Square-Root Variable Metric based Elastic Full Waveform Inversion and Uncertainty Estimation

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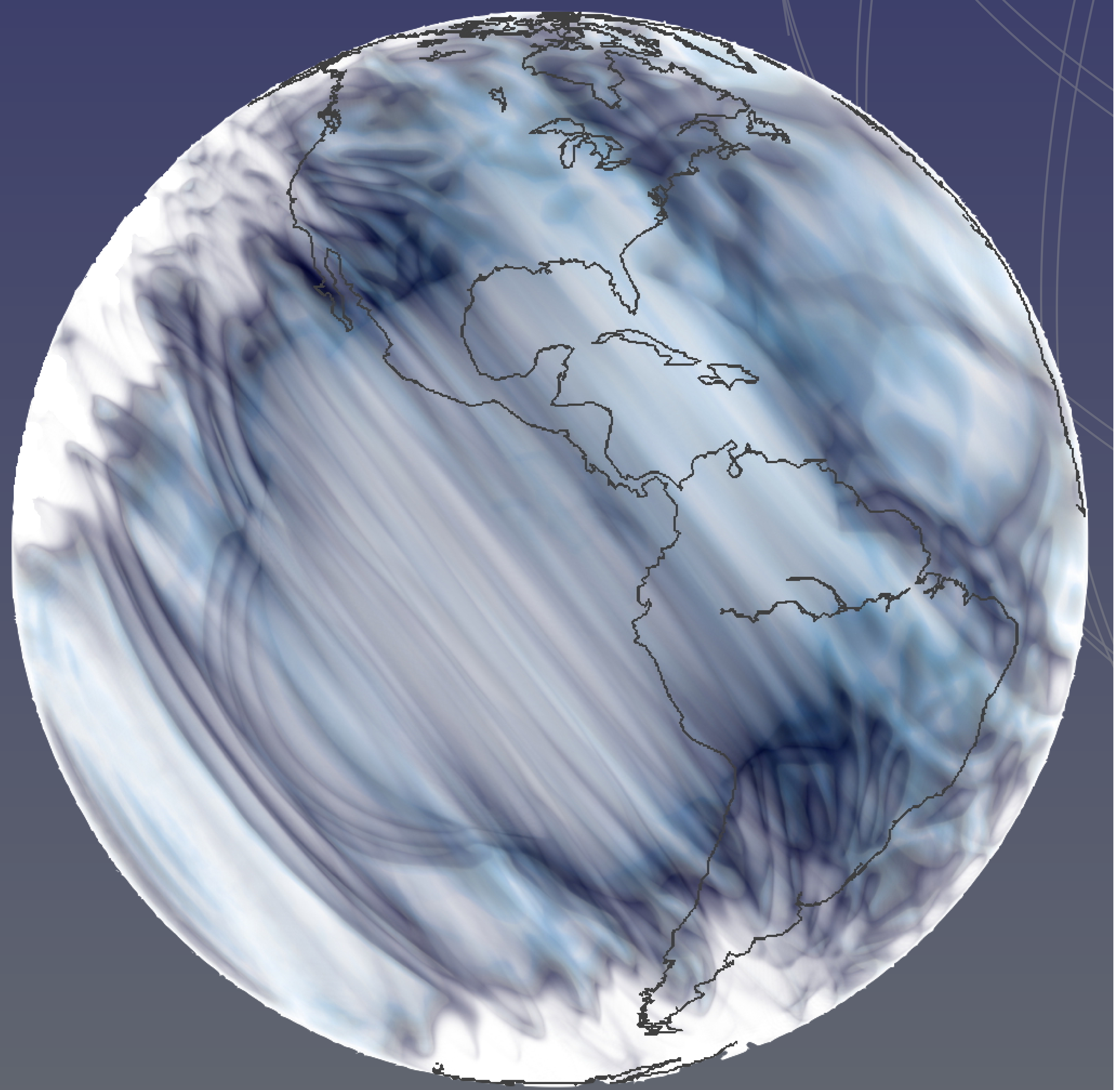

Abstract

Full-waveform inversion (FWI) is a powerful tool in inverting high-quality subsurface geophysical properties; however, its uncertainty estimation is equally important but still left behind. The uncertainty estimation is on the posterior covariance, which is Hessian-related and thus prohibitive to store for practical problems.
We investigate the application of the square-root variable metric (SRVM) method, a quasi-Newton optimization algorithm, to elastic FWI in a memory-affordable vector version. In the elastic Marmousi testing with our method, we take the state-of-the-art L-BFGS method for reference. After the final iteration we can access the posterior covariance by reconstructing the inverse Hessian over the SRVM vector series. The posterior standard deviation and a selection of random samplings of posterior models can measure uncertainties in our elastic FWI.

