Least-squares fitting of marine seismic refraction data

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Summary. An iterative procedure is presented for fitting waveform data from a marine seismic refraction experiment. The wavefunction from the explosive source is known and the crustal structure is refined using the damped least squares procedure. The damping parameter serves the dual purpose of stabilizing an under-constrained inversion and improving the linearity by suppressing high frequencies. The synthetic seismograms and their model differentials are calculated using the WKBJ seismogram method. Both the synthetic seismograms and the linear algebra are sufficiently straightforward that the computations can be performed on an array processor. The inversion procedure is then sufficiently rapid that interactive computations are possible. The technique is illustrated using the FF2 refraction data from the Fanfare cruise of the Scripps Institution of Oceanography. These data had been interpreted previously by trial-and-error using the reflectivity method. Starting from two different, simple models, the inversion procedure obtains essentially one unique model. Its features are very similar to the previous model.

Introduction

The use of synthetic seismograms in the interpretation of refraction data is now well established. Following the pioneering papers by Helmberger (1968) and Fuchs & Müller (1971), the Cagniard–de Hoop–Pekeris and reflectivity methods have been widely used to compute synthetic seismograms. Seismic models are refined iteratively to obtain a reasonable fit between the synthetics and data. In general the iterations have been determined by trial-and-error and the fit has been measured visually rather than quantitatively. While this procedure has been remarkably successful (e.g. Spudich & Orcutt 1980), it is usually extremely tedious and expensive. Recently some attempts have been made to automate the inversion process

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The overall objective of an inversion procedure using waveform data is to find the model parameters, \( m \), which minimize, in some sense, the difference between the observed data, \( d(t, x_i) \), and theoretical seismograms, \( u(t, x_j, m) \). In the most general case, the model parameters could include the velocity, density and attenuation structures, and the source location and mechanism. Normally, of course, we make the a priori assumption that some model parameters are well known or alternatively that some parameters are unimportant. For instance, in the example in this paper we are concerned with the P-wave velocity structure which we will assume to be one-dimensional (1-D). The source-time functions will be assumed known although variations in their amplitude and time will be considered. Other model parameters are ignored. In principle, the techniques described in this paper can be extended to more general situations including 3-D structures and unknown source mechanisms. The success of the procedure will obviously depend on the quality and quantity of data, and the efficiency of the numerical methods.

The method used to calculate the synthetic seismograms, \( u(t, x_j, m) \), depends on the data set, \( d(t, x_i) \), the model, \( m \), the information required from the inversion and computing considerations. In general, the parameterization of the model and the choice of synthetic method may be difficult. Only a few necessary conditions are known for whether a data set is compatible with a given model. For instance, travel-time curves can only take certain forms in laterally homogeneous models. Sufficient conditions for testing the compatibility of the data set and model parameterization are unknown. Normally, therefore, an a priori choice of model parameterization and synthetic method must be made. The adequacy of the model parameterization can only be judged by the success of the inversion. The adequacy of the synthetic method can either be determined on theoretical grounds or by comparison with a more accurate method. Conversely, the inversion may fail because the model parameterization is inappropriate, because the synthetic method is inadequate or because the data are too noisy.

For a given model, \( m \), virtually any method of calculating theoretical seismograms, \( u(t, x_j, m) \) is only approximate. This may be due to approximations deliberately made in the interests of efficiency, e.g. ray theory, or because of practical limitations in the numerical methods, e.g. finite difference methods. For instance, using the Cagniard–de Hoop–Pekeris method (Helmberger 1968), the model must be approximated by homogeneous, plane layers. Only a finite number of generalized rays can be included. Often to simplify the computations, the far-field approximation is made. Further approximations have been employed to increase the computational efficiency (Mellman 1980). Similarly with the reflectivity method (Fuchs & Müller 1971) homogeneous plane layers are usually used. No ray expansion is necessary but the synthetic seismograms are band-limited in horizontal slowness and frequency. While every effort should be made to minimize these inaccuracies, e.g. we should not use geometrical ray theory at caustics, in the real world we must always live with approximations. In some cases, while it is impossible to reduce these approximations, it may be known what effect they have on the theoretical seismograms. For instance, body-wave seismograms calculated using ray methods will only model a small time window of the full seismogram. Reflectivity and finite-difference seismograms will be band limited. End-point errors due to limited slowness windows will occur at known times. Before fitting the synthetic seismograms to the real data, it is naturally advisable to pre-process the data to reflect as far as possible the approximations and errors in the theory. Thus we fit \( u(t, x_j, m) \) to the modified data \( A \{ d(t, x_i) \} \) where \( A \) is the pre-processing or approximation
operator which mimics, as far as possible, any approximations made in \( u(t, x_j, m) \). For instance in the simplest case \( A[\ ] \) could be a windowing and filtering operation. More complicated procedures can be envisaged. Note, of course, we have to apply \( A[\ ] \) to the data because the inverse operator which could be applied to the theory, is unknown, unstable or meaningless.

In this paper, we assume that the WKBJ seismogram algorithm (Chapman 1978; Dey-Sarkar & Chapman 1978) is adequate for the calculation of synthetic seismograms. The numerical algorithm includes smoothing and later (equation 19) we shall describe the specific form of operator, \( A[\ ] \), employed. The choice of the WKBJ seismogram was motivated by the simplicity and efficiency of the algorithm which allows the 'differential' seismograms to be simply calculated in a reasonable computing time. For the example in this paper, we were able to test the accuracy of the synthetic seismograms against a more accurate method — the 'reflectivity' method (Fuchs & Müller 1971) — before proceeding with the inversion, as the waveform data had been interpreted previously (Spudich & Orcutt 1980). Normally, of course, this procedure would be impossible and we would have to test the adequacy of the WKBJ seismograms periodically during the inversion using a more accurate but expensive method. Others (Brown 1982, 1983; Shaw 1983, Given & Helmberger 1983; Shaw & Orcutt 1985) have also used WKJB seismograms in inversion procedures. The theory is summarized in the next section.

It is clear that at sufficiently high frequencies, fitting seismic waveforms is a very non-linear problem. If the synthetic seismograms and the data contain narrow, high-frequency pulses that do not align, the operation of perturbing the model to increase the correlation between the data and synthetics is obviously non-linear. For small perturbations the pulses will still not align but suddenly for some finite perturbation the pulses will align and the fit will improve (Fig. 1a). We have not yet been specific about what we mean by a good fit but for the purpose of illustrating the strong non-linearity, the least squares difference between waveforms can be considered. How can we pseudo-linearize the problem? If the data and synthetic seismograms are filtered to remove the high frequencies, the pulses will broaden. Now the data and synthetic seismograms will overlap. Perturbing the model will shift the broad pulses slightly and alter the fit (Fig. 1b). Thus, provided the low-frequency components of the data are used, the system is pseudo-linear. As the fit improves and the model

![Figure 1](https://academic.oup.com/gji/article-abstract/82/3/339/606013/1)

Figure 1. An example of fitting (a) broad-band and (b) narrow-band pulses. The solid curves are the data and the dashed curves are the theoretical seismograms which are shifted in time by \( \delta t \) until a good fit is obtained. The misfit \( \phi \), is defined in the text (25) and is zero for a perfect fit.
approaches the ‘correct’ one, the system becomes pseudo-linear for higher frequencies. In order to use linear perturbation theory we proposed originally to use only the low frequencies in the data and theory. As the correct model was approached the pass-band would be increased. Fortunately, we found that the damped, least squares method (Levenberg 1944) achieves the required low-pass filtering. In the sections following the WKBJ seismogram theory, we describe the misfit function used in the least squares method, the differential seismograms used in the linear perturbation theory, and the computational methods used to solve the damped, least squares problem. Finally we use the data from Spudich & Orcutt (1980) as an example of the procedure developed in this paper. They interpreted the waveform data using the reflectivity method and a trial-and-error procedure. Using the same data and the computational methods developed in this paper, we obtain essentially one unique model. We also investigate the effect of permitting perturbations to the relative amplitudes and times.

WKBJ seismogram

The so-called ‘WKBJ seismogram’ was introduced by Chapman (1976, 1978) and Dey-Sarkar & Chapman (1978). The basic theory has been given before so we will just give a brief outline. We follow the standard procedure of expanding the displacement and forces in vector cylindrical harmonics (Takeuchi & Saito 1972) to obtain an ordinary differential equation with independent variable, \( z \). The dependent variables are the displacement and traction harmonic coefficients which are continuous as a function of depth, \( z \), even at an interface (first-order discontinuity). The differential equation is solved with appropriate boundary and source conditions to find the harmonic coefficients at the receiver. Then the inverse Fourier and Bessel transforms are evaluated to obtain the displacement at the receiver. If we approximate the Bessel function by its asymptotic form (Abramowitz & Stegun 1965, equation 9.2.1) to obtain the far-field approximation, the inverse transforms can be written

\[
\mathbf{u}(t) = \frac{1}{2s^2/x^{1/2} \pi^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} -\omega^2 \left( \frac{\pi}{|\omega|} \right)^{1/2} \\
\times \exp [i \omega (px-t) + i \pi \text{sgn} (\omega)/4] p^{1/2} R(\omega, p, z) dp d\omega.
\]

(1)

The transformed response, \( R(\omega, p, z) \) is found from the solution of the differential equation and, of course, depends on the source terms. For notational simplicity we have rotated the cylindrical coordinate system so that the receiver is at zero azimuth. The source terms, e.g. the moment tensor components, used in \( R(\omega, p, z) \) are in this rotated coordinate system. Thus the azimuthal dependence of the solution is now included in the source terms and not through the Fourier series.

In order to use the WKBJ seismogram algorithm it is necessary to assume that the zeroth-order Langer asymptotic expansion (Chapman 1974) is valid in every layer and that the zeroth-order WKBJ asymptotic expansion (Richards 1971) is valid at every interface. In addition we assume that a ray expansion can be made at every interface (Kennett 1974). For acoustic or SH-waves, the complete ray expansion can be written in a compact form by grouping rays in kinematic and dynamic groups (Hron 1971, 1972; Chapman 1977). A similar expression has not been obtained for the complete ray expansion of the P-SV system. We have therefore adopted the following symbolic notation for the complete ray expansion
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response for the P-SV system:

\[
R(\omega, p, z) = \frac{1}{2(2\pi)^{3/2}} \sum_{\text{rays}} \left\{ q_{\alpha}^{-1/2} \left[ p^2 \hat{m}_{xx}(\omega) + q_{\beta}^2 \hat{m}_{zz}(\omega) \pm 2pq_{\alpha} \hat{m}_{xz}(\omega) \right] \right. \\
\times \left[ R_{ray}^{PP}(p) \exp \left[ i\omega T_{ray}^{PP}(p) \right] \right] u^P + R_{ray}^{PS}(p) \exp \left[ i\omega T_{ray}^{PS}(p) \right] u^S \\
+ q_{\beta}^{-1/2} \left[ p q_{\alpha} \left[ \hat{m}_{xx}(\omega) - \hat{m}_{zz}(\omega) \right] \pm \Omega_0 \hat{m}_{xz}(\omega) \right] \\
\times \left[ R_{ray}^{SP}(p) \exp \left[ i\omega T_{ray}^{SP}(p) \right] \right] u^P + R_{ray}^{SS}(p) \exp \left[ i\omega T_{ray}^{SS}(p) \right] u^S \right\} .
\]

The summation is over all possible rays where each ray is defined by the sequence of ray segments and reflection/transmission coefficients. We have divided the rays into four classes depending on the ray type leaving the source and the ray type arriving at the receiver. These types, P- or SV-rays, are indicated by the superscripts P and S. Thus the function \( R_{ray}^{PS}(p) \) is the product of all the reflection and transmission coefficients on a ray leaving the source as a P-ray and arriving at the receiver as an SV-ray. Similarly the function \( T_{ray}^{PS}(p) \) is the sum of all the phase terms for the ray.

