Square-Root Variable Metric based nullspace shuttle: a characterization of the non-uniqueness in elastic full-waveform inversion

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Key Points:

- We apply a square-root variable metric (SRVM) scheme to study the nullspace shuttle.
- The vector-version SRVM method is memory-efficient and amends to large-scale geophysical inverse problems.
- The nullspace shuttle helps characterizing the non-uniqueness of ill-posed seismic inverse problems.

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Abstract

Full-waveform inversion (FWI) is for most geophysical applications an ill-posed inverse problem, with non-unique solutions. We examine its non-uniqueness by exploring the nullspace shuttle, which can efficiently generate an ensemble of data-fitting solutions. We construct this shuttle based on a quasi-Newton method, the square-root variable-metric (SRVM) method. The latter provides access to the inverse data-misfit Hessian in FWI for large-scale applications. Combining the SRVM method with a randomised singular value decomposition, we obtain the eigenvector subspaces of the inverse data-misfit Hessian. Its primary eigenvalue and eigenvector are considered to determine the null space of inversion result. Using the SRVM-based nullspace shuttle, we can modify the inverted result a posteriori in a highly efficient manner without corrupting the data misfit. Also, because the SRVM method is embedded through elastic FWI, our method can be extended to multi-parameter problems. We confirm and highlight our approach with the elastic Marmousi example.

1 Introduction

Full-waveform inversion (FWI) is an important tool in estimating the seismic parameters of the Earth from observed waveform data. As an inverse problem, FWI attempts to seek the "optimal" model which minimizes the data misfit, defined most commonly as the least-squares residual between observed and synthetic data (Tarantola, 2005). The ever-increasing capabilities in data acquisition and computation enable FWI to constrain seismic models with increasing resolution (Fichtner & Leeuwen, 2015; Fichtner, Zunino, & Gebraad, 2018; Virieux & Operto, 2009). However, due to the limitations of data coverage and the uncertainties in measurements or theories, FWI is an ill-posed problem with non-unique solutions (Fichtner & Zunino, 2019; Fichtner et al., 2018; Tarantola, 2005; Trampert & Van Der Hilst, 2005). Indeed, the non-uniqueness of solutions is common to all geophysical inverse problems using actual measurements (Backus & Gilbert, 1967; Parker, 1977, 1994), with particularly challenging problems such as in seismic, finite-source, magnetic and gravity inversions (Leweke, Michel, & Telschow, 2018; Mai et al., 2016; Michel & Fokas, 2008; Snieder & Trampert, 1999; Vasco, Lane, & Majer, 1993, see, e.g.,). Thus, further insights can be gained by investigating and quantifying the associated model space.

Regarding the non-uniqueness in FWI solutions, the nullspace of the model space provides a collection of models a posteriori within a small misfit tolerance (Deal & Nolet, 1996; Fichtner & Zunino, 2019). Due to its efficiency, the projection of model changes onto the

nullspace is termed as the "nullspace shuttle", which is guided by the prior information but imposed onto the inverted image a posteriori. The nullspace shuttle exploits the underdetermined nature of the ill-posed problem in seismic inversion. Deal and Nolet (1996) project the model changes onto the space spanned by the nullspace eigenvectors of the data-misfit Hessian. To attack large-scale realistic problems, they obtain the eigenvalues and eigenvectors of the data-misfit Hessian by an iterative method named LSQR (Nolet & Snieder, 1990; Paige & Saunders, 1982; Scales, 1987). Hereafter, Rowbotham and Pratt (1997) use the nullspace shuttle to introduce the anisotropy parameter a posteriori to improve the inversion solutions. Deal, Nolet, and van der Hilst (1999) project the difference between the tomographic model and the temperature model onto the nullspace to remove the traveltime violation caused by the temperature components. Trampert and Spetzler (2006) investigate the finite-frequency effects of surface wave tomography in the nullspace. More recently, de Wit, Trampert, and Hilst (2012) generalize the nullspace shuttle to estimate the bounds of the tomographic image to produce a collection of acceptable models. And finally, Fichtner and Zunino (2019) employ a Hamiltonian approach to explore the effective nullspace in nonlinear inverse problems where also the forward modeling equations are nonlinear and the misfit functional non-quadratic.

