

A TRADE-OFF SOLUTION OF REGULARIZED GEOPHYSICAL INVERSION USING MODEL RESOLUTION AND COVARIANCE MATRICES

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Abstract

Regularization is necessary for inversion of ill-posed geophysical problems. Appraisal of inverse models is essential to a meaningful interpretation of these models. Because uncertainties are associated with regularization parameters, extra conditions are usually required to determine proper parameters for assessing inverse models. Commonly used techniques for assessment of a geophysical inverse model derived, generally iteratively, from a linear system are based on calculating the model resolution and the model covariance matrices. Because the model resolution and the model covariance matrices of the regularized solutions are controlled by the regularization parameter, a direct assessment of inverse models using only the covariance matrix may provide incorrect results. To find a proper regularization parameter, we consider an objective function that is the trace of a weighted sum of model resolution and model covariance matrices in the vicinity of a regularized solution where the linearity of inverse problems is normally held. Using the singular value decomposition, we derive explicit formulas to calculate a regularization vector and a weighting vector that result in a minimized objective function. With the optimum regularization vector and weighting vector, we obtain a trade-off solution between model resolution and model covariance in the vicinity of a regularized solution. The unit covariance matrix can then be used to calculate an error bar of the inverse model. We apply these formulas to inverse models of both synthetic and real surface-wave data.

Introduction

Geophysical inverse problems in general are ill-posed problems except for a few specific designed problems such as determining residual mass based on residual gravity anomalies. Nonuniqueness and instability of geophysical inverse solutions are reflections of the ill-posed nature of geophysical inverse problems. There are always infinite solutions that will fit the observed data at a given data-misfit criterion. The fundamental reason of the ill-posed nature is that there are always limited data available for us to determine an earth model that possesses infinite parameters (Backus and Gilbert, 1967, 1968). To seek a meaningful solution from limited geophysical data, therefore, other measures must be included in inversion of geophysical data. The solution should be found based on a criterion associated not only with the data space but also with the model space.

The concept of the model resolution introduced by Backus and Gilbert (1967, 1968) formed a foundation of inverse geophysical problems. Regularization (Tikhonov and Arsenin, 1977) and/or constraints [e.g., Parker (1975) on the theory of ideal bodies for gravity interpretation and Oldenburg (1983) on funnel functions] are conditions that are superposed onto the inverse problems in the model space. They can reduce instability of inversion and the size/dimension of the model space to increase the chance of obtaining a meaningful solution.

The art of superposing regularization and/or constraints provides numerous opportunities to geophysicists who can solve geophysical inverse problems with their knowledge of the nature of a specific data set and an earth model. To reduce instability of geophysical inverse problems with some *a priori* information on the earth model (e.g., Li and Oldenburg, 1996, 2000), a regularized solution that minimizes data misfit and a length of difference between an earth model and a reference model is normally sought [Zhdanov, 2002; detailed discussion can also be found in Oldenburg and Li (2005)]. The regularization parameter with these inverse methods can be determined by Tikhonov's method or the *L*-curve method (Lawson and Hanson, 1974; Tikhonov and Arsenin, 1977; Hansen, 1992, 1998). Applications of *L*-curve in inversion of geophysical data can be found in much of the literature (for example, Hansen, 1992; Li and Oldenburg, 1999).

When no *a priori* information on the earth model is available, common practice is to seek a regularized solution that minimizes data misfit and a length of an earth model, for example, a regularized least-squares solution (Levenberg, 1944; Marquardt, 1963). The regularization parameter acts as a constraint on the model space (Tarantola, 1987) and can be determined by a trial-and-error method, especially because the number of unknowns is small after discretizing an earth model (e.g., Xia et al., 1999, 2002, 2003 on surface-wave inversion) or assuming a specific nonlayered earth model (Xia et al., 2006, on surface-wave inversion for a compressible Gibson half-space). The trade-off solution, equivalently, is a smooth solution calculated by a truncated inverse of a data kernel (Parker, 1994; Hansen, 1998) with the singular value decomposition (Lanczos, 1961; Golub and Reinsch, 1970).

Appraisal of inverse models is critical to geological interpretation of these models because uncertainties are associated with regularized solutions. For the regularized least-squares inversion, a method for resolution analysis based on evaluating the spatial distribution of the upper bounds of the model variations was introduced by Zhdanov and Tolstaya (2006). The other existing techniques for assessment of a geophysical inverse model derived from a linear system are based on calculating the model resolution (Wiggins, 1972) and the model covariance matrices (Tarantola, 1987; Menke, 1984). The model resolution and the model covariance matrices of the regularized solutions are controlled by the regularization parameter. Because of complexity of objective functions of geophysical inverse problems in general, the regularization parameter could vary dramatically in the vicinity of a solution. Therefore, the regularization parameter determined by previous mentioned techniques may result in good model resolution or covariance of solutions but not both.