We have assumed that the source can be represented by a second-order moment tensor. Remember that the moment components, e.g. \( m_{xx}(t) \) or its spectrum \( m_{xx}(w) \), are in the rotated coordinate system where the receiver is at zero azimuth, i.e. the receiver is in the \( x-z \) plane. The azimuthal dependence of the solution, i.e. the radiation pattern in the horizontal plane, arises from the transformation of the moment components in fixed geographic coordinates. Other terms evaluated at the source have a subscript zero. The alternative signs on the source terms depend on whether the ray is leaving the source downwards (upper sign) or upwards (lower sign). The \( z \)-axis is measured positive upwards. The notation for the horizontal slowness, \( p \), and the vertical slownesses, \( q_\alpha \) and \( q_\beta \), has been widely used and \( \Omega = q_\beta^2 - p^2 \).

The displacement vector is \( u = (u_x, u_z)^T \). The vectors, \( u^P \) and \( u^S \), are the basic vectors at the receiver. They are

\[
u^P = q_{\alpha}^{-1/2} \left( \begin{array}{c} p \\ \pm q_\alpha \end{array} \right) \quad (3a)
\]

\[
u^S = q_{\beta}^{-1/2} \left( \begin{array}{c} q_\beta \\ \pm p \end{array} \right)
\]

where the upper sign refers to an upgoing ray at the receiver and the lower sign refers to a downgoing ray. The reflection/transmission coefficients used in \( R_{ray}^{PP}(p) \) etc. must, of course, be with respect to these basic vectors. If the receiver is on a free surface we combine the incident and two reflected rays to obtain

\[
u^P = \frac{2q_{\alpha}^{1/2}}{\beta^2(4p^2 q_\alpha q_\beta + \Omega^2)} \left( \begin{array}{c} 2pq_\alpha \\ \Omega \end{array} \right) \quad (3b)
\]

\[
u^S = \frac{2q_{\beta}^{1/2}}{\beta^2(4p^2 q_\alpha q_\beta + \Omega^2)} \left( \begin{array}{c} \Omega \\ -2pq_\alpha \end{array} \right)
\]

In the example in this paper, the source and receiver are both in the fluid layer, i.e. the ocean. Thus only P-waves are possible at the source and receiver, and the source is restricted to an isotropic, pressure source. In order to simplify and abbreviate the following expres-
sions we will adopt these restrictions now. Nevertheless we should emphasize that all the
techniques can be applied to the more general expression (2). In the oceanic case, expression
(2) reduces to
\[ R(\omega, p, z) = \frac{m(t)}{2\alpha_0^2 (\rho \rho_0 q_0)} \sum_{\text{rays}} R_{\text{ray}}^{PP} (p) \exp \left[ i \omega T_{\text{ray}}^{PP} (p) \right] u^p \]  
(4)
where \( m(t) \) is the diagonal element of the moment tensor, i.e. minus the pressure volume
integral. Substituting expression (4) in (1), reversing the order of the integrals and summa-
tion, evaluating the frequency integral first, we obtain the WKBJ seismogram
\[ u(t, x, z) = -\frac{m''(t)}{2v^2 \lambda v^2 (\rho \rho_0) \alpha_0^2} \star \operatorname{Im} \left\{ \Lambda(t) \sum_{\text{rays}} \sum_{t = \Delta t} \frac{p^{1/2} R_{\text{ray}}^{PP} (p) u^p}{q_0^{1/2} \left| \partial_p T_{\text{ray}}^{PP} \right|} \right\}. \]  
(5)
The only further approximation made to obtain result (5) is to restrict the range of the
\( p \)-integral so \( T_{\text{ray}}^{PP} (p) \) is real (corresponding to travelling ray segments with no evanescent
parts). Apart from this restriction, the result remains valid whatever the form of \( R_{\text{ray}}^{PP} (p) \) and
\( T_{\text{ray}}^{PP} (p) \). The innermost summation is evaluated at solutions of
\[ t = \partial_{\text{ray}}^{PP} (p, x) = \Delta \]
(6)
The time series, \( \Lambda(t) \), has been defined by Dey-Sarkar & Chapman (1978).

Formally, expression (5) is the WKBJ seismogram. However, both the innermost sum-
mation and the time series, \( \Lambda(t) \), contain singularities and for numerical purposes we must
smooth these results. Then we obtain
\[ u_s(t, x, z) = -\frac{m''(t)}{2v^2 \lambda v^2 (\rho \rho_0) \alpha_0^2 \Delta t} \star \operatorname{Im} \left\{ \Lambda_s(t) \sum_{\text{rays}} \sum_{t = \Delta t} \frac{p^{1/2} R_{\text{ray}}^{PP} (p) u^p}{q_0^{1/2} \left| \partial_p T_{\text{ray}}^{PP} \right|} \right\}. \]  
(7)
where the subscript \( s \) indicates the smoothed time series. The innermost summation in
expression (5) has been smoothed by a boxcar \( 2\Delta t \) long. The summation and integral in
expression (7) are evaluated by summing the integrals over all intervals defined by
\[ t = \partial_{\text{ray}}^{PP} (p, x) \pm \Delta t. \]  
(8)
To evaluate the convolution operator, \( \operatorname{Im}[\Lambda_s(t)] \), we use a rational approximation for a
smoothed version of the analytic series. Details of the rational approximation can be found
in Chapman & Drummond (1982). The analytic time series, \( \Lambda(t) \), is smoothed three times
by a boxcar \( 2\Delta t \) long before the rational approximation. Thus overall the expression (5) has
been smoothed by a boxcar four times to obtain (7). This smoothing must be included in the
approximation operator, \( A \), applied to the experimental data.

The source and receiver
The source terms in expressions (2) and (5) can either be determined theoretically, by direct
observation at a range where complications due to the propagation are minimal, or as part of
the inversion scheme. In this paper we use a theoretical source function. The explosive
source function has been used successfully by Spudich (1979) and Spudich & Orcutt (1980).
It is essentially the same as that used by Helmberger (1967, 1968) which was based on the
work of Arons (1948, 1954) and Weston (1960). It is described in some detail in appendix A of Spudich & Orcutt (1980). It depends on the shot weight and depth which vary for different ranges. We denote the different ranges by \( x_i \) and for simplicity write the appropriate source function, calculated according to Spudich & Orcutt (1980, appendix A), as \( m_i(t) \). The subscript \( j \) implies that the appropriate shot weight and depth are used.

The source is sufficiently shallow that it is convenient to include the free-surface reflection in an effective source function. In principle, the free-surface reflections should be included as another set of rays in which, compared with the rays that leave the source downwards, the phase function \( T_{PP}(p) \) is increased by \( 2d_0\alpha_0 \) (where \( d_0 \) is the source depth and we assume homogeneity above the source) and the function \( R_{PP}(p) \) is negated by the free surface reflection coefficient. However, in the interest of economy it is simpler to approximate the extra phase by \( 2d_0/\alpha_0 \) and include the free surface reflection as a second source pulse. Thus we obtain an effective source function of

\[
m_j(t) = m_j(t - 2d_0/\alpha_0)
\]

and we only include downgoing source rays in the ray summation. This approximation assumes the vertical slowness, \( q_0/\alpha_0 \), differs little from \( \alpha_0^{-1} \). It is valid for the data considered in this paper as, with the source in water, the velocity contrasts are large and the rays are almost vertical at the source.

Expression (7) is for the displacement of the medium. The data analysed in this paper were collected using a hydrophone system. Therefore we replace (7) by

\[
\begin{align*}
P_j(t, x, z) &= -\frac{m_j''(t)}{2^{7/2} \pi^{1/2} \alpha_0^2 \Delta t} \left( \frac{\rho}{\rho_0} \right)^{1/2} \\
&\quad \times \operatorname{Im} \left\{ \Lambda_j(t) \sum_{\text{rays}} \sum_{t = \theta_{PP}} \int \left( \frac{p}{q_0 q_0} \right)^{1/2} R_{PP}(p) dp \right\}.
\end{align*}
\]

(10)

The hydrophone does not, of course, measure the true pressure. The calibration of the hydrophone and recording systems has been described in Spudich (1979) and Spudich & Orcutt (1980). It is assumed to be the same for all ranges. We represent the transfer function of the measurement system as a convolution with the time series, \( r(t) \), say.

Like the source, the receiver is sufficiently close to the surface that we should include the free-surface reflection. Again, to avoid an extra set of rays, we approximate the phase delay by \( 2d/\alpha \) (\( d \) is the depth of the receiver) and include the delayed ray in an effective receiver response

\[
r(t) - r(t - 2d/\alpha).
\]

(11)

The depth, \( d \), remained fixed at 46 m for all recordings.

Thus the theoretical response (10) should be modified to include the effective source function (9) and the receiver transfer function (11). In order to simplify the following development, we use a shorthand notation for this modified response:

\[
P_j(t, x_j) = s_j(t) \ast \sum_{\text{rays}} W(t, R_{PP}, T_{PP}),
\]

(12)

where the summation is over rays travelling downwards from the source and upwards to the receiver. The source/receiver function is

\[
s_j(t) = [m_j''(t) - m_j''(t - 2d_0/\alpha_0)] \ast [r(t) - r(t - 2d/\alpha)].
\]

(13)
The function $W(t, R^{PP}_{ray}, \tilde{T}^{PP}_{ray})$ is essentially the result of the WKBJ algorithm:

$$W(t, R^{PP}_{ray}, \tilde{T}^{PP}_{ray}) = \frac{1}{\pi^{1/2} x^{1/2} \pi^{1/2} \alpha_{o}^{3} \Delta t} \left( \frac{\rho}{\rho_{o}} \right)^{1/2}$$

$$\times \text{Im} \left\{ \Lambda_{s}^{*}(t) \sum_{t = \hat{R}^{PP}_{ray}} \int \left( \frac{p}{q_{o}q_{o}a_{o}} \right)^{1/2} R^{PP}_{ray}(p) dp \right\}.$$  \hspace{1cm} (14)

It depends, of course, on other variables such as the receiver position. For simplicity we have not included in this shorthand notation these variables which will be treated as known. Although we have referred to the source and receiver functions as known theoretically, in fact the absolute amplitude is unknown. Only the relative amplitudes between different shots and the shape of the response is known reasonably well. Therefore we introduce an unknown scaling parameter, $c$, into expression (12). Note that this parameter is independent of the shot and is one unknown for the entire data set. Finally, we introduce parameters to allow for errors in the relative amplitudes and timing, $c_{j}$ and $t_{j}$. Thus

$$P_{s}(t, x_{j}) = c_{j} \delta_{j}(t - t_{j}) \sum_{\text{rays}} W(t, R^{PP}_{ray}, \tilde{T}^{PP}_{ray}).$$  \hspace{1cm} (15)

These parameters can vary from their theoretical values of $c_{j} = 1$ and $t_{j} = 0$ to allow for errors in the calibration of the source and receiver, and for timing errors due to faulty positioning and topographic corrections. While it is possible to combine the parameters $c$ and $c_{j}$, it is convenient to keep them separate as $c$ is completely unknown while $c_{j}$ should be approximately unity.

