves, both from the directed source and mode conversion at interfaces). We didn’t observe any worsening of grid boundary effects or other numerical artefacts when introducing elasticity. Hence, we retained the same finite-difference parameterization as for the acoustic experiments (see Table A.1).
Elastic stochastic model SET-X (the P-wave velocity was taken as 1.7 times the P-wave velocity of model SAT and the S-wave velocity was set to its P-wave velocity). (a) 2D elastic FDTD synthetic seismic gather (particle velocity in x-direction) for a point force in x-direction with a 100 Hz dominant frequency Ricker-type source-time function. The wavefield is considerably more complicated than in model SAT and exhibits strong interference and phase modification. A clear S-wave arrival covering later portions of the wavefield is visible in both the x and the z components of motion. (b) The same as (a) but showing the particle velocity in z-direction. (c) and (d) show a sample trace at a depth of 104 m (shown in diagram b as the red curve) in the time and in the frequency domain. Misfits are higher than in model SAT.
**Stochastic model (stochastic, elastic, transmission type: SET).** – We start with an elastic version of model SAT, which we call SET. The average NRMSD is ~7.4% for the x-component of the wavefield when using an omni-directional (explosive, or pressure only) source (see Table A.3). Changing to an x-directed source yields a significant S-wave component arriving shortly after the direct P-wave arrival and strongly interfering with later portions of the gather (indicated by the arrows in Fig. A.4a, b). Mode conversions as well as interference between P- and S-waves render the wavefield highly complex. This results in errors being significantly larger than in the case of an explosion source in an acoustic medium. The average NRMSD increases to ~21.6% for the x-component of the wavefield. As can be seen in a sample trace at a depth of 104 m and its spectrum for model SET-X (Fig. A.4c, d), deviations between the 2D and the filtered 3D solution are larger than in the simple acoustic case SAT.

<table>
<thead>
<tr>
<th>Summary of synthetic modelling study</th>
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<tbody>
<tr>
<td><strong>Model ID</strong></td>
</tr>
<tr>
<td>GAR</td>
</tr>
<tr>
<td>SAT</td>
</tr>
<tr>
<td>BAT</td>
</tr>
<tr>
<td>SET(e)</td>
</tr>
<tr>
<td>BET(e)</td>
</tr>
<tr>
<td>SET(x)</td>
</tr>
<tr>
<td>BET(x)</td>
</tr>
</tbody>
</table>

Table A.3: Average NRMSD between filtered 3D (using the straight-ray time domain implementation of Eq. (A.7) and 2D FDTD synthetic data for full seismic gathers (corresponding to one source position and 60 traces). Errors for associated elastic experiments are given for the x- and the z-component of the wavefield. See Table A.1-Table A.2 for an explanation to which types of simulations the model abbreviations correspond.

**Block model (blocky, elastic, transmission-type: BET).** – Next, we consider an elastic version of model BAT, which will subsequently be abbreviated with BET. Simulations employing an omni-directional explosion source yield an average NRMSD of ~16.1% for the x-component of the wavefield (see Table A.3). However, using an x-directed source (Fig. A.5a, b), average NRMSD soars to values of ~30.0%. A sample trace in a depth of 104 m and its spectrum for model BET-X, shown in Fig. A.5(c, d), reveal the major deviations between the 2D and the filtered 3D solution in the time domain and in
the frequency domain. Even a considerable phase discrepancy is observed (Fig. A.5). Generally, the z-component of the wavefield is slightly less affected in terms of average NRMSD (see Table A.3) and again, receivers located behind the low velocity zone seem to exhibit the highest errors.