In this paper, we consider an objective function that is the trace of a weighted sum of model resolution and model covariance matrices in the vicinity of a regularized solution. Using the singular-value decomposition, we derive an explicit formula to calculate a regularization parameter and a weight that result in the minimum of the objective function. We find a trade-off solution between model resolution and model covariance with an optimum regularization parameter and the weight in the vicinity of a regularized solution. The covariance matrix can then be used to calculate an error bar of the inverse model. We apply the formula to inverse models of surface-wave data.

Data Resolution Matrix and Model Resolution Matrix

Let us consider an overdetermined system

$$\mathbf{G}\mathbf{m}^{\text{true}} = \mathbf{d}^{\text{obs}}, \quad (1)$$

where \mathbf{G} is an $m \times n$ matrix ($m > n$ in both cases, m denotes the number of data and n the number of unknowns), and \mathbf{m}^{true} and \mathbf{d} are model and data vectors, respectively. \mathbf{G} stands for a data kernel that embodies \mathbf{m}^{true} and includes the experimental geometry. Letting \mathbf{H} be a generalized inverse of \mathbf{G} , we can estimate model \mathbf{m}^{est}

$$\mathbf{m}^{\text{est}} = \mathbf{H}\mathbf{d}^{\text{obs}}. \quad (2)$$

Substituting Equation 2 (estimate \mathbf{m}^{est}) into Equation 1, we obtain

$$\mathbf{d}^{\text{pre}} = \mathbf{G}\mathbf{m}^{\text{est}} = \mathbf{G}[\mathbf{H}\mathbf{d}^{\text{obs}}] = [\mathbf{G}\mathbf{H}]\mathbf{d}^{\text{obs}} = \mathbf{N}\mathbf{d}^{\text{obs}}. \quad (3)$$

Matrix $\mathbf{N} = \mathbf{G}\mathbf{H}$ is the $m \times m$ data-resolution matrix (Minster et al., 1974). The data-resolution matrix is only determined by the data kernel and any a priori information added to the problem. It is therefore independent of actual values of the data (Menke, 1984). Equation 3 shows the predicted values \mathbf{d}^{pre} are weighted averages of the observed data \mathbf{d}^{obs} . Matrix \mathbf{N} is the weighting function. Each predicted datum is a weighted average of observed data with a row vector as a weighting function. For example, the i th estimated data $d_i^{\text{pre}} = \sum_{j=1}^m n_{ij} d_j^{\text{obs}}$, where n_{ij} is the j th element of the i th row of matrix \mathbf{N} . If data have a

natural ordering, a graph of elements of a row vector of \mathbf{N} varying with column indices provides a sharpness of resolution. If the corresponding row vector is spike-like, the measured datum is well predicted. Otherwise, if the corresponding row vector is broad, the measured datum is poorly predicted. The best scenario is $\mathbf{N} = \mathbf{I}$ (\mathbf{I} is the unit matrix), then each measured datum is perfectly predicted.

Geophysical data would not be perfectly predicted using a regularized least-squares method because the generalized inverse of the solution is $\mathbf{H} = [\mathbf{G}^T\mathbf{G} + \lambda\mathbf{I}]^{-1}\mathbf{G}^T$, where \mathbf{G} is the Jacobian matrix of the model with respect to earth parameters, superscript T denotes the matrix transposition, λ is a regularization parameter, and \mathbf{I} is the unit matrix. The regularization parameter also controls the direction of iterations and speed of convergence (Marquardt, 1963). The regularization parameter acts as a constraint on the model space (Tarantola, 1987, ch. 4). The regularization parameter varies with iterations in surface-wave inversion algorithms depending on behaviors of an objective function. When iterations converge to a local or global minimum, the regularization parameter λ approaches zero (Xia et al., 2005). Therefore, the data-resolution matrix \mathbf{N} in these cases can be written

$$\mathbf{d}^{\text{pre}} = \mathbf{G}\mathbf{H}\mathbf{d}^{\text{obs}} = \mathbf{N}\mathbf{d}^{\text{obs}} = \mathbf{G}[\mathbf{G}^T\mathbf{G} + \lambda\mathbf{I}]^{-1}\mathbf{G}^T\mathbf{d}^{\text{obs}} \approx \mathbf{G}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T\mathbf{d}^{\text{obs}}, \quad (4)$$

where the data-resolution matrix $\mathbf{N} = \mathbf{G}[\mathbf{G}^T\mathbf{G} + \lambda\mathbf{I}]^{-1}\mathbf{G}^T \approx \mathbf{G}[\mathbf{G}^T\mathbf{G}]^{-1}\mathbf{G}^T$.

Equation 4 shows that in general, data cannot be perfectly predicted because \mathbf{N} is not the unit matrix. Narrow peaks along the main diagonal of the matrix suggest that the data can be well predicted. Data associated with larger diagonal values are those needed to define an inverse model for a given problem. Data associated with smaller diagonal values are those we do not have to have in defining an inverse model. In other words, an inverse model cannot be estimated accurately if some necessary data, which possess higher diagonal values of the matrix \mathbf{N} , are not available for a given problem.

