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SUMMARY

We compare inversions of Rayleigh wave dispersion curves for shear wave velocity depth profiles based on the L2-norm (Occam’s Inversion) and L1-norm (TV Regularization). We forward model Rayleigh waves using a finite-element method instead of the conventional technique based on a recursion formula and root-finding. The forward modeling naturally leads to an inverse problem that is overparameterized in depth. Solving the inverse problem with Occam’s Inversion gives the smoothest subsurface model that satisfies the data. However, the subsurface need not be smooth and we therefore also solve the inverse problem with TV Regularization, a procedure that does not penalize discontinuities. The use of such a regularization scheme for such an overparameterized inverse problem means blocky subsurface models can be obtained without fixing the layer boundaries in advance. This represents an entirely new philosophy for surface wave inversion.

INTRODUCTION

Obtaining a depth profile of shear wave velocity from surface wave dispersion curves is one of the oldest geophysical inverse problems, with research dating back to at least Dorman and Ewing (1962). A standard approach to the problem involves parameterizing the subsurface as a small number of homogeneous layers with fixed boundaries. The shear wave velocities of the layers are then found through a regularized inversion of an overdetermined system of equations (Gabriels et al., 1987; Xia et al., 1999). The system is overdetermined since the number of data points defining the dispersion curve is larger than the small number of layers used to parameterize the subsurface.

A different approach to the inversion of surface wave dispersion curves is to overparameterize the subsurface with many thin layers and find the smoothest model. This methodology, known as Occam’s inversion, has been advocated by Constable et al. (1987) and deGroot-Hedlin and Constable (1990). The inverted model is found by imposing smoothness constraints on the solution. This is accomplished by penalizing the L2-norm of a roughening operator (e.g., first or second derivative) applied to the model.

Although there may be reasons to expect the subsurface to be smooth, many instances exist when the subsurface may in fact be discontinuous. Moreover, the depths of the discontinuities may not be known in advance. For this situation, we develop an inversion approach that penalizes the L1-norm of the first derivative of the model, known as the Total Variation (TV) Regularization. We first discuss the forward modeling of Rayleigh waves with a finite-element method that naturally leads to an overparameterized subsurface model. We then compare subsurface models obtained using Occam’s inversion (L2-norm) and TV Regularization (L1-norm). For a synthetic example, we find that TV Regularization is able to reconstruct a blocky, discontinuous model without prior knowledge of the location of layer boundaries.

RAYLEIGH WAVE FORWARD MODELING

We forward model Rayleigh waves using a method originally put forward by Lysmer (1970) and recently discussed by Masterlark et al. (2010) and Haney (2010; submitted to Geophysics). For Rayleigh wave modes, we discretize the depth dependence of the mode shapes using a finite set of basis functions. The horizontal \( r_1 \) and vertical \( r_2 \) depth shapes are discretized as

\[
\begin{align*}
\mathbf{r}_1(z) &= \sum_{K=1}^{N} r_1^K \phi_K(z), \\
\mathbf{r}_2(z) &= \sum_{K=1}^{N} r_2^K \phi_K(z).
\end{align*}
\]

Here, we use linear basis functions as in Lysmer (1970). For a non-uniform 1D spatial discretization with element thicknesses \( h_k \) spanning the depth interval \([0, z_{N+1}]\), these basis functions are mathematically defined as

\[
\phi_K(z) = \begin{cases} 
\frac{(z - z_{K-1})}{h_{K-1}} & \text{if } z_{K-1} \leq z \leq z_K, \\
\frac{(z_{K+1} - z)}{h_K} & \text{if } z_K \leq z \leq z_{K+1}, \\
0 & \text{otherwise}.
\end{cases}
\]

By organizing the vector of unknown nodal displacements with alternating vertical and horizontal coefficients as

\[
\mathbf{v} = [ \cdots r_1^{-1} r_1^{-1} r_1^K r_1^K r_2^K r_2^K r_2^{-1} r_2^{-1} ]^T,
\]

the complete system is a generalized quadratic eigenvalue problem in terms of the wavenumber \( k \)

\[
(k^2 B_2 + k B_1 + B_0) \mathbf{v} = \omega^2 M \mathbf{v},
\]

where \( \omega \) is the angular frequency, \( B_2, B_1, \) and \( B_0 \) are stiffness matrices only dependent on the elastic properties \( \lambda \) and \( \mu \), and \( M \) is the mass matrix only dependent on density \( \rho \). All four of the matrices are real-valued and symmetric (Lysmer, 1970), a property that takes on an important role in the development of the inverse problem. The structure of the matrices \( B_2, B_1, B_0, \) and \( M \) is discussed in detail by Lysmer (1970).