Fig. A.5: Elastic block model BET-X (the P-wave velocity was taken as 1.7 times the P-wave velocity of model BAT and the S-wave velocity was set to its P-wave velocity). (a) 2D elastic FDTD synthetic seismic gather (particle velocity in x-direction) with a point force in x-direction with a 100 Hz dominant frequency Ricker-type source-time function. (b) The same as (a) but showing the particle velocity in z-direction. (c) shows a sample trace at a depth of 104 m (marked in red in b), (d) and (e) in in the frequency domain (spectral amplitudes and phases). Misfits are significant. As opposed to most other models, where phases tended to match each other relatively well, here even a slight phase distortion can be observed.
Fig. A.6: Gradient model GAR. (a) Model geometry and reflection-type source-receiver setup. The model includes a velocity gradient from 2000 to 3000 m/s embedded between two layers of lower velocity. 80 receivers at a lateral spacing of 2 m are spread over a total length of 160 m. Minimum offset from the source is 40 m. Density is set to a constant value of 2600 kg/m³. (b) 2D acoustic FDTD synthetic seismic gather obtained using a 100 Hz Ricker-type explosion source. The second event overlaps the first event at a distance of around 190 m. A weak inter-bed multiple is visible at a time of around 250 ms. (c) Sample trace at a distance of 150 m in the time domain shown by the first red line in diagram (b). The second event, which has traveled through the velocity gradient, is under-corrected as its ray path is bent and the straight-ray assumption is violated. (d) Normalised amplitude spectrum of a sample trace at a distance of 210 m (shown as second red line in diagram (b)). 2D data are drawn in red and filtered 3D data are drawn in black. At locations where the first and second reflection events overlap, a particularly poor performance of the transformation filter at low frequency can be observed.
Acoustic Reflection Case

Gradient model (gradient, acoustic, reflection-type: GAR). – To highlight the effects of overlapping arrivals on the filtering error, we designed an additional reflection type experiment, involving a pressure source in a purely acoustic medium having constant density of 2600 kg/m$^3$. It is referred to as model GAR and is representative of a shallow marine seismic survey with a typical end-on acquisition geometry. The 1D layered model entails a linear velocity gradient zone, with velocity values ranging from 2.0 to 3.0 km/s, embedded between two low velocity layers, each having a wavespeed of $V_p = 1.0$ km/s. This strong impedance contrast generates two overlapping reflections from the top and bottom of the gradient zone (Fig. A.6a). The recording array comprises 80 receivers at a horizontal spacing of 2 m, spread over a total length of 160 m. The seismograms show a rather complicated interference pattern at receiver distances between 180 m and 220 m (Fig. A.6b). Arrivals associated with the reflection from the lowermost interface have traveled through the velocity gradient and follow a curved path, which strongly violates the straight-ray assumption. Consequently, the straight-ray based 3D-to-2D filter performs very poorly on the second arrival (see the example trace in a distance of 150 m in Fig. A.6c), which is under-corrected by about 15% throughout the gather. The $NRMSD$ increases erratically at receivers that recorded the overlap of the second and the first reflection. This is illustrated, for example, by a frequency-domain trace at a distance of 210 m, shown in Fig. A.6(d), which indicates particularly poor performance at low frequencies. The average $NRMSD$ value for the whole gather is $\sim$15.2% (see Table A.3).

A.4 Inversion Experiments

In order to examine the influence of approximate 3D-to-2D data transformation on the model reconstruction with a full waveform inversion routine, we performed acoustic and elastic cross-well test inversions for the block models (BAT, BET). We synthesised 3D and 2D seismograms for 15 source positions in the left well at a vertical spacing of 8 m, starting at a depth of 16 m. The 60 receivers straddle the right well which is 100 m away, as shown in Fig. A.7. The same FDTD code as for the previous simulations was employed to generate the input 3D and 2D seismograms.
Both filtered 3D and true 2D data were then inverted with a 2D finite element frequency-domain (FEFD) full waveform inversion code (Manukyan et al., 2012a). The main advantage of using a frequency-domain approach is, that it is more efficient when multiple sources are considered (Pratt, 1999), and that it helps to tame the non-linearity problem by starting the inversion at low frequencies and progressing to higher frequencies as iterations proceed (Brossier et al., 2009). Our FEFD forward code employs a rectangular grid, perfectly matched layer boundary conditions (Basu and Chopra, 2003; Zheng and Huang, 2002) and uses the PARDISO direct matrix solver to invert the system matrix (Schenk and Gärtner, 2004). The optimization scheme is based on a Gauss-Newton type approximation of the inverse Hessian matrix and locally minimises the $L_2$-norm misfit. The model update can be written as (Maurer et al., 2009; Pratt, 1999):

$$m^{i+1} = (J^T J + \alpha^2 I + \beta^2 L^T L)^{-1} \left[ J^T \left( (d - u) + J m^i \right) + \alpha^2 I m^i \right],$$