On the other hand, substituting Equation 1 (data \mathbf{d}) into Equation 2, we obtain the model-resolution matrix (Wiggins, 1972) for an overdetermined system ($m > n$) with the regularized least-squares method

$$\mathbf{m}^{\text{est}} = \mathbf{H}\mathbf{G}\mathbf{m}^{\text{true}} = [\mathbf{G}^T\mathbf{G} + \lambda\mathbf{I}]^{-1}\mathbf{G}^T\mathbf{G}\mathbf{m}^{\text{true}} = \mathbf{R}\mathbf{m}^{\text{true}}, \quad (5)$$

where the model-resolution matrix $\mathbf{R} = [\mathbf{G}^T\mathbf{G} + \lambda\mathbf{I}]^{-1}\mathbf{G}^T\mathbf{G}$ is an $n \times n$ matrix.

When iterations converge to a local or global minimum, the regularization parameter λ approaches zero and $\mathbf{R} \approx \mathbf{I}$, which means the model can be nearly perfectly resolved. For most real-world cases, Equations 4 and 5 provide a practical way to describe how well measured data can be predicted and how well model parameters can be resolved, respectively. In the same way as the data-resolution matrix, each row of the model-resolution matrix acts as a weighting function to assess how well model parameters are resolved. For example, the i th estimated model parameter is the weighted average of the true model parameters with the i th row of matrix \mathbf{R} as the weighting function. Narrow peaks along the main diagonal of the model-resolution matrix suggest that the model parameters can be well resolved. When $\mathbf{R} \approx \mathbf{I}$, however, errors associated with an inverted model are usually extremely high. So we need to find a trade-off between model resolution and variance. In other words, we should find acceptable regularization parameters in terms of model resolution and variance.

A Trade-off between Model Resolution and Variance

For a linear system, if data are assumed to be uncorrelated, the unit covariance matrix of an inverted model is $\mathbf{C} = \mathbf{H}\mathbf{H}^T$ (Tarantola, 1987; Menke, 1984). Therefore, the unit covariance matrix of a regularized least-squares solution is

$$\mathbf{C} = \mathbf{H}\mathbf{H}^T = [\mathbf{G}^T\mathbf{G} + \lambda \mathbf{I}]^{-1}\mathbf{G}^T([\mathbf{G}^T\mathbf{G} + \lambda \mathbf{I}]^{-1}\mathbf{G}^T)^T. \quad (6)$$

With the singular value decomposition $\mathbf{G} = \mathbf{U} \Lambda \mathbf{V}^T$, where \mathbf{U} and \mathbf{V} are a semi-orthogonal and an orthogonal matrix, respectively, Λ is a diagonal matrix that holds singular values Λ_i , $i = 1, 2, \dots, n$ (Golub and Reinsch, 1970), and $\mathbf{G}^T\mathbf{G} + \lambda \mathbf{I} = \mathbf{V}(\Lambda^2 + \lambda \mathbf{I})\mathbf{V}^T$, we can rewrite the model-resolution matrix (Equation 5) and the unit covariance matrix in the following forms:

$$\mathbf{R} = \mathbf{V} \Lambda^2 [\Lambda^2 + \lambda \mathbf{I}]^{-1} \mathbf{V}^T, \text{ and} \quad (7)$$

$$\mathbf{C} = \mathbf{V} \Lambda^2 [\Lambda^2 + \lambda \mathbf{I}]^{-2} \mathbf{V}^T, \text{ respectively.} \quad (8)$$

Because of linearity of inverse problems in a vicinity of a solution, we can estimate model resolution and variance with Equations 7-8 in a vicinity of a solution if a proper regularization parameter can be found. In general, a regularized least-squares solution results in an erratic unit covariance matrix because of the uncertainty of the regularization parameter in a vicinity of a solution, which will be demonstrated with the following synthetic example. Therefore, we seek a solution with a constraint on the regularization parameter, which provides a trade-off solution between model resolution and covariance.

As Equations 7-8 indicate, the regularization parameter affects only the diagonal elements of the model resolution and the unit covariance matrices. Based on the concept of a trade-off between the model resolution and variance (Backus and Gilbert, 1967, 1968), we define an objective function Φ as the trace of the weighted sum of \mathbf{R} and \mathbf{C} :

$$\begin{aligned} \Phi &= \text{trace}[(1 - \alpha)\mathbf{C} + \alpha(\mathbf{I} - \mathbf{R})] \\ &= \text{trace}[(1 - \alpha)(\mathbf{V} \Lambda^2 (\Lambda^2 + \lambda \mathbf{I})^{-2} \mathbf{V}^T) + \alpha(\mathbf{I} - \mathbf{V} \Lambda^2 (\Lambda^2 + \lambda \mathbf{I})^{-1} \mathbf{V}^T)] \\ &= \text{trace}[\mathbf{V}\{(1 - \alpha)\Lambda^2 (\Lambda^2 + \lambda \mathbf{I})^{-2} + \alpha(\mathbf{I} - \Lambda^2 (\Lambda^2 + \lambda \mathbf{I})^{-1})\}\mathbf{V}^T] = \min, \end{aligned} \quad (9)$$

where λ and α are a regularization parameter vector and a weighting factor vector, respectively, as we discuss in the following. Minimizing Φ will find the optimum λ and α that provide us a trade-off solution between the model resolution and variance.