We attempt here to define the nullspace shuttle in elastic FWI based on the Square-Root Variable Metric (SRVM) method (Hull & Tapley, 1977; Morf & Kailath, 1975; Williamson, 1975) together with randomized singular value decomposition (SVD) (Halko, Martinsson, & Tropp, 2011; Liberty, Woolfe, Martinsson, Rokhlin, & Tygert, 2007). Tarantola (2005) unburies the fact that SRVM may allow for model resolution analysis and posterior sampling. The original SRVM methods are formulated in a matrix version. Luo (2012) and Liu, Peter, and Tape (2019) rewrite the SRVM method into a vector version to make it memory-affordable for large-scale FWI problems. Liu and Peter (2019) furthermore incorporate the randomized SVD into the vector-version SRVM approach.

Given a problem which is linear or linearized around the optimum, the model uncertainties can be measured with the resolution (Boschi, 2003) or covariance (Soldati & Boschi, 2005) matrices. Based on these studies, in this paper, rather than indirectly building the nullspace shuttle with the nullspace eigenvectors of the data-misfit Hessian (Deal & Nolet, 1996), we directly build the shuttle with the first, primary eigenvector of the inverse data-misfit Hessian. Our research is similar to Meju (2009), who proposes to find a collection of acceptable models with the inverse Hessian by using extremal bound analysis.

Subsequently, we construct a number of different models which all conserve the data misfit within a small misfit tolerance by drawing random samples from the posterior distributions (Bui-Thanh, Ghattas, Martin, & Stadler, 2013; Tarantola, 2005; Zhu, Li, Fomel, Stadler, & Ghattas, 2016). This way, we unite the deterministic and probabilistic approaches for model appraisal. Because the SRVM method can be employed as optimization scheme in acoustic and elastic FWIs (Liu, 2019; Liu & Peter, 2019), it is straightforward to extend this approach to a SRVM-based multi-parameter nullspace shuttle.

In the following, we briefly review the nullspace shuttle method. Then, we introduce the SRVM-based inverse data-misfit Hessian retrieval and combine it with the randomized sampling. Next, we propose the SRVM-based nullspace shuttle and construct a set of conservatively filtered models a posteriori. Finally, we verify our approach through a numerical demonstration for exploration benchmarks.

2 Theories and Methods

2.1 Review of the nullspace shuttle method

The nullspace shuttle method for geophysical tomography was originally proposed by Deal and Nolet (1996), and then got several applications (de Wit et al., 2012; Fichtner & Zunino, 2019; Rowbotham & Pratt, 1997). The term nullspace shuttle as introduced by Deal and Nolet (1996) refers to the operator which allows to move from one solution to another without corrupting the data fit. While Fichtner and Zunino (2019) refer to the shuttle "paths", Deal and Nolet (1996) and this paper talk about the shuttle "vehicles". Based on the SVD regarding the data-misfit Hessian or the sensitivity matrix, this approach is used to generate a collection of models with permissible changes but conserve data misfits. We start with the forward problem

$$\mathbf{d} = \mathbf{f}(\mathbf{m}), \quad (1)$$

which predicts the observed seismograms $\mathbf{d}$ from a given seismic model $\mathbf{m}$. The linearized forward problem reads

$$\delta \mathbf{d} = \mathbf{G} \delta \mathbf{m}, \quad (2)$$

with $\delta \mathbf{m} = \mathbf{m} - \mathbf{m}_0$, $\delta \mathbf{d} = \mathbf{d} - \mathbf{d}_0$, and $\mathbf{G} = \partial \mathbf{f}(\mathbf{m}) / \partial \mathbf{m}$ being the Fréchet derivative or the sensitivity matrix. The normal equation in the least-squares sense reads

$$\mathbf{G}^T \mathbf{G} \delta \mathbf{m} = \mathbf{G}^T \delta \mathbf{d}, \quad (3)$$

where $\mathbf{G}^T$ is the transpose of $\mathbf{G}$, and $\mathbf{G}^T \mathbf{G}$ is also known as the Gauss-Newton approximation to the data-misfit Hessian (Pratt, 1999; Virieux & Operto, 2009).