(A.9)

where $m^{i+1}$ are the estimated (inverted) model parameters for the $i$-th iteration, $J$ is the Jacobian matrix including partial derivatives of the data with respect to the model parameters, $I$ is the identity matrix, $L$ is a Laplacian smoothing operator and $d$ and $u$ are the observed and predicted data, respectively. The parameters $\alpha$ and $\beta$ govern the damping and smoothing, which are applied to regularise the inverse problem. Unlike many other algorithms, our optimization scheme employs explicit expressions to compute the sensitivities in $J$ (Zhou et al., 2012; Zhou and Greenhalgh, 1999).

Our inversion strategy closely follows the one described by Marelli et al. (2012). The FEFD forward solver employed in the waveform inversion code is significantly more sensitive to grid dispersion than the previously used FDTD code. Therefore, the FEFD forward grid was refined to a grid spacing of 0.125 m (FDTD: $dh = 0.5$ m), corresponding to more than 50 grid points per minimum wavelength. The width of the inversion cells was set to $dh_{inv} = 2.5$ m, which corresponds to half the minimum S-wave wavelength, i.e., the expected resolving capability of the inversion algorithm. To concentrate exclusively on the deleterious effects of data filtering, and not to be concerned with other issues such as the unknown source, we assumed all sources to be known as Ricker-type
wavelets with a central frequency of 100 Hz. The inversion frequencies were chosen accordingly between 40 and 150 Hz (see Table A.4). In this range we inverted for five groups of four frequencies each, starting with 40 and 70 Hz, and proceeding to higher frequencies, roughly following the “simultaneous approach” described by (Brossier et al., 2009). In order to stabilise the inverse problem, regularization in the form of damping was applied. This is equivalent to keeping the inversion result close to a preferred model (e.g. Maurer et al., 1998), which, in our case, is the model from the previous iteration. Within any given frequency group, damping was decreased from a large value ($\alpha^2$ equals 900 times the median diagonal value of $J^TJ$) to a small value ($\alpha^2$ equals 60 times the median diagonal value of $J^TJ$) with increasing iterations, reverting to a high damping value each time a new frequency group was used. As a starting model, we used a highly smoothed version of the true model, which approximates the model that could be obtained using simple traveltime tomography.

<table>
<thead>
<tr>
<th>Iterations</th>
<th>Inversion Frequencies [Hz]</th>
</tr>
</thead>
<tbody>
<tr>
<td>1 - 8</td>
<td>40, 50, 60, 70</td>
</tr>
<tr>
<td>9 - 16</td>
<td>60, 70, 80, 90</td>
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<tr>
<td>17 - 24</td>
<td>80, 90, 100, 110</td>
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<tr>
<td>25 - 32</td>
<td>100, 110, 120, 130</td>
</tr>
<tr>
<td>33 - 40</td>
<td>120, 130, 140, 150</td>
</tr>
</tbody>
</table>

Table A.4: The frequency schedule employed in the waveform inversions. Frequencies are chosen to approximately match the bandwidth of the synthetic data.

The effect of 3D-to-2D transformation is analysed by comparing the model space $NRMSD$ between the true and the reconstructed model for both the 2D-2D (i.e., inverting 2D synthetics with a 2D algorithm) and the 3D-2D (i.e., inverting filtered 3D synthetics with a 2D algorithm) case. Besides the $NRMSD$, which represents an averaged deviation over the whole modelling domain, we give the maximum deviations at and close to the low-velocity anomaly (see Table A.5). Together with the source and the receiver borehole regions, the low velocity zone is generally affected the most.
Table A.5: Deviations between the true model and the reconstructed model in the 2D-2D case (i.e. from 2D inversion of 2D data) and in the 3D-2D case (i.e. from 2D inversions of filtered 3D data). The NRMSD is normalised by the maximum velocity of the true model. Note that $x-x$ corresponds to an $x$-directed source and the wavefield component in $x$-direction. Maximum deviations are computed in the area of the low-velocity anomaly, where they are highest, while excluding the artefacts around the boreholes.

