

Grid search inversion of teleseismic receiver functions

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SUMMARY

Reliable inversion of teleseismic receiver functions (RFs) for crustal and upper-mantle structure is difficult due to the non-linearity and non-uniqueness of the problem. We report here on an approach, based on the degrees of freedom in the signal, that produces models with similar complexity to the data. The approach mitigates the non-uniqueness and overcomes the difficulties of non-linear minimization. The method begins with an initial forward modelling exercise to determine layer numbers and inter-layer properties that are input to the grid search method. The grid search uses heuristics to reduce the search space size and yields a suite of acceptable models for the crustal and upper-mantle structure, based on a misfit measure derived from the pointwise uncertainties of the RF estimate. We compare our grid search method with a standard iterative inversion method, using data from the IRIS network station SACV, on Santiago Island in Cape Verde, to demonstrate the wider range of models our method can produce.

Key words: Body waves; Hotspots; Crustal structure.

INTRODUCTION

Teleseismic *P* waves that are incident upon the crustal section below a seismic station contain the combined effects of the earthquake source, the propagation through the medium and the instrument response and produce *P*-to-*S* conversions at crustal boundaries as well as multiple reverberations in the shallow layers. By deconvolving the vertical component from the radial component, the effects of the source, the far-field path and the instrument can be removed, leaving a signal composed of primarily *P*-to-*S*-wave conversions and reverberations below the seismic station. The result is known as the receiver function (RF; Fig. 1) (e.g. Phinney 1964; Burdick & Langston 1977; Langston 1977, 1979).

RFs have been used in numerous different geological settings to study crustal structure. Examples are: magma lenses within the crust (e.g. Sheetz & Schlue 1992), the Moho (e.g. Sheehan *et al.* 1995), the top of a subducting slab (e.g. Langston 1981) and other upper-mantle discontinuities (e.g. Kosarev *et al.* 1984). They have also been used to determine structure in several ocean island settings (e.g. Li *et al.* 2000, 2003; Collins *et al.* 2002; Leahy & Park 2005).

RFs are most sensitive to sharp velocity contrasts and, although studied using incident *P* waves, are most sensitive to the shear wave velocity structure beneath the station. The sensitivity to shear wave structure is due to the fact that at steep incidence, the *P*-to-*S* conversion amplitude is dominated by the large *P*-to-*S* impedance contrasts at layer boundaries (Ammon *et al.* 1990). They are inherently non-unique because of their sensitivity to the depth–velocity ratio, and therefore they contain little absolute velocity information.

Some constraints on absolute depths might be gained when reverberative phases can be identified in the waveforms (e.g. van der Meijde *et al.* 2003). Further constraints on absolute velocity and therefore depth may be obtained through the addition of *a priori* information (Ammon *et al.* 1990). However, a practical limitation in the application of *a priori* information in RF analysis results from the fact that the *P*-wave structure is usually known best, whereas *P* RFs are most sensitive to shear wave velocities.

Given typical crust and shallow mantle wavespeeds, an RF pulse emanating from a *P*-to-*S* (*Ps*) conversion at depth *h* kilometres appears at about *h*/10 s after the zero-lag peak. Thus, for crustal and shallow mantle structure studies, only the first 15 s or so of an RF contain direct *Ps* information. In view of the fact that broad-band seismological signals contain only about 1 degree of freedom per second of statistical information (Silver & Chan 1991), this suggests that there is very little independent information in RF traces.

This motivates a strategy for RF inversion. The previous reasoning suggests that only about 15 independent structural parameters may be constrained by a trace. What is a suitable way to parameterize them? We turn to geological reality to guide our choice. The crust is dominantly layered, comprising rock units ranging from metre to kilometre thicknesses. On the scale set by the wavelength of a 1 s teleseismic body wave, ~5 km in the crust, layer boundaries are essentially discontinuities. Therefore, a series of constant velocity layers, separated by boundaries where wave speeds and densities change, is a suitable model for crustal structure. For each layer, we require v_P , v_S , ρ and a thickness to specify its properties; each layer contains four degrees of freedom. Thus, the seismogram's total information content roughly translates into about four layers worth of information.

Material properties greatly constrain possible values for v_P , v_S , ρ , and thickness. We expect $5.8 \leq v_P \leq 9 \text{ km s}^{-1}$,

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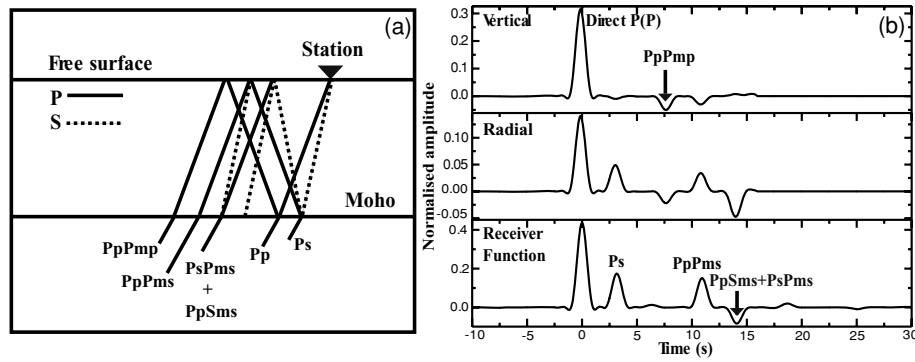


Figure 1. (a) Simplified ray diagram identifying the major P -to- S converted phases, which comprise the receiver function for a single layer over a half-space. (b) Vertical and radial synthetic seismograms and the corresponding receiver function calculated for a single layer over a half-space.

$1.6 \leq v_P/v_S \leq 2$, ρ to depend on a Nafe–Drake or Birch's Law relation on either v_P or v_S , and layer thickness to be $1 \leq h \leq 50$ km. Discretizing these ranges into perhaps five intervals leads to about 125 choices per layer, and 1×10^{10} possibilities for all four layers. This is a rather large space to explore, but heuristics can reduce its breadth substantially. The first heuristic is the structure of the RF itself; this gives rise to three primary pulses per layer: the Ps , $PpPs$ and $PsPs$ arrivals (see Ammon *et al.* 1990, for notation). This structure makes a rough assessment of the number of layers fairly easy and the time lags between the Ps arrivals from different layers determinable. These lags, along with a layer's v_P and v_S , now completely specify the layer thickness for a given slowness p . Thus, there are only two free parameters per layer, v_P and v_S . With this heuristic, among four layers, there are now about 10^5 possibilities to investigate. Consequently, grid search is feasible given present computer speeds.

The grid search method, we describe is based on a fast synthetic seismogram calculation step given a structure, processing with any standard RF estimation procedure from the synthetic, and evaluation of a misfit to a target RF. On account of the data characteristics in our data set, we use a multi-taper spectral correlation (MTC) of Park & Levin (2000) to calculate our RFs, but in practice, any RF method can be used.

The description of the grid search method follows in the following sections and is demonstrated using a synthetic test. Subsequently, we make a comparison between the models produced with this method and those produced using a standard inversion method (Ammon *et al.* 1990), to demonstrate the advantages of this new method.