It is interesting to note that the matrix in the parenthesis $\{\}$ is a diagonal matrix with the i th element (> 0), so we obtain

$$\begin{aligned} \Phi &= \sum_{i=1}^n \sum_{j=1}^n \phi_i v_{ij}^2 \text{ with} \\ \phi_i &= (1 - \alpha_i) \Lambda_i^2 [\Lambda_i^2 + \lambda_i]^{-2} + \alpha_i (1 - \Lambda_i^2 [\Lambda_i^2 + \lambda_i]^{-1}), \end{aligned} \quad (10)$$

where λ_i and α_i are the i th element of the regularization parameter vector and of the weighting vector, respectively; v_{ij} is the element of matrix \mathbf{V} at the i th row and the j th column. These unique characteristics of the objective function Φ revealed by the singular value decomposition makes minimizing Φ extremely simple. To minimize Φ , we only need to minimize each coefficient ϕ_i (Equation 10), which leads us to find the following λ_i and α_i that minimize ϕ_i :

$$\lambda_i = 0.5(\sqrt{\Lambda_i^4 + 4\Lambda_i^2} - \Lambda_i^2) \text{ and} \quad (11)$$

$$\alpha_i = 2(2 + \Lambda_i^2 + \lambda_i)^{-1}, \text{ } (0 < \alpha_i < 1). \quad (12)$$

Here we assume that treatment of extremely small singular values ($\Lambda_i \approx 0$) has been done using the truncated SVD (e. g., Oldenburg and Li, 2005) or simply by altering these values by adding a small positive constant. We can show $0 < \lambda_i < 1$ with relationships of three sides of a right triangle, two sides of the right angle of which are Λ_i^2 and $2\Lambda_i$.

After an inverse solution is found by the regularized least-squares inversion, we can calculate the best model resolution and unit covariance matrices in the trade-off criterion (Equation 9) using Equations 7-8 with the regularization parameter determined by Equation 11. In practice, we can estimate the standard deviation of an inverse model with the formula

$$\Delta m_i = \Delta d \sqrt{\sum_{j=1}^n \gamma_j v_{ij}^2}, \quad (13)$$

where Δm_i is the i th element of the standard deviation $\Delta \mathbf{m}$ of an inverse model, $\gamma_j = \Lambda_j^2 [\Lambda_j^2 + \lambda_j]^{-2}$, and Δd is the data standard deviation, which could be replaced by a threshold of terminating iterations.

A Synthetic Example

The synthetic data are calculated based on the model (Table 1) from Xia et al. (1999). Based on the data-resolution matrix, Xia et al. (2008) selected 14 data points that possess diagonal values of 0.175 and higher to perform an inversion. The initial model was the same used in Xia et al. (1999) with the same initial regularization parameter ($\lambda_0 = 1$). The inversion results (column 4 in Table 2) are superior to results from Xia et al. (1999) and possess almost perfect model resolution (Table 3), especially for layers 4 and 5. As pointed out in the previous section, the unit covariance matrix indicates a tremendous error associated with the half-space (column 7 in Table 3), which we know is not correct based on our knowledge of the synthetic model. An extra iteration starting from this model with regularization parameters and weighting factors (Table 4) determined by Equations 11 and 12 can produce a trade-off model between model resolution and variance (column 5 in Table 2). Model variance is dramatically reduced at the cost of reducing model resolution. The Euler distance between the trade-off model (column 5 in Table 2) and the model from selected data (column 4 in Table 2) is 1.8 m/s. With Equation 13, we can estimate a standard deviation in the trade-off model assuming data are uncorrelated and using the threshold of terminating iterations (1.0 m/s) as the standard deviation of data. The maximum standard deviation of the trade-off model associated with the half-space is ± 3.7 m/s (column 7 in Table 4). The trade-off solution provides an acceptable reasonable model in terms of model resolution and variance.

Table 1. Earth model parameters (Xia et al., 1999).

Layer number	v_s (m/s)	v_p (m/s)	ρ (g/cm ³)	\mathbf{H} (m)
1	194.0	650.0	1.82	2.0
2	270.0	750.0	1.86	2.3
3	367.0	1400.0	1.91	2.5
4	485.0	1800.0	1.96	2.8
5	603.0	2150.0	2.02	3.2
The half space	740.0	2800.0	2.09	infinite

Table 2. Inversion results of synthetic data. The unit is in m/s. Relative errors are in parentheses.

True	Initial	Inverted (Xia et al., 1999)	Inverted with selected data (Xia et al., 2008)	Trade-off solution
194	230	194 (0)	194	195
270	272	272 (1)	270	271
367	330	351 (4)	367	368
485	397	539 (11)	485	486
603	453	535 (-11)	601	601
740	1036	741 (0)	740	739

Table 3. Model resolution and variance (diagonal elements of R and C) of a synthetic example.