Introduction

The uncertainty estimation in elastic FWI is Hessian-related. We use a quasi-Newton method named SRVM to approach the inverse Hessian during the iterative inversion process. We write SRVM into a matrix-free vector version, making it memory affordable. The size of one SRVM vector equals that of the model, and the vector number equals the iteration number. Theoritically, the vector-version SRVM can collect up the second-order derivative information from the initial model to the final inverted model. After the inversion converges, we can approximate the inverse Hessian from the stored SRVM vectors and scalars recursively, and then access the posterior covariance matrix. To facilitate the analysis on the posterior information, we incorporate SRVM with Randomized Sigular Value Decomposition (RSVD), yielding an efficient RSVD-SRVM approach in uncertainty estimation.

Theory and Method

The derivation of the vector-version SRVM is based on the DFP algorithm, which reads

$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\mathbf{B}_k \Delta\mathbf{g}_k \Delta\mathbf{g}_k^T \mathbf{B}_k}{\Delta\mathbf{g}_k^T \mathbf{B}_k \Delta\mathbf{g}_k} + \frac{\Delta\mathbf{m}_k \Delta\mathbf{m}_k^T}{\Delta\mathbf{g}_k^T \Delta\mathbf{m}_k}, \tag{1}$$

with $\mathbf{B} = \mathbf{H}^{-1}$ the inverse Hessian, $\Delta\mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$ and $\Delta\mathbf{m}_k = \mathbf{m}_{k+1} - \mathbf{m}_k$. To ensure the positive-definite property of $\mathbf{B}$, SRVM reads:

$$\mathbf{S}_{k+1}\mathbf{S}_{k+1}^T = \mathbf{S}_k \left(\mathbf{I} - (1/P_k)\mathbf{S}_k^T \mathbf{y}_k \mathbf{y}_k^T \mathbf{S}_k\right) \mathbf{S}_k^T, \tag{2}$$

with $\mathbf{B}_k = \mathbf{S}_k\mathbf{S}_k^T$.To make Eq. (2) matrix-free, we express a vector-verion SRVM workflow as

Algorithm 1 SRVM vector-version workflow

1: **for** $k \leftarrow 0$ to n **do**
2: $\quad\Delta\mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$ ▷ Gradient update
3: $\quad\mathbf{y}_k = \mu_k \mathbf{g}_k + \Delta\mathbf{g}_k$
4: $\quad\mathbf{w}_k = \mathbf{S}_k^T \mathbf{y}_k$ ▷ Vectors
5: $\quad\beta_k = \mathbf{S}_k^T \Delta\mathbf{g}_k$
6: $\quad P_k = \mathbf{w}_k^T \beta_k$ ▷ Scaling factors
7: $\quad Q_k = \mathbf{w}_k^T \mathbf{w}_k$
8: $\quad\nu_k = \frac{1-\sqrt{1-Q_k/P_k}}{Q_k/P_k}$
9: $\quad\mathbf{S}_{k+1} = \mathbf{S}_k \left(\mathbf{I} - \frac{\nu_k}{P_k}\mathbf{w}_k\mathbf{w}_k^T\right)$ ▷ Matrix update
10: $\quad\mathbf{B}_{k+1} = \mathbf{S}_{k+1}\mathbf{S}_{k+1}^T = \mathbf{S}_k \left(\mathbf{I} - \frac{\nu_k}{P_k}\mathbf{w}_k\mathbf{w}_k^T\right)\left(\mathbf{I} - \frac{\nu_k}{P_k}\mathbf{w}_k\mathbf{w}_k^T\right)^T \mathbf{S}_k^T$
11: **end for**