Deal and Nolet (1996) propose to build a set of conservatively filtered models by projecting the model changes onto the generalized nullspace eigenvectors of $\mathbf{G}^T \mathbf{G}$. They take an iterative method named LSQR (Paige & Saunders, 1982) for eigen-decomposition. However, even with the knowledge of the full eigenvectors, we cannot directly define the nullspace from $\mathbf{G}^T \mathbf{G}$ due to the following reasons: (i) the definition of the full nullspace is not feasible because it would require many more eigenvectors than those of the effective nullspace (Fichtner & Zunino, 2019); (ii) in practical applications, data noise may be mapped into the nullspace, making the definition more elusive. Rather than directly deriving from the nullspace eigenvectors, Deal and Nolet (1996) attack this problem from another direction. That is, they first select the eigenvectors that define the range of $\mathbf{G}^T \mathbf{G}$, and then subtract the constructed resolution matrix from an ideal resolution matrix, i.e., the identity matrix, to get the nullspace shuttle. That is, given a tolerance $\eta \geq 0$, the perturbations around the "optimal" model $\tilde{\mathbf{m}}$ may still conserve the data fit as (Fichtner & Zunino, 2019)

$$\mathbf{f}(\tilde{\mathbf{m}} + \delta \mathbf{m}_{null}) \leq \mathbf{f}(\tilde{\mathbf{m}}) + \eta, \quad (4)$$

in which $\delta \mathbf{m}_{null}$ denotes the nullspace shuttle in the model space.

2.2 Constructing the inverse Hessian via a vector-version SRVM approach

In Newton's method, the relationship between the model perturbation $\Delta \mathbf{m}$ and the gradient $\mathbf{g}$ is

$$\Delta \mathbf{m} \approx -\mu \mathbf{H}^{-1} \mathbf{g}^T = -\mu \mathbf{B} \mathbf{g}^T, \quad (5)$$

where μ is the one-dimensional search step, $\mathbf{H}$ the Hessian, and $\mathbf{B}$ the inverse Hessian. The standard Davidon-Fletcher-Powell (DFP) method (Fletcher & Powell, 1963) gives an iterative approximation to the inverse Hessian

$$\mathbf{B}_{k+1} = \mathbf{B}_k - \frac{\mathbf{B}_k \Delta \mathbf{g}_k \Delta \mathbf{g}_k^T \mathbf{B}_k}{\Delta \mathbf{g}_k^T \mathbf{B}_k \Delta \mathbf{g}_k} + \frac{\Delta \mathbf{m}_k \Delta \mathbf{m}_k^T}{\Delta \mathbf{g}_k^T \Delta \mathbf{m}_k}, \quad (6)$$

with $\Delta \mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$ and $\Delta \mathbf{m}_k = \mathbf{m}_{k+1} - \mathbf{m}_k$. A workflow of a vector-version SRVM algorithm (Liu et al., 2019) is expressed as

Algorithm 1 SRVM vector-version workflow

```

1: for  $k \leftarrow 0$  to  $n$  do
2:    $\Delta \mathbf{g}_k = \mathbf{g}_{k+1} - \mathbf{g}_k$  ▷ Gradient update
3:    $\mathbf{y}_k = \mu_k \mathbf{g}_k + \Delta \mathbf{g}_k$ 
4:    $\mathbf{w}_k = \mathbf{S}_k^T \mathbf{y}_k$  ▷ Vectors
100 5:    $\beta_k = \mathbf{S}_k^T \Delta \mathbf{g}_k$ 
6:    $P_k = \mathbf{w}_k^T \beta_k$  ▷ Scaling factors
7:    $Q_k = \mathbf{w}_k^T \mathbf{w}_k$ 
8:    $\nu_k = \frac{1 - \sqrt{1 - Q_k / P_k}}{Q_k / P_k}$ 
9:    $\mathbf{S}_{k+1} = \mathbf{S}_k \left( \mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right)$  ▷ Matrix update
10:    $\mathbf{B}_{k+1} = \mathbf{S}_{k+1} \mathbf{S}_{k+1}^T = \mathbf{S}_k \left( \mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right) \left( \mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right)^T \mathbf{S}_k^T$ 
11: end for