DISPERSION CURVE INVERSION

Although Lysmer (1970) fully addressed the forward modeling of Rayleigh waves, the inverse problem was not investigated. As shown in Masterlark et al. (2010), Lysmer’s method can be extended to address inversion as well. The matrix-vector formulation of the forward problem is well-suited for developing
the inversion using straightforward perturbation theory. It can be shown that the perturbation in phase velocity \( c \) due to perturbations in the material properties at fixed frequency is given by

\[
\frac{\delta c}{c} = \frac{1}{2k^2Uc^2} \left( N \sum_{i=1}^{N} \frac{\partial (k^2B_2 + kB_1 + B_0)}{\partial \mu_i} \delta \mu_i \right) + \frac{N}{k^2} \sum_{i=1}^{N} \frac{\partial (k^2B_2 + kB_1 + B_0)}{\partial \lambda_i} \delta \lambda_i - \omega^2 \sum_{i=1}^{N} \frac{\partial M}{\partial \rho_i} \delta \rho_i.
\]

(6)

Note that, for the application discussed here, the eigenvector \( \vec{v} \), wavenumber \( k \), and phase velocity \( c \) all correspond to the fundamental mode; however, equation (6) applies individually to each mode and therefore it is useful for the inversion of higher modes. The matrices appearing in equation (6) are the same as those in the forward problem, equation (5). Thus, the connection between the forward and inverse problems is clear using the matrix-vector notation. Equation (6) is the discrete version of the continuous relations found in Aki and Richards (1980). The derivatives of matrices with respect to the material properties shown above represent the derivatives applied to each individual matrix element.

Evaluated over many frequencies, the above equation results in a linear matrix-vector relation between the perturbed phase velocities and the perturbations in material properties

\[
\frac{\delta c}{c} = K_{\mu}^{\beta} \frac{\delta \mu}{\mu} + K_{\lambda}^{\beta} \frac{\delta \lambda}{\lambda} + K_{\rho}^{\beta} \frac{\delta \rho}{\rho},
\]

(7)

where \( K_{\mu}^{\beta}, K_{\lambda}^{\beta}, \) and \( K_{\rho}^{\beta} \) are the phase velocity kernels for shear modulus, Lamé’s first parameter, and density, respectively. Note that the kernels shown here are for relative perturbations in the phase velocities and material properties.

Although equation (7) is a linear relation between phase velocity perturbations and perturbations in all three material properties, Rayleigh wave phase (or group) velocities are typically only inverted for depth-dependent shear-wave velocity profiles in practice. This is because the Rayleigh wave velocities are most dependent on shear wave velocity in the subsurface (Xia et al., 1999). To find the linear relation between phase velocity perturbations and shear-wave velocity, we use the following relations valid to first order:

\[
\frac{\delta \mu}{\mu} = \frac{2 \delta \beta}{\beta} + \frac{\delta \rho}{\rho},
\]

(8)

and

\[
\frac{\delta \lambda}{\lambda} = \left( \frac{2\alpha^2}{\alpha^2 - 2B^2} \right) \frac{\delta \alpha}{\alpha} - \left( \frac{4B^2}{\alpha^2 - 2B^2} \right) \frac{\delta \beta}{\beta} + \frac{\delta \rho}{\rho},
\]

(9)

where \( \alpha \) is the compressional wave velocity and \( \beta \) is the shear wave velocity. In matrix-vector form, equation (8) and (9) become

\[
\frac{\delta \mu}{\mu} = \frac{2 \delta \beta}{\beta} + \frac{\delta \rho}{\rho},
\]