METHOD

In routine processing, individual RFs are stacked. This process, either intrinsically (if time domain) or by jackknife (if frequency domain; see Efron 1982; Efron & Tibshirani 1986), yields a point-wise uncertainty for the RF estimate at either 1 or 2σ level. Thus, an acceptable fit of a synthetic RF must only fit within these bounds rather than rigorously reproducing the mean waveform. There may be many slightly different velocity–depth models that produce synthetic RFs satisfying this condition, with the grid search enumerating them at the chosen granularity.

The grid search begins with a simple forward modelling exercise to build an initial velocity–depth model, upon which to base the grid search. Initially, a two-layer velocity model is chosen, gradually building up the requisite number of layers to explain all of the arrivals in the first 10 s after the direct P arrival. This contains

the information on the shallow crustal and upper-mantle structure, which is of particular interest.

We use two heuristics to reduce the size of the search space. The first is the lag between successive Ps peaks, discussed earlier. This eliminates the need to iterate over layer thicknesses. The second is the relative amplitude ratio of the successive peaks, which dominantly depends on the interlayer v_S ratio (Julià *et al.* 2000). This allows one to transfer velocities in an overlying layer to the layer below. Densities are calculated either by velocity–density relations or impedance contrast from the overlying layer and not independently varied.

The grid search method presented here, like previous grid search methods (e.g. van der Meijde *et al.* 2003) allows Poisson's ratio to vary. However, unlike the previous methods, it also allows the P -wave velocity in the crust to vary too.

The pulses related to P -to- S conversions can be used to estimate the depth at which they were produced. For a plane wave arrival at any horizontal slowness p , the time lag Δt between the direct P arrival and the P -to- S conversion at the base of a layer of thickness h can be shown to be

$$\Delta t = h \left(\sqrt{v_S^{-2} - p^2} - \sqrt{v_P^{-2} - p^2} \right) \quad (1)$$

(Zhu & Kanamori 2000). Approximating to a zero-slowness arrival,

$$\Delta t = h \left(\frac{1}{v_S} - \frac{1}{v_P} \right). \quad (2)$$

v_P and v_S are the P - and S -wave speeds in the layer, respectively. Similarly, the lag accrued in any layer h_i between the Ps conversion at the base of the layer and the P wave at the layer's top (or the Ps conversion from the top) is

$$\Delta t_i = Ps_i - Ps_{i-1} = h_i \left(\frac{1}{v_{S,i}} - \frac{1}{v_{P,i}} \right). \quad (3)$$

Thus this equation (or the exact equation (1) that depends on slowness, if it is known) may be used with the constraints of the model determined using forward modelling to produce a grid search of other possible models that match the observed data. The initial forward model allows the number of layers to be determined and therefore the times and Δt_i for the Ps phases corresponding to the conversions at each of these layers. Whereas the amplitude of the Ps arrival is sensitive to the S -wave velocity contrast across the boundary, the amplitudes of the multiples are controlled by both the S -wave velocity and the density contrast, that is, the impedance contrast across the boundary (Julià 2007; Cassidy 1992). Thus, the forward modelling also provides the S -wave velocity contrast ratio

necessary to produce the amplitude of each P_s arrival. For example, in a three-layer case, a range of initial layer 1 P -wave velocities are used: 5.4–6.4 km s⁻¹ in 0.2 km s⁻¹ increments. Each layer will also have a range of v_P/v_S ratios, from 1.75–1.90 in 0.05 increments. For layer 1, the P -wave velocity and v_{P1}/v_{S1} for that layer in this iteration are used to calculate the S -wave velocity. These values are then used with the Δt between the direct P and the first P_s arrival, to calculate the depth to the layer. The S -wave velocity contrast ratio from forward modelling between layers 1 and 2 is used with the layer 1 S -wave velocity to give the layer 2 S -wave velocity, which uses the v_{P2}/v_{S2} for this iteration and layer 2, to calculate P -wave velocity. As with layer 1, these values are used with Δt (where in this instance, Δt is the time difference between the P_{S1} arrival and the P_{S2} arrival), to calculate the thickness of the second layer. Layer 3, begins as layer 2, with the S -wave velocity contrast and the S -wave velocity for layer 2 producing the S -wave velocity for layer 3 and so on, as for layer 2, etc.

Finally, the density in each layer is calculated using standard velocity–density conversions. Where forward modelling suggests density may vary differently to these standard relations, different conversions may be used in the grid search. The density relation for the crustal layers used in this study is $\rho = 1.72 + 0.337 \times v_S$ (Christensen & Salisbury 1975) and for the mantle layers, $\rho = (v_P + 1.87)/3.05$ (Birch 1961). Another relation used in structural inversions from RF waveforms (Ammon *et al.* 1990) is $\rho = 0.77 + 0.32 \times v_P$ (Berteussen 1977).

Misfit function

The grid search produces a suite of possible models that produce synthetic RFs to match the data. However, to determine the acceptable models requires a choice of misfit function. A misfit function provides a way of quantifying the disagreement between the observations and each synthetic RF within a tolerance, which is a level of misfit that is considered to be acceptable, so that when a model achieves that level, it may be said that the model adequately honours the demands of the measurements and, thus, is acceptable (Parker 1994).

In trying to match interacting waveforms, the best error function is the L2 norm (Mellman 1980); thus, the statistic used here to determine the misfit is chi-squared (χ^2):

$$\chi^2 = \frac{1}{\sum w(i)} \sum_{i=1}^N w(i) \times \left[\frac{d(i) - s(i)}{\sigma(i)} \right]^2, \quad (4)$$

where N is the total number of data points, $d(i)$ are the observed RF value and pointwise uncertainties $\sigma(i)$ and $s(i)$ are the synthetic ones. This gives a simple objective way to compare models: the model with the smallest value of χ^2 is the best model. To emphasize the importance of the direct P arrival at 0 s and the following 10 s, we apply weighting to the χ^2 values in the form of an exponential envelope and calculate the χ^2 between –2.5 and 15 s only. The envelope is chosen such that there is a maximum weight of 1 at 0 s, decreasing to 0.32 at –2.5 s and 0.41 at 15 s. The weighting is calculated as follows: $w(i) = \exp(-|t|/2.2)$ for t less than 0 s

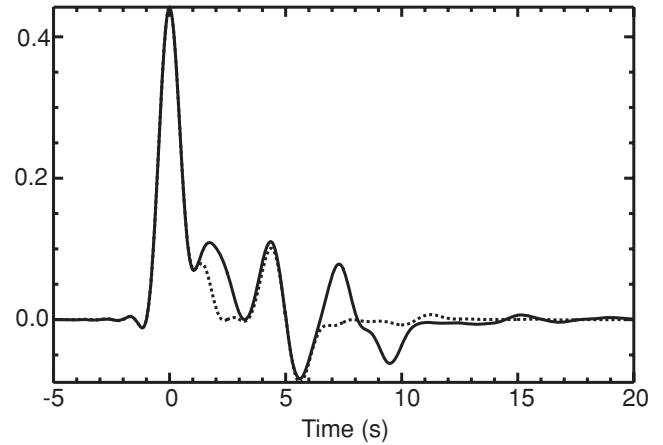


Figure 2. Synthetic ‘data’ receiver function to be modelled in the synthetic test, generated from the three-layer model shown in Table 1 (black line). Also shown is the synthetic receiver function generated by the top two layers of the three-layer model (dotted black line).

and $w(i) = \exp(-|t|/16.6)$ for t greater than or equal to 0 s. The final χ^2 value is then weighted by the $\Sigma w(i)$. This weight acts to increase $\sigma(i)$ for ‘unimportant’ parts of the waveform.