```

In the vector-version SRVM algorithm, we only need to keep one vector $\mathbf{w}_k$ and one scalar $\frac{\nu_k}{P_k}$ additionally per iteration, which is memory-efficient even for large-scale problems. The initial guess of $\mathbf{S}_0$ is an identity matrix $\mathbf{I}$ such that all the operations are expressed in vectors except for those regarding $\mathbf{S}_{k+1}$ and $\mathbf{B}_{k+1}$. Note that in the SRVM-based elastic FWI, we determine the search direction with the gradient via a matrix-vector product operation $\mathbf{S}_{k+1} \mathbf{S}_{k+1}^T \mathbf{g}_{k+1}$, which is finally in a vector version (Liu et al., 2019). Once the SRVM-based FWI converges after n iterations, we have $\mathbf{B}_{n+1}$, a positive-definite approximation to retrieve the inverse Hessian over all the iterations (Liu & Peter, 2019), as follows

$$\mathbf{B}_{n+1} = \mathbf{B}_0 + \sum_{k=0}^n \left(\frac{\Delta \mathbf{m}_k \Delta \mathbf{m}_k^T}{\Delta \mathbf{g}_k^T \Delta \mathbf{m}_k} - \frac{\mathbf{B}_k \Delta \mathbf{g}_k \Delta \mathbf{g}_k^T \mathbf{B}_k}{\Delta \mathbf{g}_k^T \mathbf{B}_k \Delta \mathbf{g}_k} \right), \quad (7)$$

in which $\mathbf{B}_0$ is usually chosen as an identity matrix $\mathbf{I}$, an initial guess of the inverse Hessian. Also, $\mathbf{B}_0 = \mathbf{I}$ acts as a stabilizer to ensure a sufficiently stable $\mathbf{B}_k$ during iterative inversion (Nocedal & Wright, 2006). As the iterations proceed, $\mathbf{B}_{k+1}$ tends to the inverse Hessian (Tarantola, 2005). Equation (7) indicates that the history information about the gradients and the model updates only contributes to $\mathbf{B}_{n+1} - \mathbf{B}_0$, so we retrieve the approximated inverse Hessian by (Liu & Peter, 2019)

$$\mathbf{H}^{-1} = \mathbf{B}_{n+1} - \mathbf{I}. \quad (8)$$

Given the stored scalar series $\frac{\nu}{P}$ and vector series $\mathbf{w}$ in algorithm (1) over the past k iterations, we can reconstruct $\mathbf{B}_{n+1}$ via

Algorithm 2 $\mathbf{B}_{n+1}$ retrieval workflow

```

1: for  $k \leftarrow 0$  to  $n$  do
104 2:    $\mathbf{S}_{k+1} = \mathbf{S}_k \left( \mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right)$ 
3:    $\mathbf{B}_{k+1} = \mathbf{S}_{k+1} \mathbf{S}_{k+1}^T = \mathbf{S}_k \left( \mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right) \left( \mathbf{I} - \frac{\nu_k}{P_k} \mathbf{w}_k \mathbf{w}_k^T \right)^T \mathbf{S}_k^T$ 
105 4: end for

```

106 The outer product $\mathbf{w}_k \mathbf{w}_k^T$ in algorithm (2) spans a matrix, which is not easy to store
107 and operate for large-scale problems. In the next subsection, we will seek solutions from
108 randomised SVD to facilitate the information retrieval from algorithm (2).