The misfit

The inversion procedure for the waveform data should minimize the difference between the data and the theoretical seismograms. While it can certainly be argued that other conditions may be more appropriate, we have chosen to use the standard least squares criterion to define the fit. This choice is motivated by the efficiency and versatility of least squares procedures. To a certain extent, other fit criteria can be simulated by appropriate weighting in the least squares method.

A suitable measure of misfit is

$$\phi = \sum_{j} \int |A [d(t, x_{j})] - P_{s}(t, x_{j})|^{2} dt$$

where $A$ is the approximation operator. Parseval's theorem permits (16) to be rewritten in the frequency domain

$$\phi = \sum_{j} \int |\hat{A} (\omega) d(\omega, x_{j}) - \hat{P}_{s}(\omega, x_{j})|^{2} d\omega$$

where we have assumed that $A$ is a convolution operator. This expression (17) is normally more economically evaluated as the convolution in (15) is most efficiently performed in the frequency domain, i.e.

$$\hat{P}_{s}(\omega, x_{j}) = c_{j} \delta_{j}(\omega) \exp (i \omega t_{j}) \sum_{\text{rays}} \hat{W}(\omega, R^{PP}_{ray}, \tilde{T}^{PP}_{ray}).$$  \hspace{1cm} (18)

For the WKBJ seismogram outlined above, the approximation operator is 'smoothing by a
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The amplitude of the data varies significantly as a function of range and frequency. It is therefore necessary to introduce weighting functions for the data. The misfit becomes

$$\phi = \sum_{i,j} |d_{ij} \hat{A}(\omega_l) \hat{d}(\omega_l, x_j) - \hat{P}_s(\omega_l, x_j)|^2.$$  

In this paper we have used three conditions to set the weighting function. The data spectra are peaked about the bubble-pulse frequency. Spectral data below a certain level from this peak will have an insignificant effect in the least squares inversion. In order to reduce the size of the linear system, these data can be excluded from the misfit, i.e. $d_{ij}$ is set to zero for frequencies outside the significant band. For the data investigated in this paper the peak frequency is approximately 7.23 Hz, and the significant frequency band is taken as 2.54-15.04 Hz outside which the spectral amplitude is reduced by 90 per cent or more from the peak amplitude. Secondly, the amplitude of the seismograms varies significantly with range. This variation is, of course, most important information. We therefore introduce a range-dependent scaling, call it $d_i$, so that the scaled spectra, $d_i \hat{A}(\omega_l, x_j)$, have spectral peaks of roughly equal magnitude. Then the fit of a low amplitude seismogram will be as significant as a high one. Finally, we introduce a frequency-dependent scaling. The impulse seismograms (14) have in general a roughly flat spectrum. The differential seismograms which constitute the most important part of the linear system (see below), have a spectrum which generally grows with frequency. It is therefore desirable to integrate the data (and the theoretical seismograms) in order to obtain differential seismograms which have a roughly flat spectrum. This corresponds to a weighting function inversely proportional to frequency. Thus the weighting function in (21) is taken as

$$d_{ij} = \frac{id_i}{\omega_l} \quad \text{in the significant frequency band}$$
$$= 0 \quad \text{otherwise.}$$

This weighting makes the norms of the rows of the perturbation matrix approximately constant. Physically it is reasonable as we know that it will be harder to fit the high-frequency data. As we have already discussed, the system will be more linear for the lower frequencies. Thus it is advisable to reduce the significance of the high-frequency data.

The constant, $c$, in expression (18) is completely unknown. We therefore choose it to minimize the misfit (21). Defining

$$\phi_1 = \sum_{l,j} |d_{ij} \hat{A}(\omega_l) \hat{d}(\omega_l, x_j)|^2,$$

$$\phi_2 = \sum_{l,j} \text{Re} \left\{ [d_{ij} \hat{A}(\omega_l) \hat{d}(\omega_l, x_j)] * [d_{ij} \hat{C}_f(\omega) \exp(i\omega_l t_j) \sum_{\text{rays}} \hat{W}(\omega_l, R_{\text{ray}}^P, \hat{T}_{\text{ray}}^P) \right\},$$

$$\phi_3 = \sum_{l,j} |d_{ij} \hat{C}_f(\omega) \exp(i\omega_l t_j) \sum_{\text{rays}} \hat{W}(\omega_l, R_{\text{ray}}^P, \hat{T}_{\text{ray}}^P)|^2,$$
we find
\[ c = \phi_2/\phi_3. \]  

The summations in (23) are over all ranges and all significant frequencies. Substituting (24) in (21) we find the misfit is \( \phi = \phi_1 - \phi_2^2/\phi_3. \) For convenience we normalize the misfit with respect to the data and use the redefined form
\[ \phi = 1 - \phi_2^2/\phi_1\phi_3. \]

Minimizing (21) or (25) is obviously identical as \( \phi_1 \) is fixed by the data. Throughout the rest of this paper we will be using expression (25) as our misfit with (19) and (22) defining the approximation operator and weighting, respectively.

**Differential seismograms**

In order to minimize the misfit (25) it is necessary to perturb the trial model. Because the theoretical seismograms (18) are non-linear functions of the model, it is expected that the correction will have to be obtained iteratively. In order to correct the model we assume that the system is pseudo-linear and use first-order perturbation theory for the change in the theoretical seismograms. This perturbation is given by

\[
\delta P_s(t, x_j) = \delta cc_j s_j(t - t_j) \sum_{\text{rays}} W(t, R_{\text{ray}}^{PP}, T_{\text{ray}}^{PP}) \]
\[ + c \delta cc_j s_j(t - t_j) \sum_{\text{rays}} W(t, R_{\text{ray}}^{PP}, T_{\text{ray}}^{PP}) \]
\[ - cc_j s_j(t - t_j) \delta t_j \sum_{\text{rays}} W(t, R_{\text{ray}}^{PP}, T_{\text{ray}}^{PP}) \]
\[ + cc_j s_j(t - t_j) \sum_{\text{rays}} W(t, \delta R_{\text{ray}}^{PP}, T_{\text{ray}}^{PP}) \]
\[ - cc_j s_j(t - t_j) \sum_{\text{rays}} W(t, R_{\text{ray}}^{PP}, \delta T_{\text{ray}}^{PP}, T_{\text{ray}}^{PP}) \]  

or the equivalent expression in the frequency domain.

We have assumed the source functions, \( s_j(t) \), are fixed. The first term in (26) represents a simple change in the absolute scaling. As the scaling is chosen (24) to minimize the misfit, this perturbation is not needed by itself. However, it must be included to compensate for other perturbations. The second and third sets of terms represent perturbations in the relative amplitudes and times. The fourth term describes changes in the seismogram caused by perturbations in the reflection/transmission coefficients, i.e. model perturbations at the source, receiver and interfaces. In the example considered in this paper, the only discontinuities are at the ocean surface and floor. The crustal part of the model is assumed to be continuous. In this paper we will assume that the structure in the ocean and at the ocean–crust boundary is known and fixed. There would be no difficulty in including variations at this interface nor in including other interfaces in the model except the algebraic complexity of perturbing reflection/transmission coefficients. For simplicity we have not included this added complication in the test example in this paper.

Although the model is assumed to be continuous, consistent with the WKBJ approxima-
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It may contain second-order discontinuities. In fact, as we will use linear velocity interpolation (equation 31), it will contain many second-order discontinuities. In general these discontinuities will cause higher-order (lower frequency) reflections. For the data set investigated in this paper, we were able to test that the WKBJ approximation was sufficiently accurate and that these reflections could be ignored. For data with a broader frequency response, it may be necessary to model these signals (Thomson & Chapman 1984). As discussed below, it would be feasible to improve the modelling for the direct problem but to still use the WKBJ seismograms for the differential seismograms, i.e. expression (26).

The final term in expression (26) is the most interesting. This is the term that describes the changes in pulse shape and arrival times as model perturbations change the delay time, \( \tau_{\text{ray}} \). In order to obtain this term, it is necessary to differentiate expression (4) before evaluating the inverse transforms. Notice that it can be evaluated using the normal WKBJ algorithm (14) replacing \( R_{\text{ray}} \) by \( R_{\text{ray}} \delta \tau_{\text{ray}} \).

The perturbation, \( \delta \tau_{\text{ray}} \), is calculated by perturbing the delay time integral. The delay time is given by

\[
\tau_{\text{ray}}^{PP} = \int_{\text{ray}} q_x \, dz.
\]

where the notation

\[
\int_{\text{ray}}
\]

is used to indicate the integral over all segments of the ray always taken in the positive direction. For the simple turning ray used in the example in this paper, it is the integral from the turning point to the source and a similar integral from the turning point to the receiver. In order to linearize as much of the problem as possible, it is convenient to treat the depth as a function of velocity rather than velocity as a function of depth (Garmany 1979; Garmany, Orcutt & Parker 1979). Thus we rewrite integral (27) as

\[
\tau_{\text{ray}}^{PP} = \int_{\text{ray}} \left[ \alpha^2 - p^2 \right]^{-1/2} \, dz
= \int_{\text{ray}} \left( \alpha^2 - p^2 \right)^{1/2} z'(\alpha) \, d\alpha
\]

where \( z'(\alpha) = dz/d\alpha \), and the integral is over the appropriate range(s) of velocity. We treat the model as defined by the function \( z'(\alpha) \). In addition we need an initial value — as already mentioned we take the structure at the ocean floor interface as known and fixed. A disadvantage of expression (28) is that it breaks down for uniform layers and for LVZs the integral has multiple segments. These must be treated as special cases.