The $\Delta\chi^2$ statistic (Press *et al.* 1986) is used to determine the range of models that produce synthetic RFs within a 95 per cent confidence interval of the best fitting synthetic. $\Delta\chi^2$ is distributed as χ^2 with ν degrees of freedom given by the adjustable parameters in the grid search. These are: topmost layer P velocity, $v_{P,1}/v_{S,1}$; h_1 and $N - 1$ layers of $\{v_{P,i}, v_{P,i}/v_{S,i}, h_i\}$. They yield $\nu = 3 + 2(N - 1) = 2N + 1$ degrees of freedom.

Synthetic test of the grid search method

With our focus on the first 10 s of the data, and an oceanic rather than a continental setting, we use a three-layer model (Table 1) with layer thicknesses such that multiples arrive in the first 10 s. The synthetic RF produced by this model is shown in Fig. 2. This is the RF we wish to reproduce following our grid search method and shall be referred to as our synthetic ‘data’ RF. Also shown is the RF corresponding to the upper two layers of our three-layer model, to demonstrate how models would be built through forward modelling for real data. If our RF was generated from real data, we would not know how many layers contributed to the arrivals in the first 10 s, and therefore we would use forward modelling, beginning with a two-layer model and adding layers until all the arrivals have been modelled. For example, if we take the top two layers of our model in Table 1, then the synthetic RF this generates, produces a P_s arrival at ~1.2 s from the layer 1–2 boundary (this produces the shoulder on the direct- P in the three-layer model) and prominent multiples at ~4.5 and ~5.5 s. To then model the prominent peak at around 2 s, we add a third layer, which produces a P_s arrival at this time, along with multiples at ~7 and ~9.5 s. Having established the number of layers and the times of the P_s arrivals, our first step for the grid search, the forward modelling is complete, and we may now use

Table 1. Three-layer velocity–depth model for synthetic test.

Layer number	v_P (km s ⁻¹)	v_S (km s ⁻¹)	ρ (g cm ⁻³)	Thickness (km)	Poisson’s ratio
1	6.0000	3.4682	2.6900	10.00	0.25
2	7.0000	4.0462	3.0100	8.00	0.25
3	8.0000	4.6243	3.3300	∞	0.25

Table 2. Synthetic test grid search parameters.

Layer number	v_P (km s ⁻¹)	v_S (km s ⁻¹)	Δt (s)
1	$4.8 \leq v_P \leq 6.4$ by 0.4	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$\delta t_1 = 1.22$
2	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$v_{S2} : v_{S1} = 1.17$	$\delta t_2 = 0.83$
3	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$v_{S3} : v_{S2} = 1.14$	

Note: ρ (g cm³) = $0.77 + 0.32 \times v_P$ for all layers.

our starting model and arrival times to generate our suite of models for the grid search. The grid search parameter ranges and heuristic constraints are listed in Table 2.

Initially, the grid search produces 625 models (1.8 million without heuristics), which show a range of velocities and depths. The velocity–depth models are used to produce synthetic RFs for comparison with the synthetic RF generated from our starting model. χ^2 values are calculated to determine the best fitting synthetic, and the range of acceptable models is found using a significance level of 0.05 (95 per cent confidence interval). Because the synthetic data is noise free, we simulated a standard deviation using a random number generator at a signal-to-noise ratio of 10 : 1 to calculate the χ^2 misfit. For this synthetic test, there are two acceptable models. Their associated RFs compared with our starting RF are shown in Fig. 3, together with the velocity–depth models. There are only minor differences between the synthetic and the grid search result arising from the granularity of the grid search not coinciding with the values in Table 1.

The velocity–depth figure (Fig. 3b) highlights a well-known aspect of RFs, namely that it is most sensitive to the v_S structure. The v_S structure of the best fitting models is the same and very close to that of the input model, whereas the v_P model exhibits more variation. Using this simple synthetic test, we have demonstrated the success of the grid search and the misfit statistics in determining a range of best fit models that produce synthetic RFs matching our ‘data’ RF.

For comparison, we now perform a synthetic test of the inversion method, using the three-layer velocity–depth model (Table 1), as

for the grid search, but expanded to 45 layers each of 2 km thickness, that is, the first five layers correspond to layer 1, the next four to layer 2 and the remaining 36 to layer 3. We follow the same procedure as will be used for the real data inversion, first determining an appropriate smoothness parameter, which we find to be 0.1, before performing two suites of 24 inversions, one adding cubic perturbations with a maximum velocity of 0.5 km s⁻¹ and the other 1.0 km s⁻¹, with a random perturbation component equal to 0.1 and 0.2 km s⁻¹, respectively. All inversions converged after five iterations. The velocity–depth model with the lowest χ^2 value, along with its associated RF, is shown in Fig. 4. No other models were within $\Delta\chi^2$ of this value. This synthetic test shows that the inversion is adding structure to the velocity–depth model that is not required by the data. In particular, complexity is added near sharp boundaries and where there are few RF waveform constraints on the structure.

Application to real data

The data used here are from the GSN station SACV, on Santiago Islands, Cape Verde, and formed part of a wider study using data from a 2-yr passive deployment in the Cape Verde Islands (Lodge & Helffrich 2006). Here, the only prior seismic information consisted of a seismic refraction survey among three islands of the archipelago (Dash *et al.* 1976) and an offshore seismic reflection survey (Ali *et al.* 2003). This description follows the supplemental material of Lodge & Helffrich (2006), with amplifications.

The SACV data (Fig. 5) exhibit several prominent features that guide modeling. Fig. 5(a)–(d) show the forward modeling steps as the number of layers are increased. The direct P arrival at 0 s has a shoulder indicating a P -to- S conversion at ~ 1.2 s. A P -to- S conversion at this time produces multiples that correspond to the peaks at ~ 4.5 and ~ 5.5 s (Fig. 5a and Table 3; M1).

Although this two-layer model matches the amplitudes of both the P s and the multiple arrivals, it provides no explanation for the presence of the positive peak at ~ 2.2 s. To model this arrival as a P -to- S conversion requires the introduction of a deeper layer with a velocity increase across this new boundary because it is a positive peak. With a three-layer model, not only can this arrival be modelled, but it produces multiples that approximately correspond