Layer #	1	2	3	4	5	Half-space
Resolution	1.0	1.0	1.0	1.0	0.99	1.0
Variance	0.03	0.10	0.13	1.08	7.11	254

Table 4. Model resolution and variance (diagonal elements of R and C) of a trade-off solution of a synthetic example.

Layer #	1	2	3	4	5	Half-space
Resolution	0.94	0.81	0.62	0.41	0.09	0.90
Variance	0.03	0.08	0.07	0.27	0.20	13.9

Real-world Examples

Data of the first example were acquired in San Jose, California (Figure 1a), and included the well-defined fundamental and higher modes in the frequency-velocity domain (Figure 1b) (Xia et al., 2003). A 14-layer model with layer thicknesses of 1 m was used to invert the Rayleigh-wave data. Xia et al. (2008) calculated the data-resolution matrix (Equation 4 with $\lambda = 0$) of the multi-layer model with 35 data points selected from different frequencies up to the second mode to show how well each datum and each mode could be predicted. They selected 16 data points based on the data-resolution matrix that possess diagonal values of 0.45 and higher to perform inversion. Sixteen data points are near the minimum number of data necessary to solve the problem with 14 unknowns. The initial model was the same as the one used in Xia et al. (2003) with the same initial regularization parameter ($\lambda_0 = 1$). We showed inverted results from the selected data and inverted results from multi-mode data (28 data points with the fundamental-mode data up to 23 Hz, Xia et al., 2003) in Figure 2 with the best-inverted model that was obtained from “error-free” data (we labeled this model as “true” in Figure 2). Overall, inversion results of the 16 selected data are closer to the “true” model than results from multi-mode data (Xia et al., 2003).

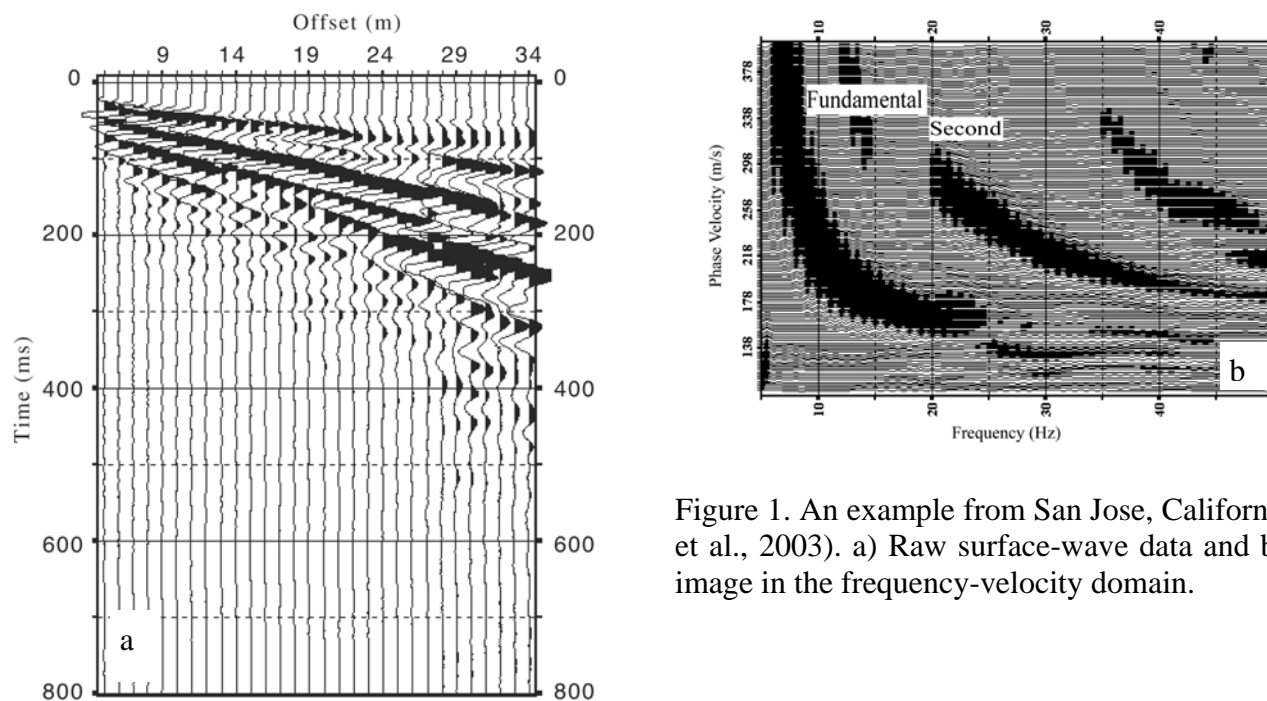


Figure 1. An example from San Jose, California (Xia et al., 2003). a) Raw surface-wave data and b) their image in the frequency-velocity domain.