2.3 Randomised SVD into SRVM approach

109
110 The SRVM method is a low-rank approach to reconstruct $\mathbf{H}^{-1} \approx \mathbf{B}_{n+1} - \mathbf{I}$. To fur-
111 ther facilitate the sampling from $\mathbf{H}^{-1}$, we employ the randomised SVD (Halko et al., 2011;
112 Liberty et al., 2007) to efficiently factorize $\mathbf{H}^{-1}$ into eigenvalues and eigenvectors. Given
113 a symmetric matrix $\mathbf{Z}$ of dimension $M \times M$ and a set of random vectors $\mathbf{X}$ of dimension
114 $M \times N_R$, where N_R is the estimated rank order of $\mathbf{Z}$, the randomised SVD runs in a workflow
115 described below

Algorithm 3 Single-pass randomised SVD algorithm

```

1:  $\mathbf{Y} = \mathbf{Z}\mathbf{X}$  ▷ Sampling  $\mathbf{Z}$  with  $\mathbf{X}$ 
2:  $\mathbf{QR} = \mathbf{Y}$  ▷ QR decomposition on  $\mathbf{Y}$ 
116 3:  $\mathbf{A}(\mathbf{Q}^T \mathbf{X}) = \mathbf{Q}^T \mathbf{Y}$  ▷ Solve for  $\mathbf{A}$ 
4:  $\mathbf{U}\mathbf{\Lambda}\mathbf{U}^T = \mathbf{A}$  ▷ SVD on  $\mathbf{A}$ 
5:  $\mathbf{V} = \mathbf{QU}$ 
117 6:  $\mathbf{Z} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^T$ 

```

118 In our application, we have $\mathbf{Z} = \mathbf{B}_{n+1} - \mathbf{I}$. The key to combining SRVM and randomised
119 SVD is how to construct $\mathbf{Y}$ from algorithm (2). For each random vector $\mathbf{x}$ within $\mathbf{X}$, we
120 have a sampled vector $\mathbf{y}$ for $\mathbf{Y}$ as

Algorithm 4 Sampling vector $\mathbf{y}$ for $\mathbf{Y}$

```

121 1:  $\mathbf{d} = -\mathbf{S}_{n+1}^T \mathbf{x} = \prod_{i=0}^n (\frac{v_i}{P_i} \mathbf{w}_i \mathbf{w}_i^T - \mathbf{I}) \mathbf{x} = \prod_{i=0}^n [\frac{v_i}{P_i} (\mathbf{w}_i^T \mathbf{x}) \mathbf{w}_i - \mathbf{x}]$ 
      2:  $\mathbf{y} = \mathbf{S}_{n+1} \mathbf{S}_{n+1}^T \mathbf{x} = \mathbf{S}_{n+1} \mathbf{d} = \prod_{i=0}^n (\mathbf{I} - \frac{v_i}{P_i} \mathbf{w}_i \mathbf{w}_i^T) \mathbf{d} = \prod_{i=0}^n [\mathbf{d} - \frac{v_i}{P_i} (\mathbf{w}_i^T \mathbf{d}) \mathbf{w}_i]$ 
122 3:  $\mathbf{y} = \mathbf{y} - \mathbf{x}$ 

```

We run such kind of random samplings on $\mathbf{Z}$ with a collection of independent $\mathbf{x}$ for n_{iter} times, with n_{iter} being the iteration number at convergence, because $\mathbf{Z}$ has already been in a low-rank form in algorithm (1). Then, we merge the resulting $\mathbf{y}$ collection into a matrix $\mathbf{Y}$ to continue the workflow in algorithm (3), whose verification can be found in Liu and Peter (2019). Finally, we can represent the inverse Hessian in a SVD form as

$$\mathbf{H}^{-1} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^T, \quad (9)$$

in which the eigenvectors of $\mathbf{H}^{-1}$ are ordered within $\mathbf{V}$ and the eigenvalues within $\mathbf{\Lambda}$. In the next subsection, we will introduce the SRVM-based nullspace shuttle from the subspace spanned from $\mathbf{V}$.

2.4 SRVM-based nullspace shuttle

In this part, we attempt to construct the SRVM-based nullspace shuttle. Deal and Nolet (1996) project the model-space changes onto the nullspace of the data-misfit Hessian $\mathbf{G}^T \mathbf{G}$. However, the estimation of the full nullspace eigenvectors is infeasible, because it would require many more eigenvectors than that of the effective-space eigenvectors (Deal & Nolet, 1996). Also, it is hard to define the noiseless nullspace eigenvectors. Finally, Deal and Nolet (1996) define the projection matrix for the nullspace shuttle by subtracting the resolution matrix constructed by the effective-space eigenvectors from the ideal resolution matrix, i.e., the identity matrix.