During the invesion, in Alg. (1), we only keep the vector $\mathbf{w}_k$ and the scalar $\frac{\nu_k}{P_k}$, and update the search direction with a matrix-vector multiplication: $\mathbf{p}_{k+1} = -\mathbf{S}_{k+1}\mathbf{S}_{k+1}^T\mathbf{g}_{k+1}$.
After the final iteration we can retrieve the inverse Hessian $\mathbf{H}^{-1} = \mathbf{B}$ from the stored $\mathbf{w}_k$ and $\frac{\nu_k}{P_k}$. We furthermore design a RSVD-SRVM combination to facilitate the sampling of inverse Hessian. The relationship between the posterior covariance and inverse Hessian reads

$$\mathbf{C}_M = (\mathbf{G}^T\mathbf{C}_d^{-1}\mathbf{G} + \mathbf{C}_m^{-1})^{-1} = (\mathbf{H} + \varepsilon\mathbf{C}_m^{-1})^{-1}, \tag{3}$$

with $\mathbf{G}$ being the Fréchet derivative, $\mathbf{C}_m$ the prior covariance, ε the prefactor for regularization. If we precondition the Fréchet derivative with $\mathbf{C}_m^{1/2}$, Eq. (3) changes into

$$\mathbf{C}_M = (\mathbf{H}\mathbf{C}_m + \varepsilon\mathbf{I})^{-1}\mathbf{C}_m \approx \widetilde{\mathbf{H}}^{-1}\mathbf{C}_m. \tag{4}$$

$\widetilde{\mathbf{H}}^{-1}$ performs on $\mathbf{C}_m$ as a "big filter" to approach $\mathbf{C}_M$. We sample the prior and posterior covariances using

$$\mathbf{m}_{prior} = \mathbf{m}_0 + \mathbf{C}_m^{1/2}\mathbf{n}, \qquad \mathbf{m}_{\mathbf{post}} = \widetilde{\mathbf{m}} + \mathbf{C}_{\mathbf{M}}^{1/2}\mathbf{n}, \tag{5}$$

with $\mathbf{m}_0$ being the initial model, $\widetilde{\mathbf{m}}$ the inverted model, $\mathbf{n}$ 2D random samplers, and $\mathbf{C}_M^{1/2} = \mathbf{V}\Lambda^{1/2}\mathbf{V}^T\mathbf{C}_m^{1/2}$ constructed from randomized SVD.