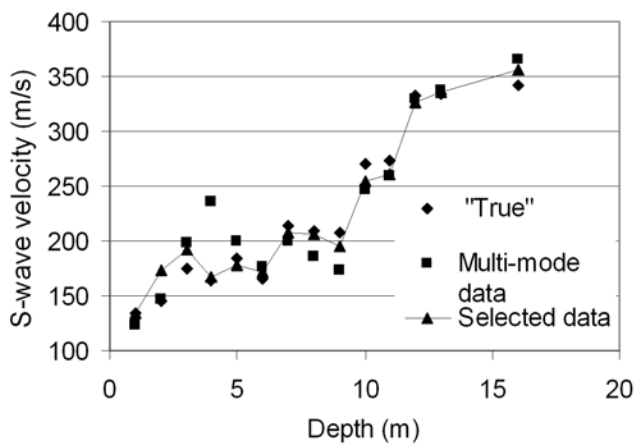


Figure 2. Inversion results of the San Jose example. Model “True” was obtained from inverting “error-free” data and “Multi-mode data” was the inverted model from 28 multi-mode data (Xia et al., 2003). “Selected data” was the inverted model from 16 data points selected based on data-resolution functions.

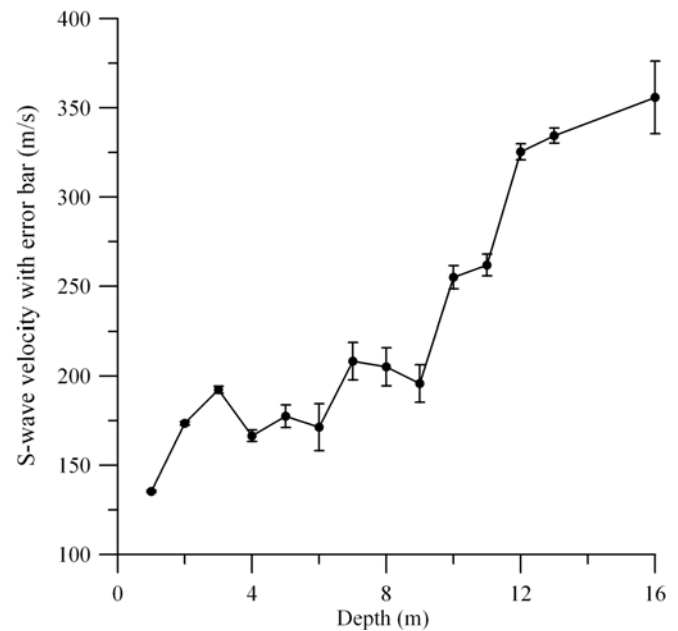


Figure 3. Inverted results of the San Jose example with an extra iteration from the inverted model of “Selected data” (Figure 2). Error bars were computed with the optimal regularization vector (Table 6).

The inversion of the 28-data set was converged to the model denoted by squares (Figure 3) with $\lambda = 10^{-1}$ (Xia et al., 2003). The inversion of 16 selected data points was converged to the model denoted by triangles (Figure 3) with $\lambda = 10^{-3}$. The inverted model from 16 selected data points possesses higher model resolution, but the model also has higher variance (diagonal elements of the model resolution and the covariance matrices, Table 5). As we discussed in the previous section, an extra iteration starting from this model with regularization parameters and weighting factors (Table 6) determined by Equations 11 and 12 can produce a trade-off model between model resolution and variance (Table 7). Model variance is dramatically reduced at the cost of reducing model resolution. The Euler distance between the trade-off model (Figure 3) and the model from selected data (triangles in Figure 2) is

Table 5. Model resolution and variance (diagonal elements of R and C) of the San Jose example.

Layer #	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Resolution	0.30	0.41	0.55	0.49	0.46	0.46	0.36	0.44	0.43	0.29	0.34	0.26	0.24	0.99
Variance	0.17	0.71	5.83	12.9	145	394	308	373	362	244	290	220	202	838

Table 6. Regularization parameters and weighting factors for the trade-off model.

Layer #	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Reg. Param.	0.72	0.52	0.26	0.18	0.05	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01	0.01
Weighting	0.44	0.65	0.85	0.90	0.98	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99

Table 7. Model resolution and variance (diagonal elements of R and C) of the trade-off model.

Layer #	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Resolution	0.03	0.05	0.08	0.12	0.11	0.14	0.09	0.09	0.09	0.03	0.03	0.02	0.02	0.34
Variance	0.01	0.03	0.13	0.31	1.22	5.23	3.33	3.48	3.37	1.28	1.14	0.63	0.54	12.6

2.4 m/s. With Equation 13, we can estimate a standard deviation in the trade-off model if assuming data are uncorrelated and using the threshold of terminating iterations (5.8 m/s) as the standard deviation of data. The maximum standard deviation of the trade-off model associated with layer 14 is ± 20 m/s (Figure 3).