Suppose we could succeed in finding the full, noiseless nullspace eigenvectors in a non-singular $\mathbf{G}^T \mathbf{G}$, then this would correspond to the subspace spanned by the last smallest eigenvalues. Subsequently, if we take the inverse of $\mathbf{G}^T \mathbf{G}$, these nullspace eigenvectors should correspond to the first largest eigenvectors of $(\mathbf{G}^T \mathbf{G})^{-1} = \mathbf{H}^{-1}$. Based on this assumption, in this paper, we propose to take the effective nullspace eigenvector(s) of $\mathbf{G}^T \mathbf{G}$ as the first largest eigenvector of $\mathbf{V}$. The definition of the nullspace eigenvector is not

142 enough, because we need to design a nullspace shuttle by constructing the conservatively
 143 filtered models a posteriori.

The uncertainty in model parameters can be measured by the resolution (Boschi, 2003) or covariance (Soldati & Boschi, 2005) matrices. Here, we consider the construction of the conservative models from the posterior samplings (Tarantola, 2005) as

$$\mathbf{m}_{post} = \tilde{\mathbf{m}} + \mathbf{C}_{post}^{1/2} \mathbf{n}, \quad (10)$$

with $\tilde{\mathbf{m}}$ being the inverted model (also known as the maximum a posteriori model), $\mathbf{C}_{post}$ being the posterior covariance matrix, $\mathbf{n}$ of zero mean and banded covariance being a 2D/3D Gaussian random sampler in the 2D/3D case (Tarantola, 2005). Strictly speaking, $\mathbf{n}$ should be a Gaussian random vector with zero mean and identity covariance. We put the banded effect into the 2D/3D Gaussian random fields to enable a diagonal representation of the prior covariance matrix for large-scale applications. The posterior covariance of a linear inverse problem with Gaussian priors is defined as

$$\mathbf{C}_{post} = (\mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \varepsilon \mathbf{C}_{prior}^{-1})^{-1}, \quad (11)$$

144 with $\mathbf{C}_d$ being the data covariance matrix, $\mathbf{C}_{prior}$ and $\mathbf{C}_{post}$ being the prior and posterior
 145 model covariance matrices, respectively, and ε being a tuning scalar upon $\mathbf{C}_{prior}$ for stabi-
 146 lization. The a priori knowledge of $\mathbf{C}_d$ and $\mathbf{C}_{prior}$ can prove helpful in seismic inversions
 147 (de Wit et al., 2012). Herein, we focus on the role of the SRVM-based inverse Hessian in
 148 the determination of the nullspace shuttle, leaving the precise estimation regarding the data
 149 covariance and prior model covariance matrices an open question for future research.

We can rewrite equation (11) as

$$\mathbf{C}_{post} = (\mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} + \varepsilon \mathbf{C}_{prior}^{-1})^{-1} = (\mathbf{C}_{prior}^{1/2} \mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} \mathbf{C}_{prior}^{1/2} + \varepsilon \mathbf{I})^{-1} \mathbf{C}_{prior}. \quad (12)$$

Absorbing $\mathbf{C}_{prior}^{1/2}$ into $\mathbf{G} \mathbf{C}_{prior}^{1/2}$ and $\mathbf{C}_{prior}^{1/2} \mathbf{G}^T$ means that the prior covariance matrix takes part in the linearized inversion of elastic FWI, leading to an approximate inverse data-misfit Hessian as $\mathbf{H}^{-1} \approx (\mathbf{C}_{prior}^{1/2} \mathbf{G}^T \mathbf{C}_d^{-1} \mathbf{G} \mathbf{C}_{prior}^{1/2} + \varepsilon \mathbf{I})^{-1}$. Then, we have

$$\mathbf{C}_{post} \approx \mathbf{H}^{-1} \mathbf{C}_{prior}, \quad (13)$$

in which the inverse data-misfit Hessian $\mathbf{H}^{-1}$ connects the prior model covariance $\mathbf{C}_{prior}$ to the posterior model covariance $\mathbf{C}_{post}$. We can thus rewrite equation (13) as

$$\mathbf{m}_{post} = \tilde{\mathbf{m}} + \mathbf{C}_{prior}^{1/2} [\mathbf{V} \mathbf{\Lambda}^{1/2} \mathbf{V}^T] \mathbf{n}. \quad (14)$$