<table>
<thead>
<tr>
<th>Summary of inversion experiments</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Used wavefield comp. (src-rec)</strong></td>
</tr>
<tr>
<td>Inverted parameters</td>
</tr>
<tr>
<td>NRMSD in $V_p$ [%], 2D-2D</td>
</tr>
<tr>
<td>NRMSD in $V_p$ [%], 3D-2D</td>
</tr>
<tr>
<td>NRMSD in $V_s$ [%], 2D-2D</td>
</tr>
<tr>
<td>NRMSD in $V_s$ [%], 3D-2D</td>
</tr>
<tr>
<td>NRMSD in $V_p$ [%], 3D-2D with noise and inversion for source</td>
</tr>
<tr>
<td>Max. dev. in $V_p$ [m/s], 2D-2D</td>
</tr>
<tr>
<td>Max. dev. in $V_p$ [m/s], 3D-2D</td>
</tr>
<tr>
<td>Max. dev. in $V_s$ [m/s], 2D-2D</td>
</tr>
<tr>
<td>Max. dev. in $V_s$ [m/s], 3D-2D</td>
</tr>
<tr>
<td>Max. dev. in $V_p$ [%], 3D-2D with noise and inversion for source</td>
</tr>
</tbody>
</table>

**A.4.1 Acoustic Inversion**

As expected from the satisfactory fit between filtered 3D and 2D synthetic seismograms in the acoustic case (BAT), model reconstructions obtained by acoustically inverting these data match each other quite well. This can be seen from similar deviations between the true and the reconstructed models in the 2D-2D case and the 3D-2D case (see Table A.5). In both cases, the low-velocity anomaly has its magnitude overestimated by $\sim 300$ m/s compared to its true velocity of 1000 m/s (see Fig. A.7a).

**A.4.2 Elastic Inversion**

As a next step, we performed an elastic waveform inversion, using the elastic model BET and inverting the wavefield's $x$-component caused by $x$-directed sources for both $V_p$ and $V_s$, while fixing the medium's density $\rho$ at its true value. While both the 2D-2D and the 3D-2D elastic model reconstructions appear slightly sharper than in the acoustic
case (especially for the low velocity zone), we observe an inferior reconstruction of the background velocity and artefacts close to the source and the receiver boreholes. The large misfit between filtered 3D and 2D synthetic seismograms clearly propagates into the reconstructed $V_p$ model in the 3D-2D case (see Fig. A.7b). Interestingly, the $V_s$ model is much less affected than the $V_p$ model (see Fig. A.7c), i.e., the $V_s$ model exhibits comparable NRMSD values in the 2D-2D and the 3D-2D case (see Table A.5), which is most likely due to the shorter periods of the S-components of the wavefield.

Fig. A.7: Comparison of reconstructed velocity models obtained by acoustic (a) and elastic full waveform inversion of FDTD synthetics propagated for 15 source locations (denoted by the black crosses) and 60 receivers (denoted by the black dots) in model BAT and BET. The $x$- and $z$-component of the wavefield are inverted for both $V_p$ (b) and $V_s$ (c); or the $x$-component only is inverted for $V_p$ only (d). The true locations of the anomalies are indicated by the black boxes. The first row shows the reconstructed models obtained by inverting 2D synthetic data, the second row displays models obtained by inverting filtered 3D synthetic data. The last row corresponds to the difference of the former two.
We observe certain artefacts in the elastic 2D-2D model reconstruction, which were not present in the acoustic 2D-2D case (e.g., the fast anomaly close to the receiver borehole at a depth of ~120 m; see Fig. A.7b). They might arise from trade-offs between $V_P$ and $V_S$ in the inversion due to the higher number of free parameters as described for example by Manukyan et al. (2012). Since it is difficult to distinguish spurious features caused by parameter trade-offs from those caused by asymptotic filtering, we performed an additional experiment with the aim to isolate the effect of filtering. To this end, we inverted the $x$-component of the wavefield for $V_P$ only, while keeping $V_S$ and $\rho$ fixed at their true values (yielding an inversion with the same number of free parameters as in the acoustic case). The 3D-2D model reconstruction still exhibits significantly more spurious features than its 2D-2D counterpart, which we can now unambiguously attribute to poor 3D-to-2D filtering. In this elastic one-component / single-parameter type inversion (Fig. A.7d), the differences between the 2D-2D and the 3D-2D case are the largest amongst all inversion experiments (see Table A.5).