Data acquired in Vancouver, Canada (Figure 4a), are used for our second example (Xia et al., 2003). Fundamental-, second- and third-mode data are well defined in the frequency-velocity domain (Figure 4b). Rayleigh-wave data were inverted using a 14-layer model with a common layer thickness of 2 m. Xia et al. (2008) calculated the data-resolution matrix (Equation 4 with $\lambda = 0$) of the multi-layer

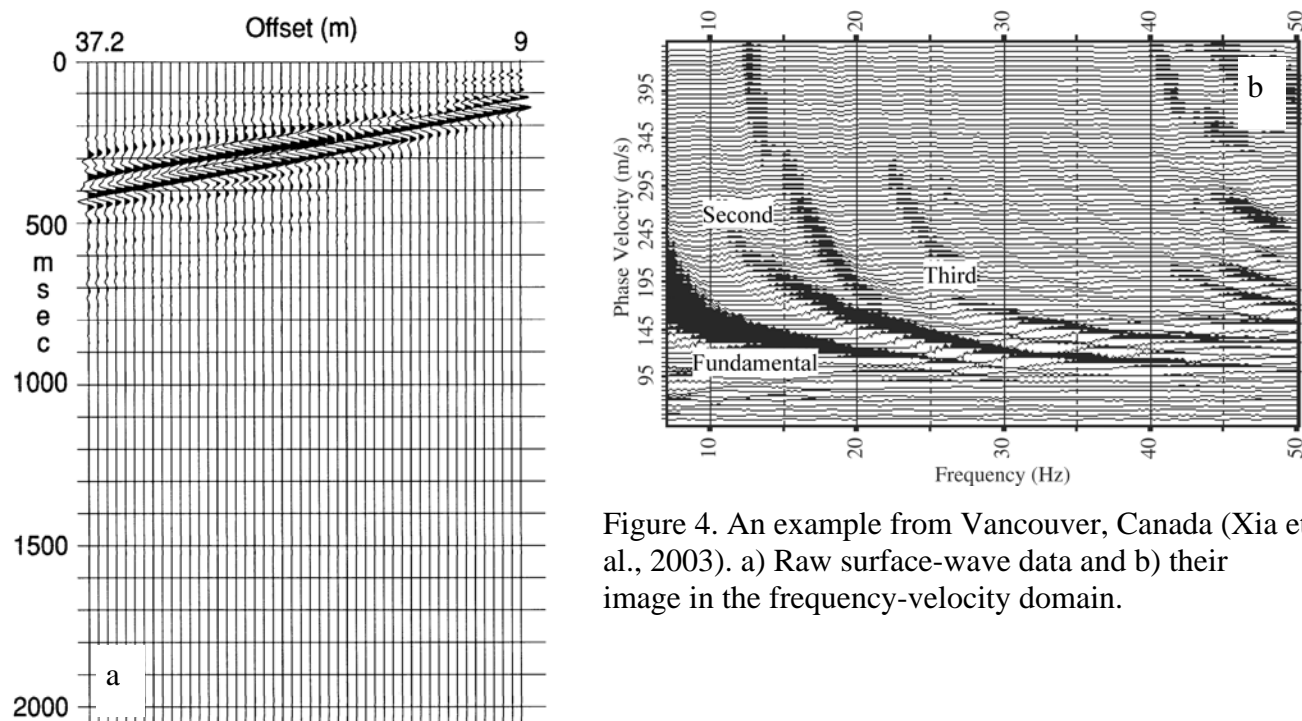


Figure 4. An example from Vancouver, Canada (Xia et al., 2003). a) Raw surface-wave data and b) their image in the frequency-velocity domain.

model to show how well each datum and each mode could be predicted. They selected 29 data points based on the data-resolution matrix that possess diagonal values of 0.35 and higher, the same range for the fundamental- and the second-mode data (53 data points) used by Xia et al. (2003), to perform an inversion. The initial model was the same as used in Xia et al. (2003) with the same regularization parameter ($\lambda_0 = 1$). Inverted results from these 29 selected data and from multi-mode data (Xia et al., 2003) were compared with the borehole measurements (Figure 5). Inversion results from the 29 selected data are closer to the borehole measurements than results from multi-mode data up to 16 m in depth. For the deeper part (> 16 m)

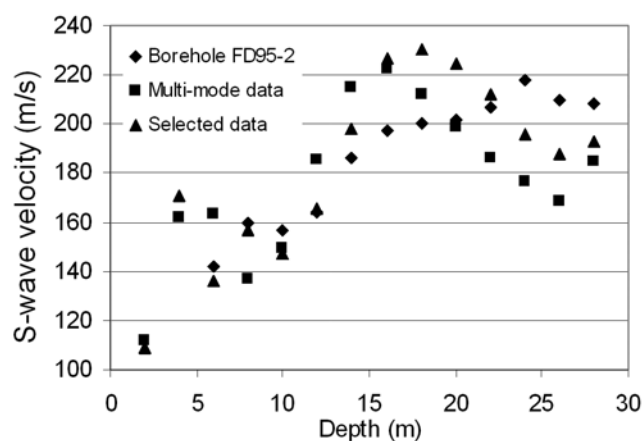


Figure 5. Inversion results of the Vancouver example. “Multi-mode data” was the inverted model from 53 fundamental- and second-mode data (Xia et al., 2003). “Selected data” was the inverted model from 29 data points selected based on data-resolution functions. “Borehole FD95-2” was S-wave velocities from direct borehole measurements (Hunter et al., 1998).