Now \( \tau_{\text{ray}}^{PP} \) is a linear function of \( z' \) and the perturbation is exactly

\[
\delta \tau_{\text{ray}}^{PP} = \int_{\text{ray}} \left( \alpha^2 - p^2 \right)^{1/2} \delta z'(\alpha) \, d\alpha.
\]

Notice that a perturbation of \( z' \) at one velocity (depth) will perturb the model at all greater depths. If the model initially has a LVZ, it will always retain it under any perturbation. Similarly a model without a LVZ will not develop one. Also a general perturbation is not permitted. The model must remain physical, i.e. velocity is a single valued function of depth. In fact

\[
\delta z'(\alpha) < - z'(\alpha)
\]
in regions where \( z'(\alpha) < 0 \) (and the opposite conditions in regions where \( z'(\alpha) > 0 \)). The perturbation in each iteration must be restrained to satisfy condition (30).

In practice the velocity function is defined at discrete points and some interpolation formula is used. For simplicity we assume linear interpolation. Thus for \( z_{i+1} < z < z_i \) we take

\[
\alpha(z) = \alpha_i + (\Delta\alpha_i/\Delta z_i)z
\]

where \( \Delta z_i = z_{i+1} - z_i \) and \( \Delta\alpha_i = \alpha_{i+1} - \alpha_i \). Using the well-known formulae (Telford et al. 1976, pp. 273-274), the contribution to the delay time from this depth element is

\[
\Delta\tilde{T}_i = (\Delta z_i/\Delta \alpha_i) \left\{ \ln \left[ \frac{1 + (1 - p^2 \alpha_i^2)^{1/2}}{1 + (1 - p^2 \alpha_{i+1}^2)^{1/2}} \right] - (1 - p^2 \alpha_i^2)^{1/2} + (1 - p^2 \alpha_{i+1}^2)^{1/2} \right\}.
\]

The total delay time is given by

\[
\tilde{T}_{ray}^{pp} = 2 \sum_i \Delta\tilde{T}_i
\]

where the summation is taken over all depth elements appropriate to the ray and the factor of 2 arises assuming a simple turning ray with upgoing and downgoing segments through each depth element. Notice that this expression (33) like (28) is linear in \( (\Delta\alpha_k/\Delta z_k) \). However, for this discretized model it is simple to perturb \( \alpha_k \). Again \( \tilde{T}_{ray}^{pp} \) is exactly linear in \( z_k \) and we have

\[
\delta\tilde{T}_{ray}^{pp} = 2 \sum_k (\Delta\tilde{T}_{k-1}/\Delta z_{k-1} - \Delta\tilde{T}_k/\Delta z_k) \delta z_k.
\]

This is the expression used in (26).

Before proceeding further, it is interesting to consider the form of the final term in (26) for a simple model. Suppose we have a model in which the velocity increases with depth (Fig. 2a). The theta function, \( \tilde{\theta}_{ray}^{pp} \), will have a minimum at the arrival time. For illustrative purposes, we have included the intermediate time series obtained before convolution with \( \Lambda'_k(t) \) in Fig. 2(b). It has an inverse square root pulse at the arrival time. We take the source functions, \( s_j(t) \), to be delta functions and so the seismograms are smoothed delta functions (Fig. 2b).

**Figure 2.** (a) Simple turning rays in a model with a smooth gradient. The model is perturbed at \( z_k \) which modifies the model between \( z_{k-1} \) and \( z_{k+1} \) and the travel-time curve for \( p > p_{k-1} \). (b) Theoretical seismograms corresponding to (a). The left diagram is the intermediate imaginary seismogram before convolution with \( \Lambda'_k(t) \). The right diagram is the impulse seismogram. The arrival is a smoothed delta function at time \( t = T \). (c) The differential of the delay-time function, \( \tilde{T}_{ray}^{pp} \). The function is zero for \( p > p_{k-1} \). (d) Differential seismograms when \( x > X(p_{k-1}) \). The left diagram is the intermediate imaginary seismogram before convolution with \( \Lambda'_k(t) \). The discontinuity at \( t = \tilde{\theta}_{k-1} = \tilde{\theta}(p_{k-1}, x) \) is caused by the end of the differential function \( \tilde{\delta}T_{ray}^{pp}/\delta z_k \) (Fig. 2c). The right diagram is the impulse differential seismogram. The arrival at \( t = T \) shifts the arrival time, and the pulse at \( t = \tilde{\theta}_{k-1} \) is a new diffracted arrival. The diagram is drawn for \( \delta z_k < 0 \). (e) Differential seismogram where \( x < X(p_{k-1}) \). Compared with (d) only the diffracted arrival at \( t = \tilde{\theta}_{k-1} \) is present.
Now suppose that we perturb the model at \( z = z_k \). The function \( \frac{\delta T_{ray}}{\delta z_k} \) (34) is a negative, monotonically increasing function of \( p \), and is zero for \( p > \alpha^{-1}(z_{k-1}) = p_{k-1} \), say (Fig. 2c). There are two distinct types of differential seismograms depending upon whether the turning point is above or below the perturbed region. For large ranges, \( x > X(p_{k-1}) \), the turning point is below the perturbed depth and the geometrical ray parameter is less than the cutoff value, \( p_{k-1} \). Thus the differential amplitude function, \( R_{ray}^{PP} \delta T_{ray}^{PP} \), is non-zero at the geometrical arrival time. At a later time given by \( \delta T_{ray}^{PP} (p_{k-1}, x) \) the cutoff in the differential amplitude function causes a gradient discontinuity. In Fig. 2(d) we show the intermediate time series and the differential seismogram, \( \delta P_x \). Note the extra time derivative, \( \dot{\delta}_1(t) \), in (26). The differential seismogram contains two arrivals — a differentiated delta function at the geometrical arrival time and a pulse at \( \delta T_{ray}^{PP} (p_{k-1}, x) \). The former has the effect of shifting the geometrical arrival as the ray has propagated through the perturbed region. The latter pulse is a diffracted arrival. As the model is perturbed it will develop into the triplication and caustics expected near \( x = X(p_{k-1}) \). For small ranges, \( x < X(p_{k-1}) \), the turning point is above the perturbed depth and the geometrical ray parameter is greater than the cutoff value, \( p_{k-1} \). Thus the differential amplitude is zero at the geometrical arrival time and we only obtain an arrival at time \( \delta T_{ray}^{PP} (p_{k-1}, x) \) (Fig. 2e). Again this develops into the triplication and caustics expected near \( x = X(p_{k-1}) \). The differential pulse at the geometrical arrival time is absent as the ray has not propagated through the perturbed depth.
The linear system

In order to improve the fit between the theoretical seismograms and the data, we solve for the linear perturbations (26). The linear system can be written in the usual fashion

\[ y = B \delta m \]  

(35)

and solved as a least squares problem. The vector \( y \) is the difference between the data and theory, i.e. the required change in the theory for a perfect fit, the matrix \( B \) contains the differential coefficients defined by linear perturbation theory (26), and the vector \( \delta m \) is the model perturbation. Using the misfit defined in equation (25) [with (19) and (22)], the elements of \( y \) are

\[
y_v = \begin{cases} 
\frac{\text{Re} \left\{ i \frac{d \left( \omega_1, x_j \right)}{\omega_1} \text{sinc}^4 \left( \frac{\omega_1}{\omega_N} \right) \frac{id \text{s} \text{c} j \left( \omega_1 \right)}{\omega_l} \exp \left( i \omega t_j \right) \hat{W} \left( \omega_l, R_{\text{ray}}^{\text{PP}}, \hat{T}_{\text{ray}}^{\text{PP}} \right) \right\}}{\text{Im}} & \text{for } j = 1 \text{ to } J \\
\frac{\text{Im} \left\{ i \frac{d \left( \omega_1, x_j \right)}{\omega_1} \text{sinc}^4 \left( \frac{\omega_1}{\omega_N} \right) \frac{id \text{s} \text{c} j \left( \omega_1 \right)}{\omega_l} \exp \left( i \omega t_j \right) \hat{W} \left( \omega_l, R_{\text{ray}}^{\text{PP}}, \hat{T}_{\text{ray}}^{\text{PP}} \right) \right\}}{\text{Re}} & \text{for } m = 2j - 1 \\
\end{cases}
\]

(36)

The index \( v \) is used to enumerate all the frequency and range data. We have only retained the significant frequencies (22) and we index these as \( l = 1 \) to \( L \). The ranges we index as \( j = 1 \) to \( J \). The index \( v \) is defined as \( v = 2L \left( j - 1 \right) + 2l - 1 \) for the real part in (36) and \( \nu = 2L \left( j - 1 \right) + 2l \) for the imaginary part. It runs from 1 to \( 2JL = N \), say.

The elements of \( \delta m \) are perturbations of the relative amplitudes and times, the model depths and the absolute amplitude. The model depths that are perturbed are \( z_k \) with \( k = 1 \) to \( K \). Thus we take

\[
\begin{align*}
\delta m_{2j - 1} &= \delta c_j \\
\delta m_{2j} &= \delta t_j \\
\delta m_{k + 2J} &= \delta z_k
\end{align*}
\]

(37)

and

\[ \delta m_{1 + K + 2J} = \delta c/c. \]

The model space has dimension \( M = 2J + K + 1 \). The absolute amplitude perturbation, \( \delta c \), is divided by \( c \) to reduce slightly the computations in the differential matrix, \( B \). The differential matrix is \( N \) by \( M \) and from expression (26), the non-zero elements are

\[
B_{\nu m} = \begin{cases} 
- \frac{i d j c \text{s} j \left( \omega_1 \right)}{\omega_l} \hat{W} \left( \omega_l, R_{\text{ray}}^{\text{PP}}, \hat{T}_{\text{ray}}^{\text{PP}} \right) \exp \left( i \omega t_j \right) / \omega_l & \text{for } m = 2j - 1 \\
d j c \text{s} j \left( \omega_1 \right) \hat{W} \left( \omega_l, R_{\text{ray}}^{\text{PP}}, \hat{T}_{\text{ray}}^{\text{PP}} \right) \exp \left( i \omega t_j \right) & \text{for } m = 2j \\
d j c \text{s} j \left( \omega_1 \right) \hat{W} \left( \omega_l, R_{\text{ray}}^{\text{PP}}, \hat{T}_{\text{ray}}^{\text{PP}} \right) \exp \left( i \omega t_j \right) / \omega_l & \text{for } m = k + 2J \\
- i d j c \text{s} j \left( \omega_1 \right) \hat{W} \left( \omega_l, R_{\text{ray}}^{\text{PP}}, \hat{T}_{\text{ray}}^{\text{PP}} \right) \exp \left( i \omega t_j \right) & \text{for } m = 2J + K + 1
\end{cases}
\]

(38)

where \( \nu \) has been defined above.

The first \( 2J \) columns of \( B \), i.e. the first two lines in expression (38), are the relative amplitude and time differentials, i.e. the second and third terms in expression (26). Note that in each group of \( 2L \) rows of \( B \) (corresponding to the real and imaginary terms at \( L \) frequencies at one range) only two of the first \( 2J \) columns of \( B \) are non-zero. The next \( K \) columns of \( B \), i.e. the third line in expression (38), are the depth differentials, i.e. the final
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(26). The final \((2J + K + 1)\)th column of \(B\), i.e. the last line in expression (38), is the absolute amplitude differential, i.e. the first term in expression (26).