By taking the first largest eigenvalue λ_1 from $\mathbf{\Lambda}$ and the corresponding eigenvector $\mathbf{v}_1$ from $\mathbf{V}$, we construct the SRVM-based conservatively filtered models a posteriori as

$$\mathbf{m}_c = \tilde{\mathbf{m}} + \mathbf{C}_{prior}^{1/2} [\mathbf{v}_1 \lambda_1^{1/2} \mathbf{v}_1^T] \mathbf{n}, \quad (15)$$

in which the term $\mathbf{C}_{prior}^{1/2} [\mathbf{v}_1 \lambda_1^{1/2} \mathbf{v}_1^T] \mathbf{n}$ is our SRVM-based nullspace shuttle. This shuttle allows for a more significant change on $\tilde{\mathbf{m}}$ but only with a very slight change on the data misfit of $\mathbf{m}_c$. In principle, we could include more eigenvalue/eigenvector pairs without much complication. However, we see later that in our numerical demonstration the eigenvalue from first to second eigenvalue drops by almost an order of magnitude. This implies that the corresponding increase on data misfit becomes much stronger in model areas spanned by the second eigenvector. Thus, we restrict the nullspace shuttle to the largest eigenvalue/eigenvector pair. Also, our method can be easily extended to multi-parameter problems, because the SRVM method is inherently embedded into the elastic FWI (Liu et al., 2019). With different random sampling vectors $\mathbf{n}$, we can efficiently generate an extensive set of $\{\mathbf{m}_c\}$ because equation (15) runs after the inversion process.

Let us further explain the SRVM-based nullspace shuttle from an uncertainty estimation (Bui-Thanh et al., 2013; Liu & Peter, 2019; Zhu et al., 2016) point of view. The square-root diagonals of $\mathbf{C}_{post} \approx \mathbf{H}^{-1} \mathbf{C}_{prior} = [\mathbf{V} \mathbf{\Lambda} \mathbf{V}^T] \mathbf{C}_{prior}$ provide a quantitative measure of the posterior uncertainty. Among $\mathbf{V}$ and $\mathbf{\Lambda}$, the first eigenvector $\mathbf{v}_1$ together with the first eigenvalue λ_1 contributes the most to the $\mathbf{C}_{post}$ based uncertainty estimation. It also means that the inverted structures associated with $\mathbf{C}_{prior}^{1/2} [\mathbf{v}_1 \lambda_1^{1/2} \mathbf{v}_1^T]$ are with the least data coverage from the data-misfit Hessian point of view. If we look further into the term $\mathbf{C}_{prior}^{1/2} [\mathbf{v}_1 \lambda_1^{1/2} \mathbf{v}_1^T] \mathbf{n}$, we will figure out that the product $\lambda_1 \mathbf{v}_1^T \mathbf{n}$ is a scalar. We can, therefore, simplify equation (15) into

$$\mathbf{m}_c = \tilde{\mathbf{m}} + \mathbf{C}_{prior}^{1/2} \mathbf{v}_1 \eta(\mathbf{n}), \quad (16)$$

in which $\eta(\mathbf{n}) = \lambda_1^{1/2} \mathbf{v}_1^T \mathbf{n}$, a scalar function regarding $\mathbf{n}$, acts as a scaling factor to $\mathbf{C}_{prior}^{1/2} \mathbf{v}_1$, and $\mathbf{C}_{prior}^{1/2} \mathbf{v}_1 \eta(\mathbf{n})$ becomes the nullspace shuttle $\delta \mathbf{m}_{null}$.