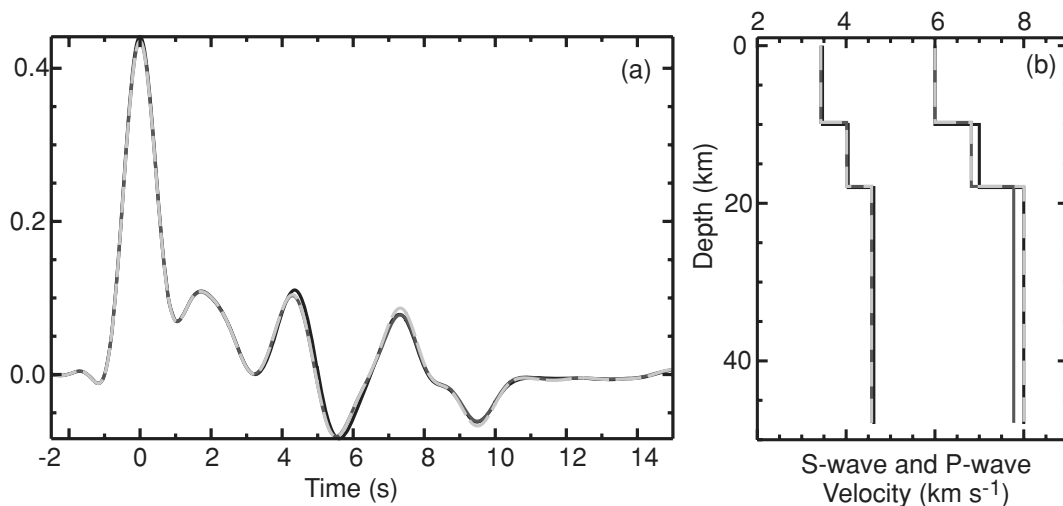


Figure 3. (a) The two best fitting synthetic RFs (dark grey line and dashed light grey line) to the synthetic ‘data’ RF (black line), as determined by the misfit function. (b) Velocity–depth models for the two best fitting synthetic RFs (dark grey line and dashed light grey line) and the ‘input’ velocity–depth model (black line).

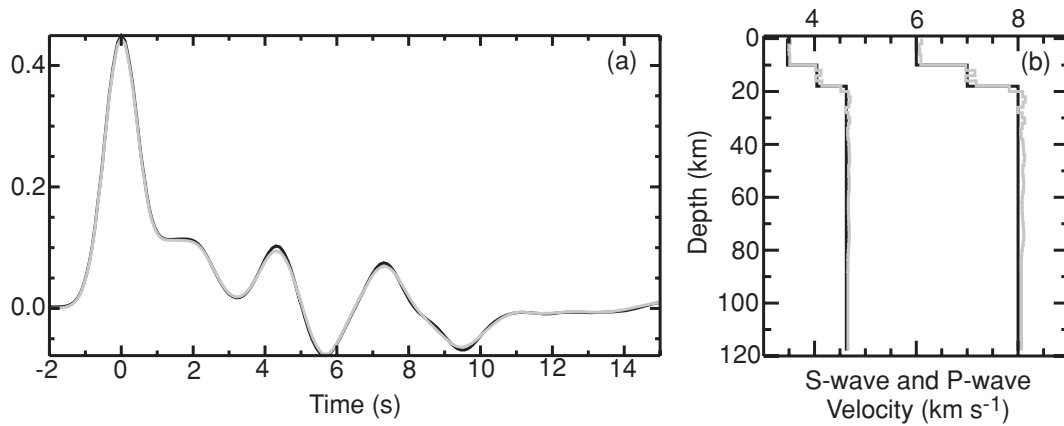


Figure 4. (a) The best fitting synthetic RF from the inversion modelling (grey line) to the synthetic ‘data’ RF of a 45-layer model (black line), as determined by the misfit function. (b) Velocity–depth model for the best fitting synthetic RF (grey line) and the ‘input’ velocity–depth model (black line).

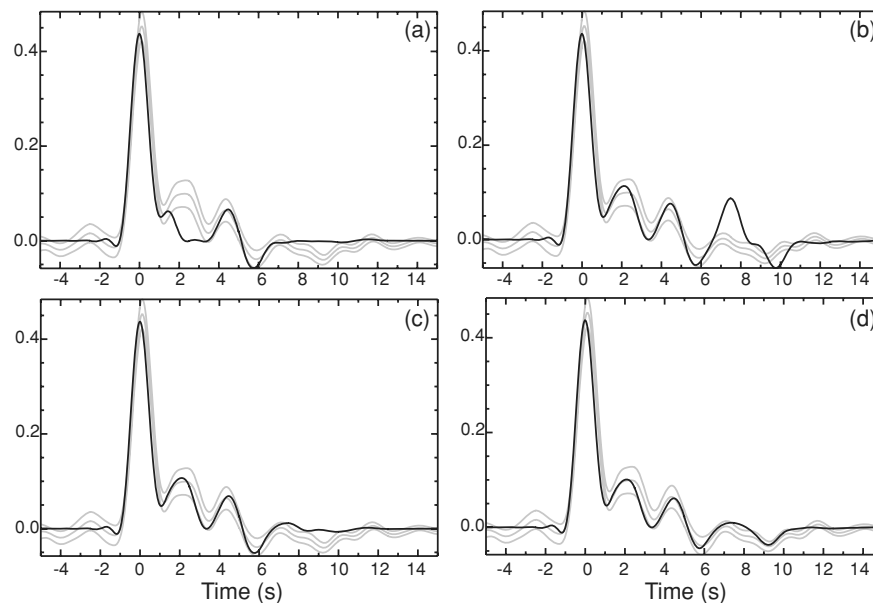


Figure 5. Forward modeling steps for Santiago island (SACV). Grey lines are the data and $\pm 2\sigma$ bounds, and the black line is the best fitting synthetic RF. (a) Best fitting synthetic RF for a two-layer model. (b) Best fitting synthetic RF for a three-layer model. (c) As (b) but with a density decrease in layer 3. (d) Best fitting synthetic RF for a four-layer model.

to the positive and negative arrival at ~ 7.5 and ~ 9.5 s, respectively (Fig. 5b and Table 3; M2).

This three-layer model clearly reproduces the timing of arrivals well, and the P_s amplitude, but not the multiple amplitudes. The amplitude of the multiples may be better modelled by reducing the density in layer 3 from 3.27 to 2.7 g cm^{-3} , while all other parameters are held constant (Fig. 5c). This leaves only the prominent negative arrival at around 9 s to be modelled. In RF analysis, a velocity inversion across a boundary produces a negative P_s arrival. If we introduce a velocity decrease from layer 3 into a layer 4, then the synthetic RF matches the data well (Fig. 5d, Table 3; M3). This four-layer velocity–depth model is used as the starting model for the grid search, with constraints tabulated in Table 4.

Initially, the grid search produces 9375 models, which show a range of velocities and depths. However, any models with a $v_p > 9 \text{ km s}^{-1}$ are excluded, as these velocities are not physically viable in the depths being considered here (Gudmundsson & Sambridge 1998). The velocity–depth models are used to produce synthetic

RFs for comparison with the data. Chi-squared values are calculated to determine the best fitting synthetic (Fig. 6), and the range of acceptable models is found using a significance level of 0.05 (95 per cent confidence interval). For Santiago, there are 317 acceptable models, the mean best fitting model is shown in Table 5, with the range of possible velocity–depth models shown in Fig. 7.