The variables (37) have different dimensions. It is therefore necessary to introduce a weighting matrix, \(H\), to compensate for the different dimensions and relative importances of the various variables, i.e.

\[
\delta m = H\delta \tilde{m} \\
\tilde{B} = BH.
\] (39)

In general, if one has sufficient \textit{a priori} statistical information to define a covariance matrix, \(C\), for the uncertainty of \(m\), then \(H\) can be computed as the upper triangular Cholesky factor of \(C\), i.e. \(C = HH^T\) (Lawson & Hanson 1974, pp. 186–187). In the simplest case, the matrix \(H\) is the diagonal matrix of the uncertainties of the elements of \(m\). The transformed variables, \(\tilde{m}\), then have unit \textit{a priori} uncertainty. This obviously compensates for the different dimensions of elements in \(\delta m\). The importance of the different model depths, \(z_k\), depends on the extent to which the model is perturbed by \(\delta z_k\). The effect of \(\delta z_k\) is spread over the model range of \((v_{k+1} - v_k)\) and the inverse of this can be used to scale the columns of \(B\).

We, in effect, use a combination of these methods although only a very crude estimate of the covariance matrix \(C\) is made. The matrix \(H\) is chosen diagonal with elements

\[
H_{mm} = \lambda_c \sqrt{\sum_v B^2_{vm}} \quad m = 2j - 1 \\
= \lambda_r \sqrt{\sum_v B^2_{vm}} \quad m = 2j \\
= \lambda_z \sqrt{\sum_v B^2_{vm}} \quad m = k + 2J \quad \text{with } k = 1 \text{ to } K \\
= \lambda_0 \sqrt{\sum_v B^2_{vm}} \quad m = 1 + K + 2J.
\] (40)

The importance of perturbations in the relative amplitudes and times, model depths and absolute amplitudes are controlled by the weighting parameters \(\lambda_c\), \(\lambda_r\), \(\lambda_z\) and \(\lambda_0\), respectively. If these parameters are zero, the perturbation in the corresponding type of variable is suppressed. If the experiment is well calibrated then we take \(\lambda_c = \lambda_r = \lambda_0 = 0\) and \(\lambda_z = 1\). In the examples in this paper, the weighting parameters were initially taken with these values and relative amplitude and time variations suppressed. The inversion by Spudich & Orcutt (1980) was achieved with this restriction. Only in later tests did we investigate the improvement in fit achieved by permitting relative amplitude and time variations. As the absolute scaling parameter, \(c\), is always chosen to minimize the fit, increasing the value of its weighting parameter, \(\lambda_0\), has the effect of suppressing all perturbations to the model, i.e. damping the iterative least squares procedure.

Although the linear system (35) is normally overdetermined, i.e. \(N \gg M\), we have no way of knowing, \textit{a priori}, whether it is ill-conditioned. It is therefore prudent to compute the
satisfaction value decomposition of \( \tilde{\mathbf{B}} \), i.e.
\[
\tilde{\mathbf{B}} = \mathbf{USV}^T
\]  
(41)

and examine the eigenvalues, \( \mathbf{S} \) (Lawson & Hanson 1974, chapter 18). In order to reduce the uncertainty of the solution, the eigenvectors corresponding to small or zero eigenvalues must be removed. The system (35) is a linear approximation to a problem that is definitely non-linear. We have found that the data eigenvectors, \( \mathbf{U} \), corresponding to small eigenvalues invariably contain more high-frequency energy. If the rows of \( \mathbf{U} \) are arranged in order of frequency, and the magnitude of elements in a column is plotted as a function of frequency, we obtain results like those illustrated in Fig. 3. In other words, the large eigenvalues correspond to low-frequency data and small eigenvalues correspond to high-frequency data.

![Figure 3. A sketch of the magnitude of elements in columns of \( \mathbf{U} \) as a function of frequency, \( \omega \). Three columns are shown corresponding to eigenvalues \( S_1 > S_2 > S_3 \).](https://academic.oup.com/gji/article-abstract/82/3/339/606013)

The separation is not, of course, sharp particularly as the data have a fairly narrow band spectrum. This relationship between the frequency and eigenvalue is extremely useful. Suppressing the small eigenvalues serves three purposes. It reduces the uncertainty of the solution and removes the high frequencies from the inverse process. As already discussed, this has the effect of linearizing a non-linear problem (Fig. 1). It can also be used to reduce the perturbation to keep the model physical.

Although some intuitive arguments can be made for the relationship between the frequency content and eigenvalue magnitude, we cannot give a rigorous proof. The relationship between eigenvalue and the ‘frequency’ content of the model perturbations (eigenvectors \( \mathbf{V} \)) is more direct but for body-waves the relationship between the ‘frequency’ content of the model and data perturbations is less obvious. For the data and models in this paper the relationship holds. If the relationship fails, the linear system (35) can be reduced to linearize the system. In other words, by only including low-frequency data, i.e. reducing the range of \( l \) in expressions (36) and (38), we improve the linearity of the system. This has the added advantage of reducing the size of the linear system (by decreasing \( L \)) and hence increasing the computational efficiency. It has the minor disadvantage of increasing the complexity of the program somewhat (how to choose \( L \) for each iteration?). We had initially planned to linearize the system this way but it proved unnecessary for the example in this paper.

The method we have chosen to use to suppress the small eigenvalues in the linear system is the damped least squares method (Levenberg 1944). Given the singular value decomposi-
tion of the matrix $\tilde{B}$ (41), the model perturbation is found using

$$\delta \mathbf{m}_\lambda = H V S (S^2 + \lambda^2 I)^{-1} U^T \mathbf{y}. \quad (42)$$

$\lambda$ is the damping parameter. Because the problem is non-linear and we are only solving the linear approximation to the exact problem, and because we have introduced the damping parameter, this model perturbation will probably not give the model that minimizes the misfit (25). In fact if the damping is too small, the misfit may increase. Therefore, the damping parameter, $\lambda$, is chosen so that the model perturbed by expression (42) minimizes, at least approximately, the misfit (25). In other words, $\lambda$ is found empirically so as to optimize the procedure of reducing the misfit (25). In addition the damping is chosen such that the model remains physical, i.e. $z_k > z_{k+1}$. We have not employed the more satisfactory but more complicated and expensive technique of non-negative least squares (Lawson & Hanson 1974, chapter 23). This method was used by Shaw (1983) and Shaw & Orcutt (1985). An advantage of using the singular value decomposition (41) over the normal equations is that multiple values of the damping parameter can be tested with little extra effort (42). Having found the optimum model perturbation, the process is repeated starting from the new model. The iterative procedure is continued until the reduction in the misfit and the perturbation to the model are insignificant.

**Computational methods**

Using the theoretical techniques described above, it is a straightforward computational problem to obtain the iterative numerical solution. In view of the number of synthetic seismograms required per iteration $[f(K + 1 + n)]$ where $n$ is the number of values of the damping parameter, $\lambda$, tested] and the size of the linear system (35) ($N \times M$), significant demands are made on the computer. Although algorithms for the various parts of the computation are well known, successful and routine application of the method depends to a large extent on the efficiency of computer programs. Therefore, in this section we discuss in some detail the program used.

If the starting model is too far from the ‘correct’ model, the iterative perturbations can easily find the incorrect local minimum of the misfit. For the bubble source and hydrophone used in the experiment analysed in this paper, the arrivals are sufficiently oscillatory that a fit can be attempted with the wrong oscillations aligned. This alignment causes a local minimum in the misfit. The problem is normally easily recognized by visual inspection of the seismograms but difficult to avoid completely in a computer program. It is therefore highly desirable that the computer program can be run interactively to allow graphical output to be inspected immediately. Note that the problem with misaligned oscillations is less likely to occur with broad-band signals.

The original code we developed was run on a VAX11/780 computer. Typically each iteration took a few minutes of CPU time (more quantitative estimates are given below). While this is not an excessive figure it made interactive execution rather tedious as in normal circumstances the elapsed time is several times greater than the CPU time. To alleviate this problem we have developed a code to run on an array processor (AP) (Floating Point Systems AP-120B) attached to the same computer. The CPU requirements are typically 10–30 times less on the AP than on the VAX. More important, the elapsed time on the AP is essentially equivalent to the CPU time (provided I/O between the AP and host is minimized), whereas on the VAX it may be considerably greater. However, using an AP introduces other constraints as the memory is normally severely limited (32K words in our case).
A major part of the computation involves the calculation of the elements of the matrix, \( B \). Unlike some inverse problems, e.g. normal modes, where the differential coefficients are obtained very easily once the forward problem is solved, the differential seismogram for each depth variable requires the same computational effort as the direct problem. Hence the desirability of using an extremely fast approximation to compute the synthetic seismograms. The WKBJ algorithm and the rational approximation operator, \( \Lambda'_c(t) \), have been discussed in some detail in Chapman & Drummond (1982). The total number of operations required to evaluate the WKBJ seismogram (14) is approximately

\[
a_1n_t + a_2n_p
\]  

[combining equations (76) and (86) in Chapman & Drummond (1982)]. The important feature about this expression (43) is that it is proportional to the number of time points in the seismogram, \( n_t \), and the number of \( p \) values in the ray tables, \( n_p \), but not to some higher-order expression such as the product, \( n_p \). The algorithms have been programmed in APAL (Array Processor Assembly Language) and the constants \( a_1 \) and \( a_2 \) are approximately

\[
a_1 = 21 \mu s
\]

\[
a_2 = 14 \mu s
\]

in terms of CPU time on the AP. In addition each seismogram must be Fourier transformed. The AP execution time is approximately

\[
a_3n_t \log_2 n_t
\]

with

\[
a_3 = 0.35 \mu s.
\]

Seismograms must be calculated for each range and depth variable. This calculation normally dominates the program. The total number of operations required to compute the elements of \( B \) (38) is approximately

\[
J(K + 1)(a_1n_t + a_2n_p + a_3n_t \log_2 n_t).
\]

Note that the direct seismograms provide the differential seismograms for relative amplitude and time and absolute amplitude perturbations with only minor extra computations.

As \( N \gg M \), the SVD of the matrix \( B \) is most efficiently obtained by first applying Householder transformations to form the upper triangular matrix \( NM^2 \) as opposed to \( 2NM^2 \) operations, Lawson & Hanson 1974, table 19.1). Often the matrix \( B \) will be too large to store in an AP. The sequential Householder triangularization algorithm (Lawson & Hanson 1974, chapter 27) permits the matrix \( B \) to be calculated and used in blocks. The seismograms for one range conveniently form a block of \( 2L \) rows. After each block (range) of data and differential coefficients is included, the matrix is upper triangularized by Householder transformations. The upper triangular matrix including the data vector is \((M + 1) \times (M + 1)\). After the \( j \)th block is included the matrix is \((2L + M + 1) \times (M + 1)\) and \( M \) Householder transformations are applied to upper triangularize the matrix again. The increase in computations caused by using the sequential Householder triangularization algorithm is only by a factor \((2L + 1)/2L\) (normally very close to unity as \( L \gg 1 \)), but the number of rows of the matrix \( B \) that must be stored simultaneously is reduced from \( N = 2LJ \) to \( 2L + M + 1 \). With this algorithm the entire matrix can be calculated and triangularized in the AP without memory or I/O difficulties.