Results

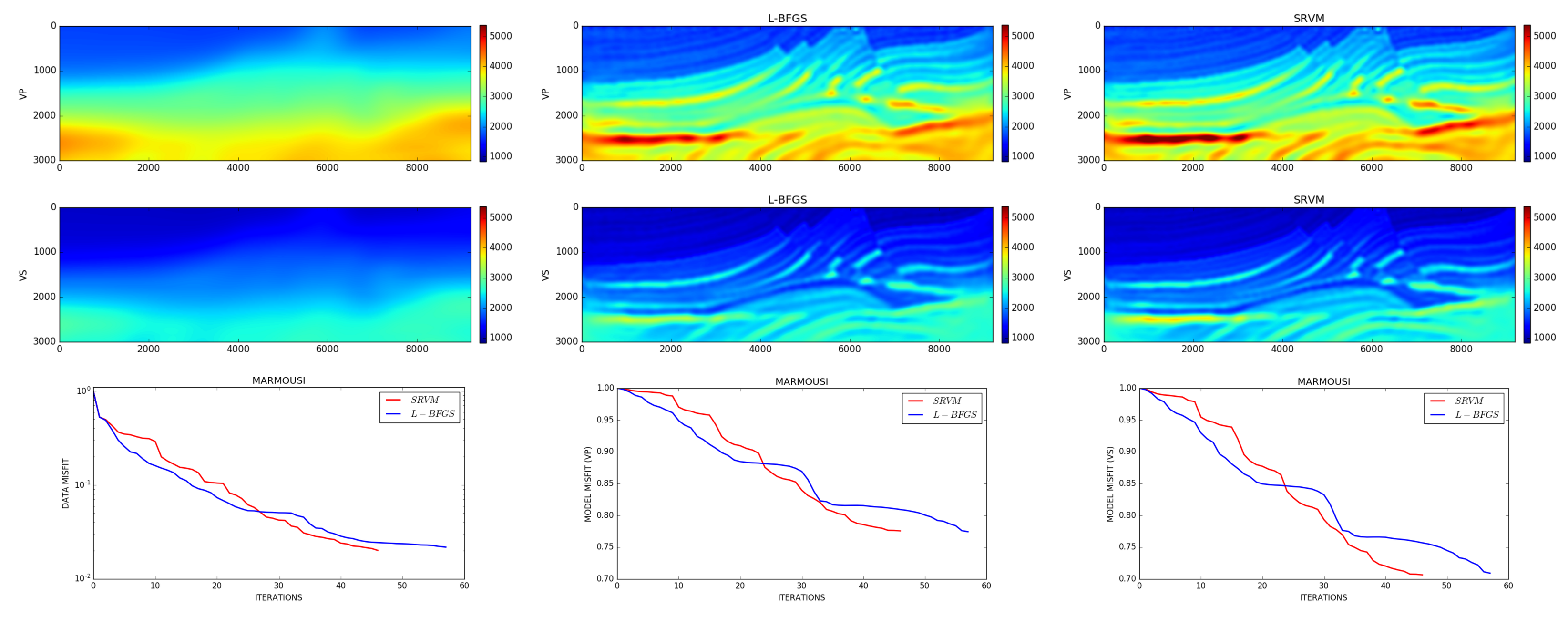

Figure 1: SRVM versus L-BFGS in the elastic Marmousi testing (no surface waves).

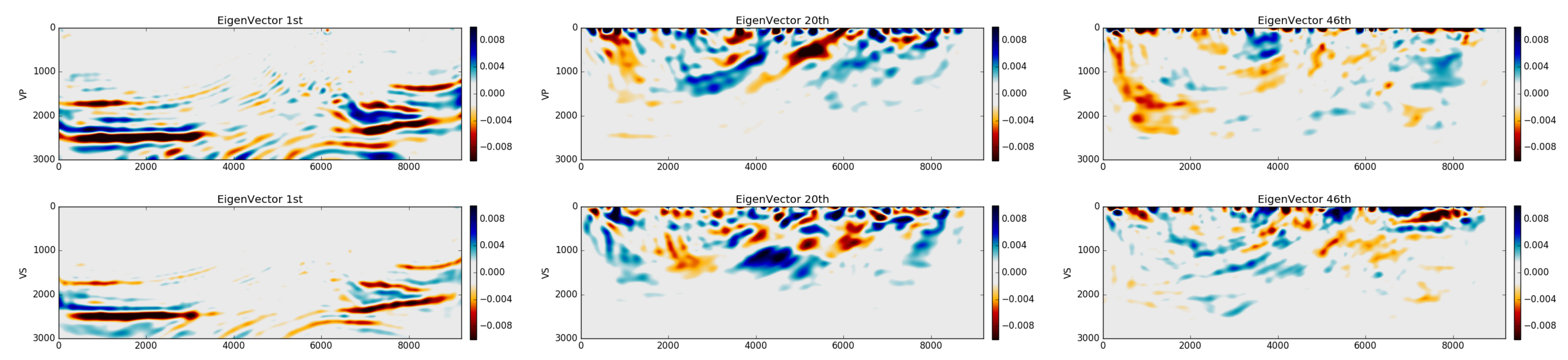

Figure 2: Examples of contributing eigenvectors of the inverse Hessian, by randomized SVD

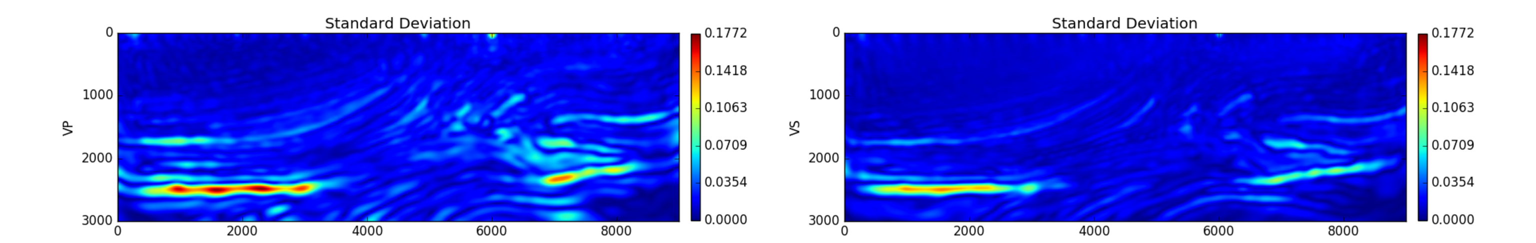

Figure 3: Standard deviation maps (from the diagonals of posterior covariance).