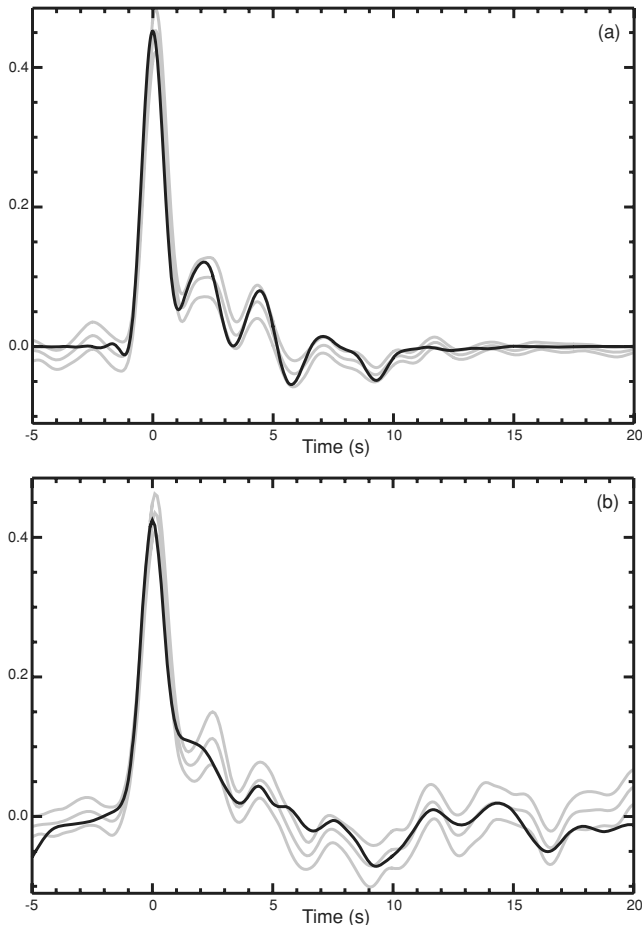
The densities derived in this methodology are potentially biased to low values because the inter layer v_s ratios in layers 1–3 are fixed to force the synthetic RFs to match the corresponding P_s amplitudes in the data. The densities derived from the density–velocity relation in each layer do not reflect the uncertainty in the P_s amplitudes. Furthermore, although Poisson’s ratio was allowed to vary, the range of acceptable velocity–depth models contain Poisson’s ratio values in each layer that range from the minimum of 0.21 to the maximum of 0.29, set up in the initial parametrization of the grid search. Thus, we cannot constrain Poisson’s ratio in any of the four layers, in agreement with previous RF studies, where the effect of Poisson’s

Table 3. Velocity–depth models for Santiago.

Layer number	v_P (km s ⁻¹)	v_S (km s ⁻¹)	ρ (g cm ⁻³)			Thickness (km)			Poisson's ratio
			M1	M2	M3	M1	M2	M3	
1	6.0000	3.4286	2.8754	2.8754	2.8754	10.1	10.1	10.1	0.25
2	6.8400	3.8889	3.0306	3.0306	3.0306	∞	8.0	8.0	0.25
3	8.1000	4.6286	–	3.2689	2.7000	–	∞	70.0	0.25
4	7.4700	4.2425	–	–	3.1497	–	–	∞	0.25

Table 4. Grid search constraints for Santiago.

Layer number	v_P (km s ⁻¹)	v_S (km s ⁻¹)	ρ (g cm ⁻³)	Δt (s)
1	$5.0 \leq v_P \leq 6.6$ by 0.4	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$0.337 \times v_S + 1.72$	$\delta t_1 = 1.26$
2	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$v_S : v_S = 1.12$	$0.337 \times v_S + 1.72$	$\delta t_2 = 0.89$
3	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$v_S : v_S = 1.19$	$\begin{cases} 1.06 \times (v_{S2} \times \rho_2)/v_{S3} \\ 1.16 \times (v_{S2} \times \rho_2)/v_{S3} \\ (v_P + 1.87)/3.05 \end{cases}$	$\delta t_3 = 6.48$
4	$1.65 \leq v_P/v_S \leq 1.85$ by 0.05	$v_S : v_S = 0.92$	$(v_P + 1.87)/3.05$	

**Figure 6.** (a) Data and $\pm 2\sigma$ bounds (grey lines) for the grid search modelling, with the best fitting synthetic receiver function from the grid search (black line). (b) Data and $\pm 2\sigma$ bounds (grey lines) for the inversion modelling with a 45-layer initial model, with the best fitting synthetic receiver function from the inversion (black line).

ratio has been determined (e.g. Sarkar *et al.* 2003; van der Meijde *et al.* 2003). These authors show that although the depth to the Moho is well constrained to ± 2 km, the Poisson's ratio can change from 0.2 to 0.3.

Overall, the grid search results suggest a crust thickened up to ~ 18 km depth overlying a high-velocity, low-density layer which overlies an LVZ at ~ 90 km.

Comparison of grid search with RF inversion

Our aim is to show that grid search yields similar structures to those retrieved using traditional inversion methods with real data as well as with synthetic tests. Consequently, we use the same data set as with the grid search, even though we do not know the actual subsurface structure. A successful outcome should show that the two methods yield similar structures given the same data. Hence, we use the same seismograms as used in the grid search. The inversion functions directly in the RF domain; so, we compute RFs from the seismograms using frequency domain division with a spectral water level (Langston 1979; Owens *et al.* 1983; Ammon *et al.* 1990), in contrast to MTC used previously.

A Gaussian width factor a of 1.5 was used, which lowers the frequency content of the signal, decreasing the importance of higher frequencies that may be due to scattering from small-scale heterogeneities. Generating the RFs with this method leads to only 31 RFs that are acceptable for generating the average azimuthal stack. However, the new average azimuthal stacked RF is remarkably similar to the one determined for the grid search, but for the increased amplitudes post 10 s (Fig. 6). The lack of amplitudes post 10 s above is a characteristic of the multiple-taper spectral correlation estimates method (Park & Levin 2000) and is not under investigation here. For an extension of the method that alleviates this problem, see Helffrich (2006).

The same initial model is used for the inversion as is used for the grid search (Table 3). It should be noted that the current inversion codes fix Poisson's ratio to 0.25, and density is always calculated using a standard velocity–density relationship ($0.32v_P + 0.77 = \rho$; Berteussen 1977). Thus, none of the final models may produce an unusually low-density layer, without also exhibiting an unusually

Table 5. Best-fitting four-layer velocity–depth model for Santiago.

Layer number	v_P (km s ⁻¹)	v_S (km s ⁻¹)	ρ (g cm ⁻³)	Thickness (km)	Poisson's ratio
1	6.2000	3.5429	2.9139	10.436	0.2576
2	7.4342	4.0185	3.0742	7.763	0.2936
3	8.8483	4.7828	2.7379	67.469	0.2936
4	7.2334	4.3839	2.9847	∞	0.2097