Although the matrix, \( B \), has \( M = K + 2J + 1 \) columns, only \( K + 3 \) columns are non-zero in each block (38). This feature can be exploited to reduce the computations in upper triangu-
Figure 4. (a) The upper triangular matrix after \((j - 1)\) blocks have been included. In the upper triangular matrix, the first \(2(j - 1)\) non-zero columns correspond to the relative amplitude and time variables, the next \(K\) to the depth variables, and the final two to the absolute amplitude variable and the data variable, \(y\).

(b) The matrix with the \(j\)th block included. The block is \(2L \times (K + 4)\) elements. Part of the upper triangular matrix (a) has been shifted two columns left. The shaded parts of the matrix are non-zero and the clear parts are zero or as yet undefined. (c) The upper triangular matrix after \(j\) blocks have been included, obtained by Householder transformations of the matrix in (b).

larizing the matrix. The procedure is illustrated in Fig. 4. Let us consider the steps in adding the \(j\)th block (range). After the \((j - 1)\)th stage is completed, the upper triangularized matrix is restricted to columns \((2J + 3 - 2j)\) to \(M\) (Fig. 4a). The differential coefficients for the relative amplitudes and times of the first to \((j - 1)\)th ranges occupy columns \((2J + 3 - 2j)\) to \(2J\) at this stage. Now the \(j\)th block is added. First the columns \((2J + 3 - 2j)\) to \(2J\) are shifted to columns \((2J + 1 - 2j)\) to \((2J - 2)\). Columns \((2J - 1)\) and \(2J\) are zeroed for the new relative amplitude and time terms. The \(j\)th block of differential coefficients is now added in columns \((2J - 1)\) to \(M\) (Fig. 4b). This composite matrix is then upper triangularized by a series of Householder transformations. Note that in the first \((2j - 2)\) transformations, the effective column length in the transformation is only three elements. Only in \((K + 3)\) transformations is the full column length needed. This completes adding the \(j\)th block (Fig. 4c). The process is repeated until all \(J\) blocks have been included. After the \(J\)th block is added, the differential coefficients for the relative amplitudes and times have been moved into their correct columns as defined by (38).

Thus by using the algorithm illustrated in Fig. 4, the number of operations is reduced from

\[
a_4(2LJ)(K + 2J + 1)^2
\]

to

\[
a_4(2LJ)(K + 3)^2
\]

plus lower-order terms. This reduction is significant as typically \(J \gg 1\) and is comparable with \(K\). It means that the relative amplitude and time variables can be included without significant extra computations — a useful feature as often we will wish to suppress variations in these variables anyway. In addition the algorithm illustrated in Fig. 4 reduces the memory requirement from \((2LJ) \times (K + 2J + 2)\) to \((K + 2J + 2)^2 + 2L(K + 4)\). Again this reduction is
significant as often the former figure exceeds the size of AP memory. The AP execution time is approximately

$$a_5 = 0.67 \mu s.$$  \hfill (49)

The modified sequential Householder triangularization algorithm (Fig. 4) is applied to the matrix $B$ (38) before it is weighted. Let us represent the complete set of Householder transformations by the matrix $Q$. The linear system (35) becomes

$$\tilde{y} = \tilde{B} \delta m$$

where

$$\tilde{y} = Qy$$

and

$$\tilde{B} = OB.$$

By design $\tilde{B}$ is an upper triangular matrix and only the first $M$ rows of (50) are significant. The variables are now weighted using the matrix $H$ defined in (40) (except that the elements of $B$ are replaced by those of $\tilde{B}$). The final linear system becomes

$$\tilde{y} = \tilde{B} \delta \tilde{m}$$

where

$$\tilde{B} = \tilde{B}H$$

and

$$\delta \tilde{m} = H \delta \tilde{m}.$$  \hfill (51)

The complete computation of the matrix $B$ (38) and transformations to reduce it to the upper triangular form $\tilde{B}$ (Fig. 4) have been programmed in APAL and VFC (Vector Function Chainer) to run on the AP with only one call from the host computer. The approximate run time is given by expression (47) plus (48). For typical values of the parameters, $(n_p = 256, n_p = 200, J = 25, K = 20, L = 65, N = 3250, M = 71)$ this reduces to about 6 s. Run on a VAX 11/780, the CPU time is about 200 s for the same parameters but the elapsed time is normally much greater. In addition, while the computation is running on the AP other computations can be performed on the host. For instance, preliminary plotting can be prepared for the new results. On the interactive graphics system we used, the output time for this plotting exceeded 6 s and so the main part of the computation is completely hidden.

Having computed the upper triangular matrix, $\tilde{B}$, the AP execution is interrupted to allow the weighting matrix, $H$, to be set. Finally the SVD of the matrix $\tilde{B}$ is performed on the AP (41) (again programmed in APAL and VFC) (Lawson & Hanson 1974, chapter 18). The operation count for the computation is approximately

$$a_5 (K + 2J + 1)^3.$$  \hfill (52)

The exact value of $a_5$ varies as the SVD algorithm is iterative but a typical value for the AP execution time is

$$a_5 = 2 \mu s.$$  \hfill (53)

Finally we test several values of the damping parameter, $\lambda$, in order to optimize the perturbation (42) approximately before proceeding with the next iteration. As the computation of the direct problem, i.e. $J$ seismograms, is only equivalent to one column of the
matrix $B$, these tests are computationally efficient. The evaluation of the perturbation (42) is a relatively minor computation (proportional to $M^2$) so, as we must test that the depth perturbations yield a physical model, it is performed on the host computer. The perturbation of the travel-time tables, the direct seismograms and the misfit are evaluated on the AP. The number of operations per test is approximately

$$J(a_1n_1 + a_2n_p + a_3n_1 \log_2 n_1) + a_6Kn_p + a_7LJ$$

(54)

where for the AP run time,

$$a_6 = 0.3 \mu s$$

$$a_7 = 2.8 \mu s.$$  

The times for the table perturbation and misfit (55) are relatively minor compared with the seismograms. With the above parameters, the AP run time per test is about 0.3 s.

Example

In order to illustrate the method, we have used the FF2 refraction data from the 1959 Fanfare cruise of the Scripps Institution of Oceanography. These data have been interpreted before using travel times (Shor, Menard & Raitt 1970) and synthetic seismograms (Spudich 1979; Spudich & Orcutt 1980). The success of the latter investigation motivated the use of this data set in these experiments.

The data collection and preliminary analysis have been thoroughly described in Spudich & Orcutt (1980) and we will only briefly describe them here. The experiment was conducted

![Figure 5. Comparison of the FF2 P data and the best fitting synthetic seismograms calculated by Spudich & Orcutt (1980). The horizontal scale is the reduced travel time (reducing velocity = 8 km s$^{-1}$) and the vertical scale is the range in kilometres. The data are the upper seismogram of each pair and are correctly positioned on the range axis whereas the lower seismogram is the synthetic and is shifted slightly. Other details are given in the text.](https://academic.oup.com/gji/article-abstract/82/3/339/606013 by guest on 27 March 2019)
over a region of gently rolling bottom and basement topography east of Guadalupe Island where the average water depth was 3.55 km. The crust is fairly normal, uncomplicated oceanic crust of about 15 Myr age. The seismic data are unreversed two-ship lines shot in 1959 by Russell W. Raitt on the Fanfare cruise of the Scripps Institution of Oceanography. Explosive charges of TNT weighing 1–45 kg were used as seismic sources and the seismograms were recorded by hydrophones suspended at a depth of about 46 m beneath the sea surface. A detailed account of the procedure and instrumentation has been given by Shor (1963). The topographic corrections have been described by Spudich & Orcutt (1980). As already discussed, the source function was calculated theoretically from the weight and depth of the explosive source. The theory has been given in appendix A of Spudich & Orcutt (1980). Finally, the calibration of the hydrophone recording system has been described by Spudich (1979).

The data set used in the inversion is shown in Fig. 5. Topographic corrections have been applied and the data have been scaled by shot weight and range for plotting. To compensate roughly for the variation in shot sizes the data have been multiplied by \((\text{shot weight})^{-0.65}\), and to reduce the range dependence multiplied by \(x^2\). The horizontal axis is the reduced travel time using the reducing velocity 8 km s\(^{-1}\). The vertical axis is the range in kilometres. Also shown in Fig. 5 are the best fitting synthetic seismograms calculated by Spudich & Orcutt (1980). By 'best fitting' we mean that the absolute amplitude parameter, \(c\), has been chosen to minimize the misfit, \(\phi\), i.e. using (24) except that the synthetics in \(\phi_2\) and \(\phi_3\) (23)

Figure 6. The \(P\) velocity models obtained using travel-time data by Shor \textit{et al.} (1970) and using synthetic seismograms by Spudich & Orcutt (1980) (plotted with respect to the left and right depth axes, respectively).
Fitting marine refraction data were calculated using the reflectivity method (Fuchs & Müller 1971). The misfit (25) is \( \phi = 0.781 \) for these synthetics. Fig. 5 should be compared with fig. 3 in Spudich & Orcutt (1980). Although these figures plot essentially the same data and synthetics, the absolute scaling of the synthetics, i.e. the parameter \( c \), is significantly different. In Fig. 5 in this paper, the scale has been chosen to minimize the misfit, \( \phi \). Spudich & Orcutt (1980) judged the fit of the waveforms visually by overlaying seismograms and chose the scale to improve this visual fitting. It is clear that in this visual procedure, the scale is chosen to make the peak amplitudes of the waveforms approximately equal even when the waveforms misfit. The slight difference in the waveforms has a significant effect on the misfit (25), and the scaling (24) is noticeably reduced. Presumably, the seismologist's eye is more impressed by the correlation of waveform amplitude than the exact alignment. The appropriateness of the least squares fit criterion (25) is certainly open to question, and the design of a better function an unsolved problem. Nevertheless we have used the least squares method as the technique is so widely developed and used. It can be modified by introducing weighting functions, particularly in the time domain (but weighting the synthetic seismograms in the time domain would require extra Fourier transforms or a convolution in the frequency domain), and the misalignment problem can be investigated by introducing relative time corrections, \( t_i \) (as we have done below).

The \( P \) velocity model used by Spudich & Orcutt (1980) to calculate the synthetics in Fig. 5, is shown in Fig. 6. The layering is, of course, an artefact of the technique used to calculate the synthetics (the reflectivity method, Fuchs & Müller 1971) and is not required by the data. On physical grounds, a continuous model would have been preferred if a synthetic technique had been available. For comparison, the layered model determined from the travel times is shown (Short et al. 1970).