We performed two additional inversions (inverting either only the $z$-component or both the $x$- and the $z$-components simultaneously for $V_P$ and $V_S$) and summarise all results in Table A.5. Since the results of the additional inversions are very similar to the previous experiments, we do not show them here.

In order to evaluate the significance of the filtering error in the more severely affected elastic case relative to other causes of error in real data, we repeated the inversion experiment on the $x$-component data for $V_P$ with 10% random (white) noise added to the seismograms. Furthermore, we assumed the source wavelets to be unknown and inverted for them using the technique described in Maurer et al. (2012). Whilst the reconstruction of the anomalies is only negligibly affected, the artefacts around the boreholes and in the background medium are mildly increased (compare Fig. A.7d, second row, with Fig. A.8), resulting in a slightly larger $NRMSD$ (see Table A.5). We infer that even in the presence of realistic levels of data noise and unknown source wavelets, the error introduced by poor 3D-to-2D transformation (difference between Fig. A.7d, first and second row) is significant – at least in the elastic case.
A.5 Discussion

As reported above, the stochastic model SAT seems rather forgiving in terms of filtering error and we speculate that this observation reflects that stochastic media – depending on their spatial wavelengths and statistical properties – can in some situations act as an effective homogeneous medium. This may rectify (straighten) the overall ray geometry and play in favour of the straight-ray assumption, which is implicit in the data transformation. The errors that we observe for our block models are generally higher. A trace-by-trace comparison of errors revealed that most of this increase originates from relatively high discrepancies at traces situated behind the low velocity zone, at which two arrivals overlap. This may be explained by the fact that low velocity zones tend to "compress" the wavefield, resulting in a higher amount of interference, while the high velocity zone rather "stretches" out the wavefield and separates events. For central receivers, the ray path is more or less straight and observed errors are relatively moderate (see the sample trace in Fig. A.3c).

When full elastic treatment and directed sources are considered, direct S-arrivals and mode conversions into different elastic phases render the wavefield much more complex, with severe interference occurring between P- and S-waves. Due to the high degree of phase modification and due to interfering and overlapping events, the filtering
errors for the elastic models SET and BET increase significantly compared to what we observe for their acoustic counterparts.

We regularly observe higher discrepancies at low frequencies, whereas at higher frequencies, the amplitudes tend to match each other better. Most likely, this reflects the inherent high frequency assumption in the 3D-to-2D transformation filter. Another reason might be that lower frequency components diffract more easily around obstacles and deviate stronger from direct ray paths, thus violating the straight-ray assumption more acutely. The fact that the low frequency end seems to be affected more severely, is particularly concerning because the low frequency components are of high importance in the optimization process, and their absence is known to exacerbate difficulties related to entrapment in local minima.

In our inversion experiment we excluded further sources of uncertainty – such as a deficient starting model and deviations from a real 2.5D geometry – making our inversion study a best case scenario. It is important to recognise that the investigated asymptotic filtering errors represent only one of multiple sources of error in the inverse problem, and its relative importance requires careful consideration.