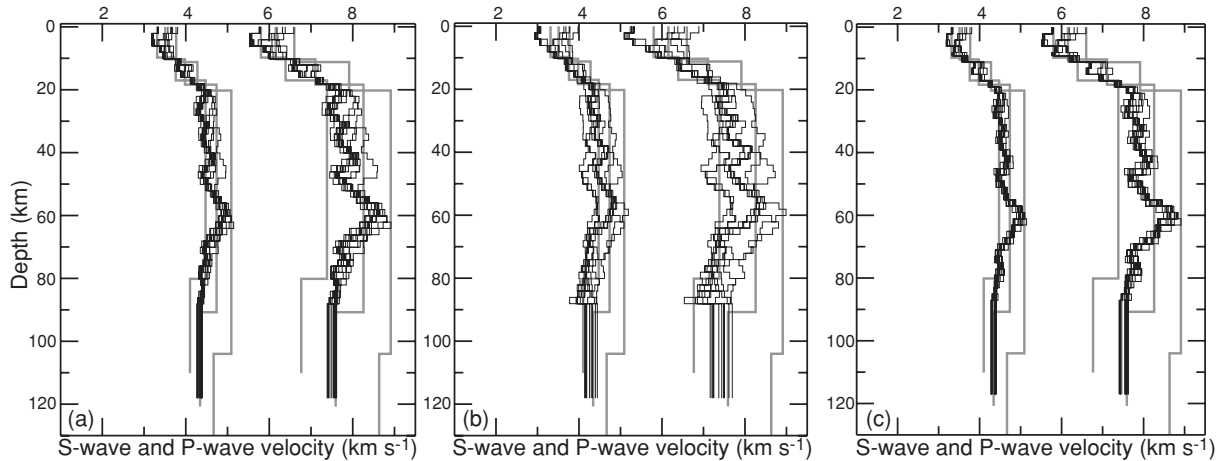


Figure 7. (a) Inversion 1: best fitting velocity models from the inversion (black lines) compared with the minimum, mean and maximum best fitting velocity models determined from the grid search (grey lines). (b) Inversion 2: best fitting velocity models from the inversion (black lines) compared with the minimum, mean and maximum best fitting velocity models determined from the grid search (grey lines). (c) Inversion 3: best fitting velocity models from the inversion (black lines) compared with the minimum, mean and maximum best fitting velocity models determined from the grid search (grey lines). In each panel, left-hand curve is S -wave velocity (v_S) and right-hand curve is P -wave velocity (v_P).

low velocity. The grid search results show that a range of Poisson's ratio are acceptable and, thus, do not constrain it within its initial boundary conditions. Therefore, using the approximately average value of 0.25 is probably not a bad approximation and should not affect the results adversely. In the inversion models, layer thickness and Poisson's ratio are fixed, shear wave velocity is varied, then Poisson's ratio is used with shear wave velocity to give P -wave velocity, and the P -wave velocity is used to give density. Once again, the χ^2 fit is used to determine the acceptable models.

As with any inversion, there is a trade-off between waveform fit and model smoothness. Model roughness is measured by summing the absolute amplitude of the velocity difference normalized by the number of layers used to compute the difference (second difference in this study) throughout the model. The waveform fit is taken from the rms residual. To estimate an appropriate value of the smoothness trade-off parameter, we inverted the waveform with 12 distinct values ranging from 0 to 1.1. Fig. 8 quantifies the trade-off between smoothness and waveform fit. Based on an analysis of Fig. 8, we chose a smoothness parameter of 0.2 to generate the smoothest models that adequately fit the data.

We performed two suites of 24 inversions, each with a smoothness parameter equal to 0.2 but with distinct sets of starting models. For each inversion, an initial model was computed by adding perturbations to the initial model used for the grid search (Table 3). Each of the total 48 inversions were allowed a maximum of five iterations, that is, sufficient iterations to produce a satisfactory fit to the data.

The 24 initial models for the first inversion were generated by adding cubic perturbations with a maximum velocity of 0.5 km s⁻¹ and a random perturbation component equal to 0.1 km s⁻¹ to the initial model used for the grid search. All 24 inversions in

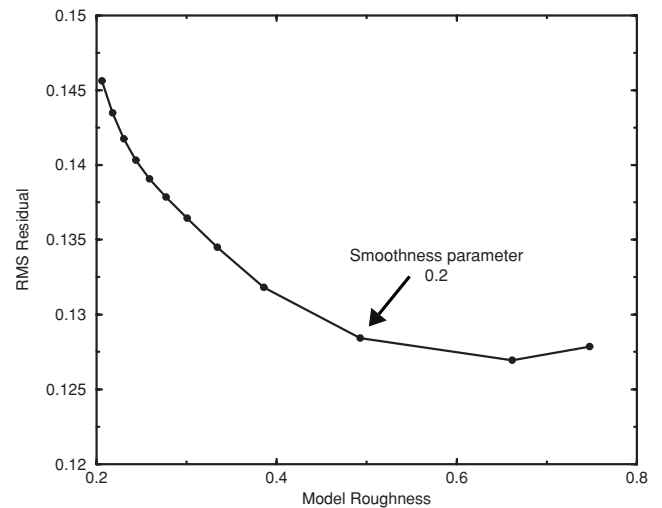


Figure 8. Smoothness/waveform fit trade-off for the 12 inversions with varying smoothness trade-off parameter. As the trade-off parameter increases, the model roughness decreases and the length of the residual vector increases. The 'knee' in the curve indicates the appropriate smoothness parameter to use for the inversions. In this example, it is 0.2.

this suite converged after five iterations. The 24 initial models for the second inversion were generated with a larger range of velocity perturbations, with 1.0 km s⁻¹ cubic perturbations and 0.2 km s⁻¹ for the random perturbations. Once again, all 24 inversions converged after five iterations. As with the grid search, χ^2 values were calculated for the fit of the synthetic RFs to the observed RF, and in this instance, none of the models produced a

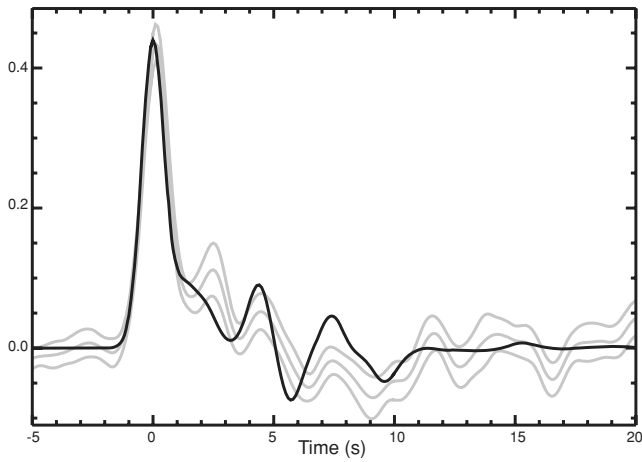


Figure 9. Data and $\pm 2\sigma$ bounds (grey lines) for the inversion modelling with a four-layer initial model (Table 3; M3), with the best fitting synthetic receiver function from the inversion (black line).

value within the $\Delta\chi^2$ range, as determined from the grid search models; that is, the inversion could not reproduce synthetic RFs that fit the observed SACV RF, as well as those produced from the grid search. To demonstrate this, the best fitting synthetic from the inversion for the four-layer model is shown in Fig. 9, which shows that the inversion is struggling to fit the prominent P_s arrival at around 2 s, while trying to minimize the amplitudes of the multiple arrivals at around 7.5 and 9.5 s. However, although an inversion for a simple four-layer model case could not fit the data as well as the grid search, often in inversions layer thicknesses are chosen to be relatively thin, which minimizes problems with layering parametrization in the inversion (Owens *et al.* 1984). Thus, to determine if the inversion cannot fit the data because of the small number of thick layers, the initial four-layer model was expanded into a 45-layer model (Table 6). This starting model is the same as the four-layer model, except that each layer has been broken down into 2-km-thick layers (except layer 1 which is 2.1, simply to keep the total thickness the same as the four-layer model).