Before proceeding with the inversion, the data must be weighted. In Fig. 7 we show the

![Figure 7](https://academic.oup.com/gji/article-abstract/82/3/339/606013)  
**Figure 7.** Comparison of the weighted FF2 \( P \) data (upper seismograms) and the smoothed, weighted data (lower seismograms). The weights relative to the first seismogram at \( x_1 = 7.95 \) km are given. Other details are as for Fig. 5 or are given in the text.
weighted data and the smoothed, weighted data. The former are the seismograms \( d_i d(t, x_i) \) where the weights have been chosen to give spectral peaks of roughly equal magnitude for all the seismograms. The weights relative to the first seismogram at \( x_i = 7.95 \) km are indicated. The second set of seismograms is \( A [d_i d(t, x_i)] \) where the approximation operator is 'smoothing by a fourth-order boxcar' (19) as required by the WKBJ seismogram theory. The initial attempts at inversion were performed on data with \( \Delta T = 0.02 \) s (\( \omega_n = 157 \) rad s\(^{-1} \)) and the appropriate smoothing is shown in Fig. 7. Final iterations in the inversion used \( \Delta T = 0.01 \) s when the effect of the approximation operator was less significant. Note that although it is not required by the reflectivity seismogram method, for consistency the data and synthetics have been smoothed by the approximation operator to calculate the misfit for Fig. 5 (with \( \Delta T = 0.01 \) s).

In Fig. 8 we have shown the average amplitude spectrum derived from the total energy of the weighted data, i.e. we have plotted

\[
\sqrt{\sum_j |d_j d(\omega_j, x_j)|^2 / J}.
\]

The spectra of the individual seismograms are all similar in form and, of course, the weights, \( d_j \), have been chosen to make the peaks of similar magnitude. The spectra are peaked about the bubble pulse frequency (7.23 Hz). In the inversion we have only used frequencies in the range 2.54–15.04 Hz giving \( L = 65 \) with \( \Delta T = 0.02 \) s and \( n_t = 256 \). This frequency band is indicated in Fig. 8.

In order to illustrate the inversion procedure, we have included two different starting models (Fig. 9). Note that both these models are chosen to be simple with continuous crustal structure but details in the transition regions differ significantly. The models are con-

![Figure 8](https://academic.oup.com/gji/article-abstract/82/3/339/606013/8233960013)
strained to fit the first arrival times approximately but are otherwise chosen arbitrarily. If the times are wrong by a significant amount (compared with the dominant period), the inverse procedure finds a local minimum of the misfit (25) with the peaks of the waveform shifted by an integral number of half-periods. This is normally obvious visually and would be less likely to occur with broader band data. We have not attempted to avoid it automatically in the computer program as it is very easy to choose an appropriate starting model interactively. One method to automate the entire procedure would be to fit the waveform envelope initially (Brown 1982; Shaw 1983; Shaw & Orcutt 1985) when misalignments by half-periods would not cause local minima in the misfit (25).

The models A and B in Fig. 9 give misfits (25) of $\phi = 0.911$ and 0.825, respectively. After seven iterations, these are reduced to $\phi = 0.717$ and 0.714, respectively. The models are shown in Fig. 10. In Fig. 11 we have compared the data and the best fitting synthetic seismograms for model A in Fig. 10. With this size figure and line thickness, the seismograms for model B in Fig. 10 would not differ visibly. Other details about Fig. 11 are identical to Fig. 5. These initial iterations were performed with $\Delta T = 0.02$ s to emphasize the low-frequency data needed to pseudo-linearize the problem. Having obtained two such similar models (Fig. 10), we attempted to improve the model using the $\Delta T = 0.01$ s’ data. The resultant model is shown in Fig. 12. With this size figure and line thickness, the models obtained from either model in Fig. 10 are not visibly different. The data and best fitting synthetic seismograms are shown in Fig. 13. A further seven iterations were needed to obtain these results and the misfit was reduced to $\phi = 0.673$. For comparison we have included the
Figure 10. Two models obtained after seven iterations from the starting models in Fig. 9, using the FF2 $P$ data with $\Delta T = 0.02 \text{s}$. Again, models A and B are plotted with respect to the right and left axes, respectively.

Figure 11. Comparison of the FF2 $P$ data and best fitting synthetic seismograms calculated using model A in Fig. 10. Other details are as for Fig. 5 or are given in the text.
Figure 12. Comparison of the $P$ velocity model obtained after seven iterations from either model in Fig. 10, and the model from Spudich & Orcutt (1980) (as in Fig. 6) (plotted with respect to the left and right axes, respectively). The FF2 $P$ data with $\Delta T = 0.01$ s were used.

Figure 13. Comparison of the FF2 $P$ data and the best fitting synthetic seismograms calculated using the model in Fig. 12. Other details are as for Fig. 5 or are given in the text.
model from Spudich & Orcutt (1980) in Fig. 12 for which, using the reflectively method, $\phi = 0.781$.

If the layered model of Spudich & Orcutt (1980) were smoothed to give a continuous crustal structure, the features would be extremely similar to those in the final model obtained by the iterative procedure (Fig. 12). Not only are similar velocity gradients obtained, but the shape (second derivative) of the transition regions have the same form. The automatic procedure has obtained a significantly better fit ($\phi = 0.673$ compared with 0.781) although this may be due to 'numerical noise' from the layered structure. It is worth emphasizing that this final model has been obtained from two dissimilar but simple starting models (Fig. 9). Given the assumptions built into the theoretical model (lateral homogeneity, no attenuation, etc.), it appears that a unique, best fitting model is well defined (we use the word 'appears' as we have not, of course, made a complete search of the model space). The complete inversion took about 2 min of processing time on the AP (and a similar time on the VAX 11/780 for control, plotting, etc.). Although an exact comparison is impossible, this figure is comparable with just one trial using the reflectivity method.

To obtain the model shown in Fig. 12 we have assumed that the relative amplitudes and times are accurate, i.e. taken $\lambda_x = \lambda_y = 0$. Considerable care was taken over the amplitude calibrations and topographic corrections, and we believe these assumptions are reasonable. Nevertheless it is interesting to investigate the effect of permitting relative amplitude and time variations, and two experiments are shown here. In both cases we take $\lambda_x = \lambda_y = 1$ and $\lambda_z = 0$ so no model perturbations are permitted. In Fig. 14 we show the best fitting seismograms obtained using model A in Fig. 9 and letting the relative amplitudes and times vary. The final values for the relative amplitudes and times, $c_j$ and $t_j$, are shown for each seismogram. The misfit for these synthetic seismograms is $\phi = 0.662$. Although this is comparable with the

![Figure 14](https://example.com/fig14.png)

Figure 14. Comparison of the FF2 P data and best fitting synthetic seismograms calculated using model A in Fig. 9 where relative amplitude and time perturbations are permitted. For each range the final value of $c_j$ and $t_j$ are indicated (the left and right numbers, respectively).
misfit obtained in Figs 12 and 13 by perturbing the model, we do not consider it a valid solution. Several of the amplitude corrections are at least 50 per cent and two have changed signs. In addition, time corrections greater than 0.02 s are thought to be unlikely. In the second experiment we used the final model from Fig. 12 with the synthetic seismograms in Fig. 13 as our starting point. In Fig. 15 we show the best fitting seismograms together with the relative amplitude and time corrections. The misfit is $\phi = 0.534$. In general the corrections are smaller than in Fig. 14 and no amplitude factor, $c_i$, has changed sign. Again we consider that the larger of these corrections are improbable in view of the care taken in the experiment, but the smaller corrections are certainly within possible bounds. Thus, although we consider the solution in Figs 12 and 13 acceptable, the misfit can be reduced further by permitting relative amplitude and time corrections. In general, if more information were available concerning the uncertainties of the different variables, it would be possible to make a more definitive statement. With the present data set, this is impossible.

The above example has shown that a linear perturbation theory of the WKBJ seismogram and the damped least squares method provide an efficient, automatic method of fitting waveform data. Apart from providing a mechanism for obtaining the best fitting model, an inverse method should also provide information concerning the uncertainty and resolution of the model. The techniques for error and resolution analysis in linear, least squares systems are well known (Lawson & Hanson 1974). Two facts discourage us from pursuing this approach in detail. Clearly the problem is non-linear and the technique only applies to linear systems. The fact that the inversion took more than 10 iterations confirms our initial assumption (Fig. 1) that the problem is non-linear. In Fig. 17 we have given model uncertainties assuming linear theory, and the error bars are obviously well outside the linear range. Secondly our intuition tells us that uncertainties which have not been modelled, particularly...
lateral inhomogeneities, will be very important. Having found the best fitting model using the damped, least squares method, the non-linear problem can be overcome by searching model space for bounds on models which fit within the errors using the 'edgehog' or similar technique (Jackson 1973). This is probably practical using WKBJ seismograms. Nevertheless, we have not included it in this paper as there would seem to be little point until the modelling can be generalized to include lateral inhomogeneities.

Therefore, the error analysis that follows is brief. A more detailed and meaningful analysis must await further developments. First, we should note that the damping parameter, \( \lambda \), used in the inversion procedure has been chosen to optimize the search for the best fitting model and not, as is sometimes the case (Franklin 1970; Jordan & Franklin 1971), from the statistics of the model and data. Having found the best fitting model, however, the damping parameter, \( \lambda \), can be used to investigate the statistics of the solution, i.e. the trade-off between model uncertainty and resolution (Der, Massé & Landisman 1970; Wiggins 1972).

For simplicity we have assumed that the uncertainty of each component of data used in the inversion, i.e. each element of \( y \), is the same. The signal to noise ratio of the data, if we assume a noise level from the record before the first arrival, is very high. However, it is probably more realistic to broaden the definition of noise to include scattered signals, etc. which we have made no attempt to model. Necessarily it is then very difficult to establish the noise level \textit{a priori}. The 'noise' can only be identified definitively if and when the signal is modelled, at which time it no longer need be treated as noise! The choice of uncertainty in the data is therefore somewhat subjective. We have followed the common procedure of estimating the standard deviation of the data from the misfit (25). Thus (Wiggins 1972)

\[
\sigma^2 = \frac{\phi_i}{(N - M_\lambda)}
\]

(56)

where the numerator is the unnormalized misfit, and the denominator is the number of data \( (N) \) reduced by the number of degrees of freedom \( (M_\lambda) \) (Wiggins 1972). The latter is given by (Wiggins 1972)

\[
M_\lambda = \sum_{m=1}^{M} \frac{S_m^2}{S_m^2 + \lambda^2}
\]

(57)

where \( S_m \) are the eigenvalues of the singular value decomposition (41). Because the system is highly overdetermined \( (N > M > M_\lambda) \) the dependence of \( \sigma \) upon \( \lambda \) is not very important. In Fig. 16 we have indicated the uncertainty (56) for the seismograms in Fig. 11. In the following analysis we have only considered the uncertainty in the model parameters and have suppressed variations in the relative amplitudes and times \( (A_2 = 1 \text{ and } A_1 = A_0 = 0) \). In Fig. 16 we have plotted the mean, integrated, weighted data spectrum, i.e.

\[
\sqrt{\sum_{j} d_{ij} \delta (\omega_i, x_j)^2 / J},
\]

and on the same scale, the uncertainty, \( \sigma \).