(10)

and

\[
\frac{\delta \lambda}{\lambda} = D_1 \frac{\delta \alpha}{\alpha} - D_2 \frac{\delta \beta}{\beta} + \frac{\delta \rho}{\rho},
\]

(11)

where \( D_1 \) and \( D_2 \) are matrices whose only nonzero elements lie on the main diagonal. Substituting equation (10) and (11) into equation (7) and setting perturbations in P-wave velocity and density to zero gives

\[
\frac{\delta c}{c} = [2K_{\mu}^{\beta} - K_{\lambda}^{\beta} D_2] \frac{\delta \beta}{\beta} = K^{\beta} \frac{\delta \beta}{\beta},
\]

(12)

which is the linear relation between phase velocity and shear wave velocity. Under the assumption of no perturbations in P-wave velocity and density, the shear-wave velocity kernel is a weighted sum of the \( \alpha \) and \( \mu \) kernels.

A similar linear relation as in equation (12) can be set up for group velocity (Rodì et al., 1975)

\[
\frac{\delta \vec{U}}{U} = K^{U} \frac{\delta \beta}{\beta}.
\]

(13)

This equation is the basis for group velocity inversion. The linear relations shown in equations (12) and (13) are usually set up in terms of absolute perturbations instead of relative perturbations. Denoting the group velocity kernel in this case as \( G^{U} \), the absolute perturbation kernel can be given in terms of the relative perturbation kernel as

\[
G^{U} = \text{diag}(\vec{U}) K^{U} \text{diag}(\vec{\beta})^{-1},
\]

(14)

where \( \text{diag}(\vec{U}) \) is a matrix with the vector \( \vec{U} \) placed on the main diagonal and off-diagonal entries equal to zero.

**OCCAM’S INVERSION**

Occam’s inversion adopts a type of regularization that yields optimally smooth solutions to the inverse problem. We employ a method based on weighted-damped least-squares. Data covariance and model covariance matrices, \( C_d \) and \( C_m \), are chosen, as in Gerstoft et al. (2006). The data covariance matrix is assumed to be a diagonal matrix

\[
C_d = \sigma_d^2 I,
\]

(15)

where \( I \) is the identity matrix and \( \sigma_d \) is the data standard deviation. For simplicity, the standard deviation is assumed to be the same for all data points. The model covariance matrix has the form

\[
C_m(i, j) = \sigma_m^2 \exp(-|z_i - z_j|/\ell),
\]

(16)

where \( \sigma_m \) is the model standard deviation, \( z_i \) and \( z_j \) are the depths of the \( i \)-th and \( j \)-th nodes, and \( \ell \) is a smoothing distance.

With the covariance matrices so chosen, group velocity inversion proceeds using the algorithm of total inversion (Tarantola and Valette, 1982; Muyzert, 2007). The \( n \)-th model update \( \vec{\beta}_n \) is calculated by forming the augmented system of equations (Snieder and Trampert, 1999; Aster et al., 2004):

\[
\begin{bmatrix}
C_d^{-1/2} \\
C_m^{-1/2}
\end{bmatrix} \begin{bmatrix}
\vec{U}_n - f(\vec{\beta}_{n-1}) + G^{U}_{n-1} (\vec{\beta}_{n-1} - \vec{\beta}_0) \\
\vec{G}_n^{U}
\end{bmatrix} = \begin{bmatrix}
\vec{U}_n - f(\vec{\beta}_0) \\
\vec{G}_n^{U}
\end{bmatrix},
\]

(17)
Rayleigh wave inversion: Occam vs. L1-norm

where $\vec{U}_0$ is the group velocity data, $f$ is the (nonlinear) forward modeling operator, and $n$ ranges from 1 to whenever the stopping criterion is met or the maximum allowed number of iterations is reached. The stopping criterion we use is (Gouveia and Scales, 1998)

$$ (f(\vec{\beta}_n) - \vec{U}_0) C_d^{-1} (f(\vec{\beta}_n) - \vec{U}_0) \leq F, \quad (18) $$

where $F$ is the number of measurements (number of frequencies where group velocity has been measured). An identical weighted-damped least-squares scheme applies for phase velocity inversion. The augmented matrix-vector relation can be passed to a conjugate gradient solver, for instance LSQR.