(Figure 5), a significant discrepancy is evident between inverted results and borehole measurements (Hunter et al., 1998). No improvement could be made in this part of the model because the longest wavelengths of the fundamental-mode, second-mode, and third-mode data are around 23 m, 11 m, and 8 m, respectively. As discussed in Xia et al. (2003), the maximum depth of investigation with these data sets is around 16 m. To accurately define S-wave velocities for the deeper part (> 16 m), lower (< 7 Hz) frequency data or extra higher-mode data are necessary.

Table 8. Model resolution and variance (diagonal elements of R and C) of the Vancouver example.

Layer #	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Resolution	0.99	0.87	0.95	0.82	0.61	0.59	0.45	0.40	0.36	0.32	0.30	0.28	0.28	0.28
Variance	0.26	3.23	14.5	37.2	141	246	324	292	263	229	214	206	200	203

Table 9. Regularization parameters and weighting factors for the trade-off model.

Layer #	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Reg. Param.	0.82	0.41	0.22	0.14	0.06	0.04	0.02	0.02	0.02	0.02	0.02	0.02	0.02	0.02
Weighting	0.30	0.75	0.87	0.93	0.97	0.98	0.99	0.99	0.99	0.99	0.99	0.99	0.99	0.99

Table 10. Model resolution and variance (diagonal elements of R and C) of the trade-off model.

Layer #	1	2	3	4	5	6	7	8	9	10	11	12	13	14
Resolution	0.32	0.23	0.24	0.16	0.11	0.09	0.05	0.02	0.01	0.01	0.01	0.01	0.01	0.01
Variance	0.06	0.21	0.46	0.56	1.00	1.12	1.15	0.53	0.35	0.29	0.27	0.26	0.25	0.25

The inversion of the 53-data-point set converged to the model is denoted by squares (Figure 5) with $\lambda = 10^{-2}$ (Xia et al., 2003). The inversion of 29 selected data point converged to the model is denoted by triangles (Figure 5) with $\lambda = 10^{-3}$. The inverted model from 29 selected data possesses higher model resolution, but the model also has higher variance (diagonal elements of the model resolution and the covariance matrices, Table 8). As we discussed in the previous section, an extra iteration starting from this model with regularization parameters and weighting factors (Table 9) determined by Equations 11 and 12 can produce a trade-off model between model resolution and variance (Table 10). Model variance is dramatically reduced at the cost of reducing model resolution. The Euler distance between the trade-off model (Figure 6) and the model from selected data (triangles in Figure 5) is 11.5 m/s. With Equation 13, we can estimate a standard deviation in the trade-off model by assuming data are uncorrelated and using the threshold of terminating iterations (8.5 m/s) as the standard deviation of data. The maximum standard deviation of the trade-off model associated with layer 6 is ± 4 m/s (Figure 6).

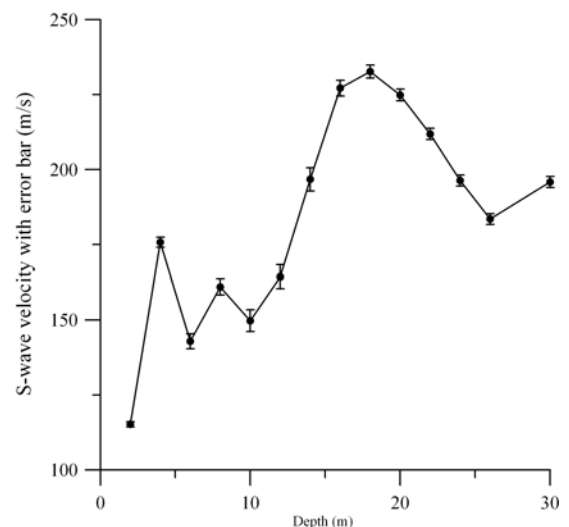


Figure 6. Inverted results of the Vancouver example with an extra iteration from the inverted model of “Selected data” (Figure 5). Error bars were computed with the optimal regularization vector (Table 9).

Conclusions

A regularized least-squares solution usually results in an erratic unit covariance matrix because of the uncertainty of the regularization parameter in the vicinity of a solution. The erratic unit covariance matrix makes it difficult to appraise an inverse model. To find a proper regularization vector, we applied the concept of a trade-off between model resolution and variance in appraisal of an inverse model. We considered an objective function that is the trace of a weighted sum of model resolution and model covariance matrices in the vicinity of a regularized solution. Using the singular value decomposition, we derived explicit formulas to calculate a regularization vector and a weighting vector that result in the minimum of the objective function. With the optimum regularization vector and the weighting vector, we can calculate the trade-off solution between model resolution and model covariance in the vicinity of a regularized solution. The unit covariance matrix can then be used to calculate an error bar of the inverse model. The synthetic example of surface-wave inversion demonstrated that a regularized solution may not provide a correct covariance matrix, and the trade-off solution is necessary for assessment of an inverse model. Two real world examples of surface-wave data also demonstrated that the unit covariance matrix with the optimal regularization and weighting vectors provides a practical tool of assessing inverse models obtained using a regularized least-squares method.

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