Perturbations in the model space are related to the data space by (42, 50)

\[
\delta m_{i\lambda} = H VS (S^2 + \lambda^2)^{-1} U^T Q y
\]

(58)

and the uncertainty in the model parameter, \( \delta m_{i\lambda} \), is given by (Wiggins 1972)

\[
\sigma_{i\lambda}^2 = H_{ii} \sigma^2 \sum_{m=1}^{M} V_{im}^2 \left( \frac{S_m^2}{S_m^2 + \lambda^2} \right)^2
\]

(59)
assuming the matrix $H$ is diagonal (40) and the data are independent, each with an uncertainty, $\sigma$. Taking a zero damping parameter ($\lambda = 0$ so $M_\lambda = K$), the uncertainties in the depth variables, $z_k$, of model A from Fig. 10 are plotted in Fig. 17. Clearly models within these error bars are outside the range of linearity, justifying our initial reservations about the validity and use of this error analysis. Although this error analysis was performed for the intermediate model obtained from inverting the $\Delta T = 0.02$ s data (model A in Fig. 10), the results would not be grossly different for the final model (Fig. 13).

Finally, we investigate the model resolution. Substituting for $y$ in (58) we can define the resolution matrix, $R_\lambda$, from

$$\delta m_\lambda = R_\lambda \delta m$$

where (Wiggins 1972)

$$R_\lambda = HVS^2 (S^2 + \lambda^2 I)^{-1} V^T H^{-1}.$$  

Each row of the matrix $R_\lambda$ represents the resolution window through which the model is seen. Differences from the identity matrix $I$, describe the averaging of this window. For simplicity, we define a single resolution parameter at each depth

$$r_{i\lambda} = \sum_{m=1}^{M} (R_{mi\lambda} - \delta_{mi})^2.$$  

By varying the parameter, $\lambda$, we can trade off resolution (62) against uncertainty (59). For $\lambda = 0$, $R_0 = I$ and $r_0 = 0$ (the depth parameters, $z_k$, are all independent and the corresponding eigenvalues non-zero), and for $\lambda = \infty$, $R_\infty = 0$ and $r_\infty = 1$. The trade-off curve for the depth at which the velocity is $5.2$ km s$^{-1}$ is shown in Fig. 18. The uncertainty plotted in Fig. 17 ($\sigma_\lambda = 0.228$ km) corresponds to the lower right end of the curve where $\lambda = 0$. Similar curves exist for all depth variables.

Figure 16. The average spectrum of Fig. 8 divided by frequency to correspond to the integrated, weighted data used in the inversion. The variance of the data assumed is indicated.
Figure 17. The variance of depths in model A in Fig. 10 obtained using the variance in the data from Fig. 16 and the narrowest resolution, i.e. \( \lambda = 0 \). Other details as Fig. 12.

Figure 18. A plot of the resolution versus variance in the depth at which the velocity is \( \alpha = 5.2 \, \text{km} \, \text{s}^{-1} \) in model A (Fig. 10).

Conclusions

In this paper we have demonstrated that a tedious and expensive inversion procedure — trial- and-error fitting of waveforms using reflectivity seismograms (Spudich & Orcutt 1980) — can
be replaced by a straightforward computer program. Similar inversions have been performed before (Mellman 1980), but the technique used in this paper is algebraically and computationally simpler. The damped least-squares method is used to stabilize the inversion procedure. No attempt is made to estimate second derivatives (Mellman 1980). Rather the damping parameter is chosen empirically to optimize approximately the damped model step. Because the forward problem can be solved as easily as computing only one column of the differential matrix, several values of the damping parameter can be tested to find this optimum step. As we find the singular value decomposition of the differential matrix, the overhead in matrix computations for different damping parameters is also small. Although with the data set (Spudich & Orcutt 1980) and the model parameterization ($K = 20$) used in this paper the system is well conditioned, in general it is useful to employ the singular value decomposition of the differential system to investigate possible ill-conditioning (Shaw 1983; Shaw & Orcutt 1985).

The WKBJ seismogram algorithm (14) is particularly suitable to use for the inversion since it is simple and inexpensive to compute. Its algebraic form is sufficiently simple that the differential seismograms are easily derived and they can be computed using the same algorithm as for the normal WKBJ seismogram. Unfortunately, and this seems to be a problem that will be shared by all methods of computing synthetic seismograms, each set of differential seismograms, i.e. a column of the differential matrix, requires essentially the same computational effort as the direct problem. Nevertheless, the WKBJ seismogram algorithm is sufficiently efficient that the computations are feasible for realistic problems. Two other methods have been widely used for computing body-wave synthetic seismograms for realistic crustal models: the Cagniard-de Hoop-Pekeris method (Helmberger 1968) and the reflectivity method (Fuchs & Müller 1971). The former has been used in a numerical inversion scheme (Mellman 1980) but the theory is sufficiently complicated that extensive approximations were necessary before a differential seismogram could be computed efficiently. The algebraic and numerical complications make the method unattractive. In addition, in order to model gradients and turning rays, the model must be approximated by many thin layers with many reflected rays. A similar model is normally used in the reflectivity method (Spudich & Orcutt 1980). To the best of our knowledge, no one has attempted to compute differential seismograms using the reflectivity method. Although the algebra is obvious, the computational burden is formidable. In order to increase the computational efficiency of the inversion, and make interactive computing possible, the computation and decomposition of the differential matrix have been programmed for an array processor. To reduce memory restrictions, the sequential Householder triangularization algorithm is used. While the use of an array processor for linear algebra and Fourier transforms is commonplace, some of the other operations are non-standard and require programming in array processor assembly language. In particular, the WKBJ seismogram (14) and singular value decomposition (Golub & Reinsch 1971) algorithms have been programmed in APAL. The entire differential matrix and decomposition are computed on the array processor with one call from the host computer.

The technique and program developed in this paper form the basis for the viable inversion of body-wave data for crustal structure. Nevertheless, much remains to be done before a versatile, complete method is available and can be used routinely. The technique described in this paper only provides the core for such a program. Many features are fairly trivial extensions of the results in this paper, but others require more research.

It is straightforward to include more rays in the WKBJ seismograms. In particular, the $S$-waves interpreted by Spudich & Orcutt (1980) could easily be modelled and the $S$ velocity structure included in the inversion. Unfortunately, of course, the WKBJ seismogram is a ray
method so the cost increases in proportion to the number of rays included. If the model
includes interfaces, reflections can be included as well as turning rays. The WKBJ seismo-
gram algorithm remains valid for partial and total reflections and head waves. It is straight-
forward to include the interface depths as variable parameters although if we allow the
velocities and densities at interfaces to vary, the problem becomes somewhat more compli-
cated. Extra differential seismograms must be included for the varying coefficients, i.e. the
penultimate term in equation (26). In addition, the perturbation of the delay time (34) is
more complicated and is no longer linear in all parameters.

A more difficult problem is probably the improvement of the misfit criterion (25). While
the least squares function is widely used, it certainly does not correspond to the measure
used by the seismologist’s eye. As discussed above, this situation could be improved by
suitable weighting in the time domain, at the expense of extra Fourier transforms in the
computations. When the misfit between waveforms is larger or the system less well con-
strained (possibly because the source is poorly known), it is useful to use the envelope to
define the misfit between waveforms (Brown 1982, 1983; Shaw 1983; Shaw & Orcutt 1985).
This introduces another non-linear operation into the theory (computing the envelope) but
normally will increase the linearity overall (the envelope will be of a longer period than the
original signal). It may be useful to employ the envelope misfit for the initial iterations when
the required perturbation is large. Equally it may be sensible to include some other data, e.g.
pulse arrival times, to make the inversion more versatile.

We have assumed in this paper that the WKBJ seismograms are sufficiently accurate. For
the example used, we were able to test this in advance. In general, however, periodic tests
must be made using a more accurate technique, e.g. the reflectivity method. It is even
feasible, particularly using an array processor, to use the reflectivity method to compute the
direct synthetic seismograms, e.g. the vector \( \mathbf{y} \). However, it seems prohibitively expensive
and probably unnecessary to compute the differential seismograms using the reflectivity
method. If the direct seismograms are calculated using the reflectivity method (extended
perhaps to include the first-order Langer asymptotic solution so that accurate calculations
can be made for the same model including second-order discontinuities, Thomson &
Chapman 1984), then the WKBJ differential seismograms will be more approximate and
even in the linear limit of infinitesimal model perturbations be in error. Some signals and
their differentials will not be included in the WKBJ seismograms. As the model is perturbed
iteratively and various values of the damping parameter are tested, the accuracy of the differ-
entials is not necessarily important. Any perturbation to the model will perturb the WKBJ
seismograms and be included in the differential seismograms even if it is not fully modelled.
We therefore would not expect the inversion scheme to be biased although it might fail to
find the best fitting model.

The WKBJ seismogram algorithm has been extended to laterally inhomogeneous media
using Maslov asymptotic theory (Chapman & Drummond 1982). Differential seismograms can
be computed for laterally varying structures using the perturbed delay time as easily as in
this paper. However, two new difficulties will arise. First the perturbation of the delay
time can no longer be written as a linear function of the model perturbation. The more
expensive ray calculations will have to be repeated although probably not for every iteration.
Secondly, of course, it will be necessary to restrict severely the number of variable parameters
in the model.

The example in this paper was sufficiently well constrained that the same final model was
obtained from two different starting models (Fig. 10). The standard damped least squares
procedure was satisfactory for finding the best misfit, and it appears to be a unique, global
minimum. In general, however, when the problem is less well constrained, more sophisticated
methods may be necessary. The 'jumping' method used by Shaw & Orcutt (1985) is of particular interest. In this method, the linear system (35) is modified so that some property of the model, $m$, is minimized rather than the model perturbation, $\delta m$. The advantage is that rather than 'creeping' from the initial model to a final model by small model perturbations, the method 'jumps' to unrelated new models.

Finally we should comment that the investigation of model uncertainty is undoubtedly unsatisfactory. It is difficult to estimate the data uncertainty. Much of the misfit is due to deterministic signals generated by scattering, etc. and is not true, random noise. In principle it could be modelled. In practice it is treated as noise. The resultant uncertainties in the model may bear no relationship to the omitted elements of the model that caused the 'noise'. In other words, the parameterization of the model and computation of synthetic seismograms are inadequate and we have no way of handling the resultant misfit. The situation can only improve if the modelling is better or if the non-modelled signals can be recognized and/or removed, e.g. stacking techniques reduce diffractions. In addition to the difficulties with the data uncertainty, using linear theory to convert it to model uncertainty is also unsatisfactory. Model space in the neighbourhood of the final, preferred model should be investigated using a general, non-linear technique such as the edgehog method (Jackson 1973). It is essential that this include lateral variations.

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