**CONSTRANDED TV REGULARIZATION**

The advantage of using an L2-norm regularization, as in the previous section, is that a closed form solution is available for a linearized phase or group velocity inversion. But the L2-norm regularization is based on the prior belief that the subsurface shear wave velocity follows a Gaussian distribution from a Bayesian statistics perspective, i.e. the model is smooth. In practice, subsurface shear wave velocity may have sharp changes or jumps, thus making the assumption of a smooth model inappropriate. Total variation (TV) regularization is a method which works well for the inversion of non-smooth or piece-wise smooth 1D curves or 2D images (Rudin et al., 1992; Chan et al., 2005). We adopt TV regularization to invert phase or group velocity from a Bayesian statistics perspective, the 1D TV-norm regularization corresponds to the prior belief that the first difference of phase or group velocity to be inverted follows a Laplace distribution (also named double exponential distribution), hence a non-smooth model or a sparse model in the difference transform domain.

In addition to the prior belief that the shear wave velocity $\vec{\beta}$ is piece-wise smooth, we might have other constraints such as bound constraints. For example, non-negativity is a special type of bound constraint. Routh et al. (2007) examined various approaches to obtain non-smooth models and models within prescribed physical bounds in addition to non-smoothness. We denote these constraints as $\vec{\beta} \in C$ where $C$ is a closed convex set. The unconstrained case corresponds to $C = R^p$ where $p$ is the dimension of the discretized $\vec{\beta}$. We will be especially interested in bound constraints given by:

$$ C = \{ \vec{\beta} : L \leq \beta^i \leq U, \forall i \}, \quad (19) $$

where $\beta^i$ denotes the $i$-th entry. Bound constraints describe the situation in which $\vec{\beta}$ has lower and upper bounds. We do not restrict the lower and upper bound to be finite. For example, the choice $L = 0$ and $U = \infty$ corresponds to non-negativity constraints.

The constrained TV-regularized inversion of Rayleigh wave phase or group velocities aims to find a shear wave velocity profile which fits the observed phase or group velocity data subject to TV and closed convex set constraints. That is, we consider the following optimization problem:

$$ \hat{\beta}(\lambda) = \arg \min_{\beta \in C} ||d - f(\vec{\beta})||^2 + 2\lambda\text{TV}(\vec{\beta}), \quad (20) $$

where $\hat{\beta}$ is the inverted model, $d \in R^n$ is the observed phase or group velocity data, $f$ the nonlinear forward modeling operator, and $\lambda > 0$ a regularization parameter which balances the trade-off between the data misfit $||d - f(\vec{\beta})||^2$ and the TV penalty. The discrete TV($\vec{\beta}$) is

$$ \text{TV}(\vec{\beta}) = \sum_{i=1}^{p-1} |\beta^{i+1} - \beta^i|. \quad (21) $$

Solving the above constrained nonlinear TV-regularized minimization problem is a challenging task. A common approach is to iteratively solve a linearized minimization problem by a linear approximation. The linear approximation entails a first-order Taylor expansion about the current solution $\vec{\beta}_n$, where the subscript $n$ represents the iteration number:

$$ f(\vec{\beta}) \approx f(\vec{\beta}_n) + G_n(\vec{\beta} - \vec{\beta}_n). \quad (22) $$

The $q \times p$ size Jacobian matrix $G_n$ is given by equation (14) for group velocity.

Starting with an initial guess $\vec{\beta}_0$, at the $n$-th iteration we solve the following constrained TV-regularized optimization problem to obtain the $n$-th model update $\vec{\beta}_n$:

$$ \vec{\beta}_n = \arg \min_{\vec{\beta} \in C} ||y_{n-1} - G_{n-1}\vec{\beta}||^2 + 2\lambda\text{TV}(\vec{\beta}), \quad (23) $$

where $y_{n-1} = d - f(\vec{\beta}_{n-1}) + G_{n-1}\vec{\beta}_{n-1}$ is the working data at $n$-th iteration.