When inverting real data, the usual procedure is to employ the waveform fit of the synthetic response computed for the final velocity model against the input data as a measure of the quality of the inversion result. As our experiments are synthetic in nature we investigate waveform misfits between our FDTD input data and FEFD synthetics for the velocity model corresponding to the last iteration. In our acoustic experiment, the waveform misfits in the 3D-2D case (17.5%) are only slightly larger than in the 2D-2D case (15.3%) but in both scenarios misfit values significantly exceed the filtering error (8.6%). Contrary, the filtering error in the elastic case (30.0%) is significantly larger than the waveform misfits (11.1% in the 2D-2D case and 21.8% in the 3D-2D case). This confirms our conclusion that filtering is a viable strategy in the acoustic case, but has to be applied with caution in elastic situations. In the case of real-data application of 2D inversion algorithms, one could think about comparing the input data to 3D synthetics obtained from the last velocity model, which may allow an ad hoc examination of errors introduced by 3D-to-2D conversion.
To assess whether frequency-domain full waveform inversion algorithms may be capable to converge to a reasonable velocity model, whenever the difference between 3D and 2D wave propagation is neglected completely (i.e. no transformation filter is applied prior to inversion) we performed two additional inversions on unfiltered acoustic and elastic 3D data. Interestingly, the inversion works rather well in the acoustic block model case (with only slightly increased $NRMSD$ values of 5.1 % in the case of unfiltered data vs. 5.0% in the case of filtered data), but fails completely in the elastic case, yielding a model far from the true one (not shown). This is in agreement with our findings that the elastic case is much more susceptible to the errors made during filtering.

A.6 Conclusions

A critical evaluation of 3D-to-2D transformation using asymptotic filters has been performed by propagating 2D and 3D wavefields through 2D models, applying the correction, and comparing 2D to filtered 3D synthetic seismograms in the time and in the frequency domain. The average normalised RMS seismogram deviations ($NRMSD$) generally stay below an acceptable value of ~10% for purely acoustic cross-hole models. The filtering approach works particularly well in acoustic stochastic media. However, when full elastic treatment is considered, mode conversions (P to S, S to P) and energy leakage into different arrivals occurs, which highly complicate the wavefield and cause severe interference between P- and S-waves. This results in a considerably increased average $NRMSD$ of up to 30% for models such as the high contrast block model involving an x-directed source.

Several full waveform inversions were performed on a model comprising a low- and a high-velocity block anomaly in a homogeneous background. The inversion results exhibited only marginal disparities between model reconstructions from 2D and filtered 3D data in the case of purely acoustic modelling and inversion. In the elastic case, the filtering error in the data space propagates to artefacts in the model space. This error is significant compared with errors that stem from random noise in the data or an unknown source wavelet, as has been shown in a corresponding inversion test.
Nevertheless, even in the presence of noise and assuming an unknown source wavelet, the inversion is stable and yields a reasonable velocity model.

There are several real-data examples of 2D full-waveform inversion using the simple asymptotic filter approach that have produced appealing high-resolution models of the subsurface. Those are in better agreement with independent geological and other geophysical observations than images derived from classical ray theory. Together with the surprisingly good performance of the filter in simple situations, as reported above, we regard those successful studies as a confirmation of the general applicability of the conventional asymptotic filter approach. Two-dimensional full waveform inversion in combination with filtering seems to be an acceptable strategy, as long as (i) the true model is two-dimensional, (ii) the recording geometry is straight (no crooked line) and perpendicular to the strike of the structures, and (iii) only a small amount of S-wave energy is contained in the data (i.e., velocity contrasts are moderate and the source is explosive). The latter two conditions are generally met in exploration type marine seismic surveys at short offsets and in some cross-well applications employing explosive sources and non-directional pressure receivers. There, the acoustic approximation is generally valid.

Nevertheless, we have shown that in the elastic case, the asymptotic filters are less effective and we observe considerable waveform misfits and artefacts in the velocity models reconstructed using an elastic full waveform inversion code. Clearly, the practitioner has to weigh the harm due to the reported filtering errors against the numerous other sources of systematic errors that lurk – such as non-repeatability of the source, poor receiver coupling, a deficient estimation of the source-wavelet, 3D out-of-plane reflectors, and arbitrary surface topography – which are unavoidable in real-world situations and likely to be much more problematic.


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Since this is the last sentence, I assume that you, the reader, have read the whole thesis; this is great, thank you for your interest (even if only in parts of it)!
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