This time, we performed three suites of 24 inversions, each with a smoothness parameter equal to 0.2 (determined from a trade-off curve of model roughness and waveform misfit as before) and with a distinct set of starting models for each suite. The first inversion as above has cubic perturbations with a maximum velocity of 0.5 km s^{-1} and a random perturbation component equal to 0.1 km s^{-1} added to the initial 45-layer model. All 24 inversions in this suite converged after five iterations. The second inversion, as before, has 1.0 km s^{-1} cubic perturbations and 0.2 km s^{-1} for the random perturbations, and again, all 24 inversions converged after five iterations. Finally, the third inversion suite assesses the layer boundary location influence on the final models by shifting them by 1 km (half a layer thickness). The 24 inversions converged after five iterations. All three suites of inversions produced synthetic RFs

with χ^2 fits lower than the best fitting synthetic determined from the grid search. However, some of these models had a $v_P > 9 \text{ km s}^{-1}$ and therefore, as with the grid search, were ruled out. This left 37 of the final 72 models left. The best-fitting synthetic RF is plotted with the average azimuthal stack and the $\pm 2\sigma$ bounds (Fig. 6b).

First, considering the fit of the synthetic RF to the data, we begin by considering the original forward modelling steps that determined the significant arrivals to be modelled. The shoulder on the direct P was the first to be modelled with the simple two-layer case and produced multiples at around 4.5 and 6 s. However, the inversion model is outside the $\pm 2\sigma$ bounds at this time. The prominent peak at ~ 2.2 s is not modelled as a peak, although the synthetic is within the bounds at this time. This smoothing of the first two P_s arrivals requires a reduction of the amplitude of the multiples at around 7.5 and 9 s. The amplitude reduction was achieved in the grid search through reducing density in the third layer. With the inversion, the reduction is achieved by making the boundaries between layers more gradational and smoothing the arrivals out. The aim here is to compare the two methods; so, it will simply be noted that the inversion fits well beyond 10 s, where the RFs used in the grid search method has no resolution. This overall analysis of the synthetic RF fit to the data is simply illustrated by considering the velocity–depth models for each of the inversion suites (Figs 7a–c). Each set of velocity–depth models is compared with the minimum, mean and maximum velocity and depth in each layer, determined from the grid search method.

The 14 models from inversion 1 show a maximum range of velocities comparable to those determined from the grid search method, although they tend to be lower than the mean velocity determined from the grid search. The notable exception to this is between 50 and 60 km depth, where the velocities increase up to almost the maximum value of the grid search before decreasing down to around 80 km depth. This behaviour seems likely to be controlled by the features in the synthetic RF, as discussed above. However, overall, the two methods show a remarkably similar velocity–depth structure, with an approximately 10-km-thick crust overlying crust thickened to around 18 km depth, then with a thick high velocity layer overlying a LVZ. In general, the inversion models do not need as high a velocity layer as the grid search, but it does overlie a LVZ. This velocity decrease also occurs at a shallower depth in the inversion models, but it is within the depth uncertainty provided by the grid search.

The 10 models from inversion 2 show much more variation than in inversion 1, but the overall shape is the same. The increase and decrease in velocity around 60 km are not as clear, and the low velocity values in the LVZ are extremely low for some models. However, overall once again the models are very similar to those produced by the grid search. Finally, the 13 models from inversion 3 are comparable with those produced from inversion 1, with the acceptable models clustering more tightly and, thus, exhibiting less extreme variation in each layer. Based on the similarity of the results of this inversion suite with those of suite 1, we conclude that the

Table 6. 45-layer velocity–depth model for Santiago.

Layer number	$v_P (\text{km s}^{-1})$	$v_S (\text{km s}^{-1})$	$\rho (\text{g cm}^{-3})$	Thickness (km)	Poisson's ratio
1	6.0000	3.4286	2.8754	2.1	0.25
2–5	6.0000	3.4286	2.8754	2.0	0.25
6–9	6.8400	3.8889	3.0306	2.0	0.25
10–44	8.1000	4.6286	2.7000	2.0	0.25
45	7.4700	4.2425	3.1497	∞	0.25

depth parametrization does not significantly affect these solutions. Evidently, the inversion technique produces velocity–depth models that agree well with those produced by the grid search technique. The linearized inversion, however, induces small-scale structure that the grid search suppresses at the same misfit level, as highlighted earlier with the synthetic inversion test (Fig. 4).

Gradational layers versus first-order discontinuities separating layers with anomalous density

Although the final results for the structure beneath SACV are very similar in their major features, regardless of whether the grid search or inversion technique is used, if we also consider the synthetic RF produced by these final velocity–depth models, then there are significant differences arising from the different ways in which each method deals with the low amplitude multiples produced by the layer 2–3 boundary.

The inversion uses gradational layers to reduce the amplitude, whereas the grid search technique uses a low density layer, that is, a reduction in impedance across the boundary, which in turn reduces the amplitudes of the multiples. The main difference between the gradient and the density solutions is that the gradient diminishes all amplitudes, whereas the density change principally affects those of the multiples. However, an arbitrary RF estimate might not yield as clear a preference for a density change as does SACV. In these cases, a further diagnostic should be used.

Cassidy (1992) showed that the amplitude of a P_s arrival created by a gradational boundary versus one created by a first-order discontinuity is dependent upon the frequency passband used to generate the RF. For $f < 1$ Hz, it is difficult to distinguish a discontinuity from a gradational zone up to 2 km thick; for $f < 0.5$ Hz this rises to ~ 3 km. Thus, broad gradational zones could be identified by comparing RFs generated using different a values. For example, Cassidy (1992) states that a gradational zone 5 km thick may be identified by an approximate doubling of the P_s amplitude for $a = 3$ relative to $a = 7$. We will now show that a density change does not lead to any frequency dependence of the results.

Using a simple two-layer model and keeping all parameters fixed except for the density in layer 2, we test three passbands, $a = 3, 5$ and 7 , corresponding to $f < 0.5, 1$ and 2 Hz, respectively (Fig. 10). This test clearly demonstrates that the amplitude decrease is not related to the frequency passband used. If modelling a RF estimate, anomalously low multiple amplitudes that are independent of frequency indicate that impedance constraints may be safely applied in a grid search for structure.

When we calculated the RF for SACV at different frequency passbands, we found no difference in the amplitude of the low amplitude multiples, thus, re-affirming our suggestion of the existence of a high-velocity, low-density layer beneath the island.

We next show how a model that contains a velocity gradient may be replaced by one with anomalous density variations. The example is from station RRRB from northern Scotland. This broadband station formed part of the SPICeD array (Kendall & Helffrich 2001). The data were used along with data from 33 other stations in the British Isles by Tomlinson *et al.* (2006) to investigate the onshore crustal and upper-mantle velocity structure there. Their study is complemented by the large number of offshore models of the velocity structure in this region.

The final velocity model (Tomlinson *et al.* 2006) has a Moho depth of ~ 25 km, overlying a gradational low velocity layer before a large velocity discontinuity at ~ 38 km. From their structural model, we calculate a synthetic RF using $a = 3$ for the Gaussian function (Ammon 1991), with the resulting RFs, velocity and density models shown in Fig. 11. This figure shows that by simply varying the density, we can reproduce the gradational RF without the need for the complexity of gradational layers. Thus, the structure below RRRB may not include a gradational layer. Coupled with our studies of the frequency dependence effect on RFs from models with anomalous density values versus the Cassidy (1992) study of frequency dependence on RFs from gradational models, we suggest that further investigations of the data from this station could differentiate between the two possibilities.