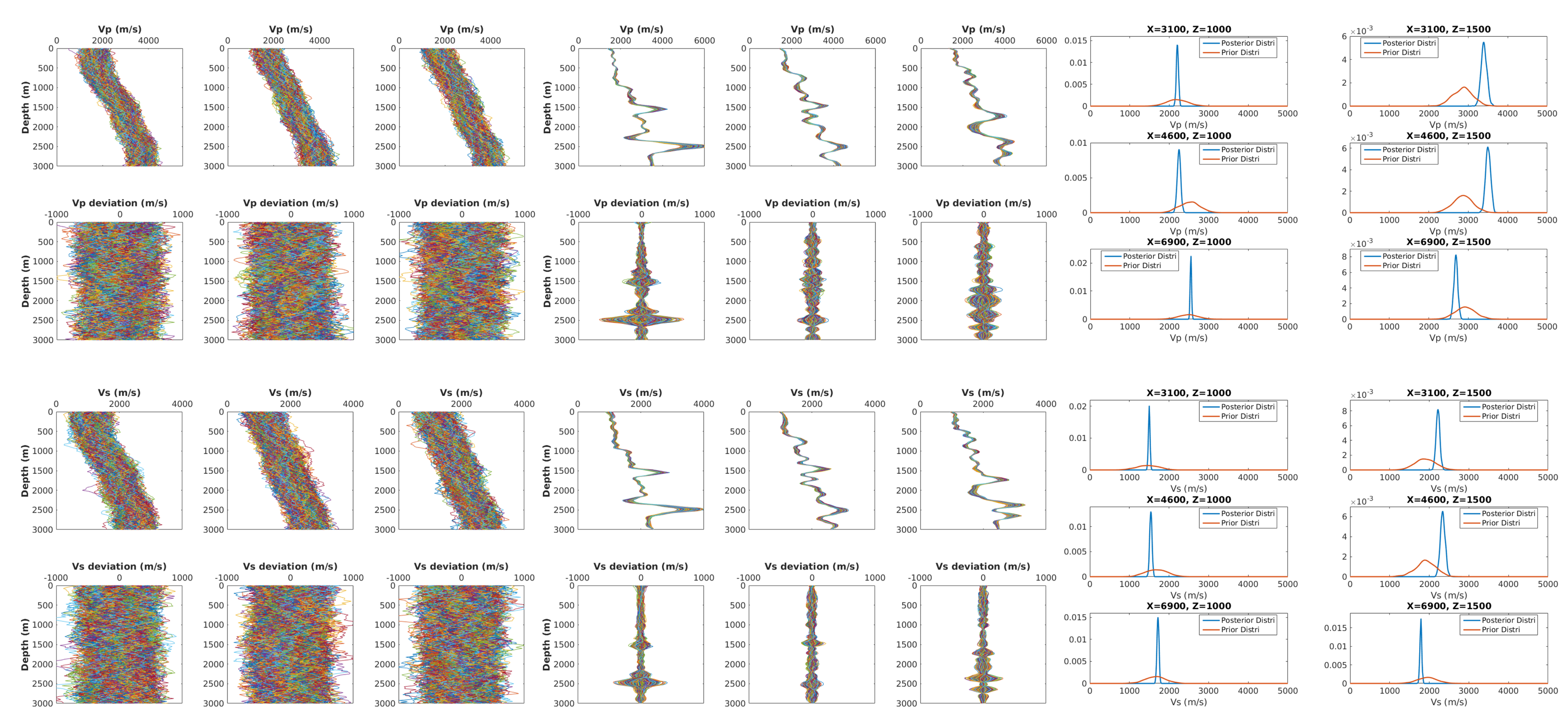

Figure 4: Comparisons of depth profiles between the (left) prior and (middle) posterior distributions of (up) V_P and (bottom) V_S, and their corresponding (right) extracted marginal distributions .

Conclusions

We compare SRVM with L-BFGS in elastic FWI. In our elastic Marmousi testing, SRVM is as good as L-BFGS in the convergence behaviors of data and model misfits, and has the advantage of reconstructing the approximated inverse Hessian from the SRVM vector series in a memory-affordable manner. The inverse Hessian acts as a "big filter" on the prior covariance to approach the posterior covariance. We can then assess the uncertainty information about elastic FWI via analyzing the posterior covariance with several tools, such as pointwise standard deviation and visualized random samples.

Acknowledgments & References

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