There is a rich literature on numerical methods for solving an unconstrained TV-regularized convex minimization problem:

$$ \min_{\vec{\beta}} ||y_{n-1} - G_{n-1}\vec{\beta}||^2 + 2\lambda\text{TV}(\vec{\beta}). \quad (24) $$

Beck and Teboullem (2009) gave a non-exhaustive list of these methods. In contrast, the algorithms for solving a constrained TV-regularized convex minimization problem (23) are gradually appearing. Routh et al. (2007) solved the optimization with non-smooth regularization and physical bounds using an interior point method. Krishnan et al. (2009) developed a primal-dual active-set algorithm for bound constrained TV deblurring problems. Chartrand and Wohlberg (2010) solved a TV regularization with bound constraints by a splitting approach, thus allowing existing TV solvers be employed with minimal alteration. Beck and Teboullem (2009) derived a fast algorithm named MFISTA for the constrained TV-based image deblurring problem. A simple version of MFISTA requires users to specify an upper bound on the Lipschitz constant of the gradient of the data misfit $||y_{n-1} - G_{n-1}\vec{\beta}||^2$:

$$ \nabla ||y_{n-1} - G_{n-1}\vec{\beta}||^2 = 2G_{n-1}^T(y_{n-1} - G_{n-1}\vec{\beta}). \quad (25) $$

For our specific problem, we do not know what this upper bound is. Hence, we are not able to apply MFISTA directly.
Rayleigh wave inversion: Occam vs. L1-norm

Figure 1: Comparison of inversion results based on TV Regularization (left) and Occam’s Inversion (right).

However, a modified version of MFISTA with a variable step size can handle the case when the Lipschitz constant is unknown.

We apply the SpaRSA algorithmic framework proposed in Wright et al. (2009) to solve problem (23). SPARSA is an iterative method. When applied to equation (23), each iteration of SpaRSA requires solving a constrained TV-denoising subproblem. We apply the FGP algorithm proposed in Beck and Teboulle (2009) for the constrained TV-denoising subproblem. The FGP algorithm is implemented in the TV_FISTA Matlab package distributed publicly by its authors.

SYNTHETIC EXAMPLE

With the implementations of Occam’s inversion and TV Regularization described above, we tested the methods for group velocity inversion with a simple subsurface model consisting of 3 layers. The subsurface model is shown as a solid blue line and labelled as the true model in Figure 1. The shallowest layer is 60 m thick and the layer beneath it is 110 m thick. The deepest layer is taken to be a halfspace. Rayleigh wave group velocity dispersion curves are modeled over the frequency band from 3-13 Hz and corrupted with 1% Gaussian noise to simulate actual data. For this range of frequencies, the individual finite-elements in the forward model are 10 m thick. The initial model for the inversions is taken to be a homogeneous halfspace and is plotted as a dashed red line in Figure 1.

The results for Occam’s inversion and TV Regularization are plotted as dash-dotted black lines in Figure 1. Both inversions were able to fit the dispersion curve for the true model to within one standard deviation. As expected, the Occam’s inversion returned an optimally smooth model that indicates the presence of a low velocity layer; however, it does not constrain the upper interface of the low velocity layer present in the true model. The inversion based on TV Regularization, on the other hand, is able to reconstruct the sharp upper interface without knowledge of the depth to the interface. Although the upper interface is reconstructed by TV Regularization, the inversion ultimately loses resolution at the lower interface due to the inherent decay of surface waves with depth.

CONCLUSION

We have discussed two methods for surface wave inversion: one an implementation of Occam’s inversion and the other based on the L1-norm. Both methods differ from standard approaches to surface wave inversion in that the subsurface model is overparameterized with many thin layers. For Occam’s inversion, the overparameterization results in an optimally smooth model. There is nothing fundamentally wrong with a smooth model. Indeed, such a model may be warranted in certain geological settings. However, an inversion based on TV Regularization is able to accurately reconstruct a blocky true model. Surface wave inversion with TV Regularization should be a valuable technique to resolve structure when a blocky subsurface is expected a priori. The ability to invert for a blocky model without advance knowledge of the location of interfaces represents an entirely new philosophy for surface wave inversion.

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