DISCUSSION AND CONCLUSIONS

The synthetic test of the grid search method demonstrates the ease and success with which this method may be applied, along with the importance of the misfit statistics. Using the input velocity–depth model in Table 1, we produce a synthetic ‘data’ RF to be modelled. The forward modelling technique is demonstrated by showing how the heuristics apply to the synthetic. Although 1.8 million models are possible, heuristics reduce this number to 625, and their subsequent synthetic RFs are compared with the ‘data’ RF, using the χ^2 fit and the $\Delta\chi^2$ statistic. We show that just two models are acceptable within our defined tolerance. Although not exact matches for the input model, due to a range of Poisson’s ratio being tested that did not include the exact Poisson’s ratio of the input model, we show that, nevertheless, the grid search produces a very good fit to the data, in terms of both the fit of the synthetic RFs to the data RFs and, also, the similarities in the velocity–depth model. The success of the

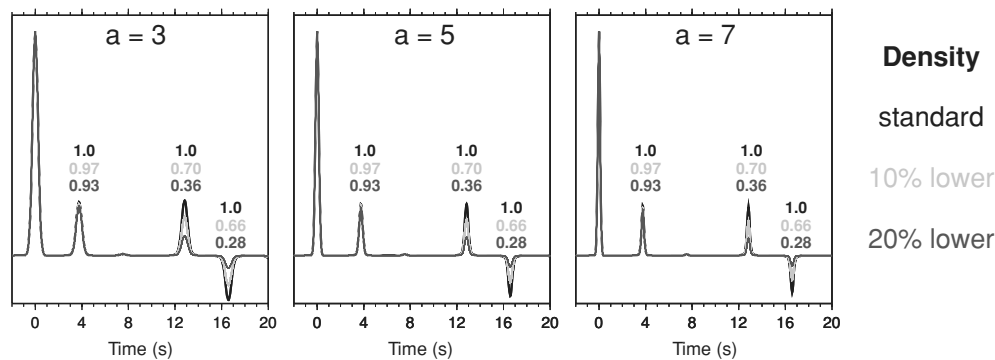


Figure 10. Synthetic test of varying layer 2 density while keeping all other parameters fixed in a two-layer model, for three frequency passbands, $a = 3$ ($f < 0.5$), 5 ($f < 1.0$) and 7 ($f < 2.0$). The numbers beside the P_s arrivals and associated multiples represent the amplitude relative to the P_s and multiples generated for a model using a density from a ‘standard’ velocity–density relation (black line).

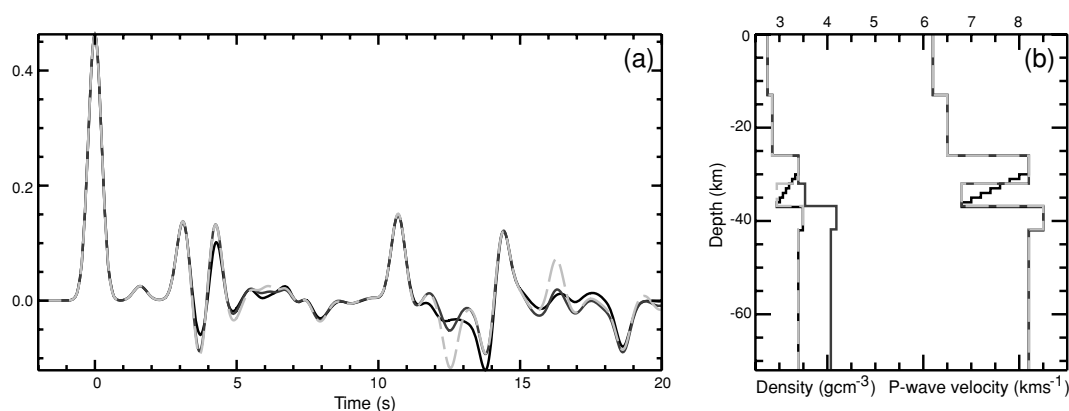


Figure 11. (a) RFs for RRRB station synthetic test. Gradational model of Tomlinson *et al.* (2006) (black line), model with a first-order discontinuity at 32 km depth (dashed light grey line) and model with a first-order discontinuity at 32 km depth and higher than ‘normal’ densities in the layers below the new first-order discontinuity (dark grey line). Note the reduction in multiple amplitude at 12.5 and 16.5 s. (b) Velocity- and density-depth models for the RFs shown in part (a).

synthetic test leads us with confidence to the comparison between this new grid search technique and the inversion technique.

One of the important differences between the grid search method and the inversion technique is that it allows the researcher to determine which are the important prominent arrivals and then to concentrate on modelling them. The inversion technique, on the other hand, trades off model roughness with fitting more details in the waveform. Although the approach does not eliminate first-order discontinuities in the model, it produces overall smoother velocity profiles. They are, however, more complexly structured and hinder insights into the structural features implicit in the RF. Results from Ammon *et al.*’s (1990) investigation of the inversion technique indicate that starting models with little similarity to the true velocity structure produce reasonable solution waveforms with reasonable solution models, something that is clearly not true for the grid search approach, which requires forward modelling to determine the number of layers in the model. However, Ammon *et al.* (1990) observe that slow initial models (average velocity is low relative to the true solution) tend to converge to slow solution models and fast initial models tend to converge to fast solution models. This, on the other hand, is not a problem for the grid search, which produces a range of models, both slow and fast; and it is simply whether or not the synthetic RF is within $\Delta\chi^2$ that is important. Overall, upon investigating their technique, Ammon *et al.* (1990) find that due to the velocity–depth trade-off, they get large suites of acceptable models that often cluster in low-, mid- and high-velocity families and suggest that a method of ruling out some of these models is the use of *a priori* information. This brings us back to the initial premise for developing the grid search method. In regions where there is no *a priori* information and the aim is to develop a simple model for the crustal and upper-mantle structure, is the inversion technique appropriate or should the grid search method be used as an alternative? Our preference is to eschew excessive structural details in this case. The sparingly parameterized grid search yields simple models that capture the information in the RF to deliver a generalized structure.

The structures determined from the same data sets are similar for the two methods: grid search and RF inversion. However, the grid search allows extra parameters or constraints to be easily added and returns a solution that is close to the data’s degrees of freedom, in number. It also allows for less restrictive density parameterizations. These factors yield better fits (in the χ^2 sense) of the prominent early

arrivals in the RF and fit the later low amplitude multiples better. In contrast, the fixed velocity–density relation and the use of many thin layers lead to large undulations in the structure that overfit the data, in a statistical sense, but that retains similar structural features to the grid search estimate, for example, for SACV, a two-layer crust overlying a fast, shallow mantle, with very similar wave speeds in the crustal layers. Further investigation of the frequency dependence of the RFs produced by gradational layers versus models with first-order discontinuities and anomalous density layers shows that the former produce RFs that are frequency-dependent (Cassidy 1992), whereas the latter are frequency independent. Although more care is required developing the initial model for the grid search, inversion requires a similar effort to construct an initial model suite and then perturbation of the final models to ensure that the solution space is adequately explored. Finally, grid search structures, being inherently parsimonious, are simpler to interpret. In poorly known areas like Cape Verde, where *a priori* constraints are few, the grid search method provides a straightforward way to estimate structure.

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