3 Numerical example

Elastic FWI mainly consists of three recursive steps: (i) gradient computation by the adjoint method, (ii) gradient update with the optimization method, and (iii) the step-length estimation with the line search. For the gradient computation, the solution to the

elastic FWI depends on the model parameterization, and subsequently the sensitivity kernels. There are different parameterization strategies (Trampert & Van Der Hilst, 2005). For our model parameters, we focus on the inversion of V_P and V_S velocities, but keep density fixed due to its weak sensitivity in waveform inversion (Virieux & Operto, 2009). For the optimization algorithm in elastic FWI, we employ the SRVM method (Liu et al., 2019) and compare its result to an L-BFGS approach as a reference (Nocedal & Wright, 2006). For the determination of the search step length, we employ the inexact line search together with the Wolfe conditions (Nocedal & Wright, 2006).

3.1 Elastic Marmousi Benchmark

We take the elastic Marmousi (Martin, Wiley, & Marfurt, 2006) benchmark for demonstration of our methods. The model is 9200 m long and 3000 m deep. Figures 1a and 1b show the true and initial models, respectively. For the initial model, we convolve the true model with a Gaussian smoother wide enough to blur imprints of the discontinuities. We extend the models with convolutional perfectly matched layers (CPMLs) (Komatitsch & Martin, 2007). There are 32 shots and 500 receivers evenly distributed. The source function is a 4-Hz Ricker wavelet. We run the numerical simulations with SPECFEM2D (Komatitsch & Vilotte, 1998), and manage the inversion workflow with Seisflows (Modrak & Tromp, 2016).

The resulting (maximum a posteriori) models by L-BFGS and SRVM-based elastic FWIs are shown in Figures 1c and 1d, respectively. For a fair comparison, we carry forward the inversions until either of them meets the stopping criterion. The red curve in Figure 1e shows that the SRVM-based elastic FWI stops at the 58-th iteration, with the normalized data-misfit minimization at 1.31×10^{-2} . The blue curve in Figure 1e shows the convergence behavior of the L-BFGS based elastic FWI as a reference. SRVM performs as good as L-BFGS in this elastic FWI example. For more details about the performance of SRVM against L-BFGS approaches in elastic FWI, we refer to Liu et al. (2019). Using the vector-version SRVM algorithm, after 58 iterations we have stored 58 SRVM scalars and vectors. We will use this set of scalars and vectors to reconstruct the data-misfit inverse Hessian for the SRVM-based nullspace shuttle. The matrix reconstruction with the scalars and vectors can be understood as a low-rank approximation of the inverse Hessian.

To facilitate the information retrieval from the SRVM-based inverse Hessian, we incorporate the single-channel randomised SVD (Halko et al., 2011) into the SRVM matrix

Figure 1: Recovery of the elastic Marmousi model for two different synthetic FWIs using SRVM and L-BFGS. Plotted are (a) the true elastic Marmousi model; (b) the initial model for elastic FWI; (c) and (d) the inverted models by L-BFGS and SRVM-based elastic FWIs, respectively; and (e) the data misfit convergence curves of L-BFGS and SRVM-based elastic FWIs (*Left* panel: V_P , *Right* panel: V_S velocities, in m/s).

retrieval algorithm. Because the rank order of the factorized matrix by randomised SVD is the same with that of the original matrix, we choose the set of random samplers composed of 58 independent 1D random vectors. Note that 1D random vectors are qualified for the randomised SVD (Halko et al., 2011) and it avoids the more time-consuming generation of 2D/3D random samplers. Figure 2a shows the eigenvalues of the SRVM-based inverse Hessian. The rest of Figure 2 displays five different eigenvectors associated with different eigenvalues. An interesting observation is that the energy distributions of the eigenvectors gradually move from the bottom to top of the subsurface model as the eigenvector order increases. We can reason this tendency from the inverse of $\mathbf{H}^{-1}$, i.e., the Hessian, in which the energy distribution should fade away from top to bottom as the eigenvector order increases (Bui-Thanh et al., 2013; Zhu et al., 2016).

As discussed in equation (16), we explore to construct the nullspace shuttle via the first, primary eigenvector of $\mathbf{H}^{-1}$. We start with the investigation of the standard deviation maps from the square-root diagonals of the posterior covariance $\mathbf{C}_{post}$, which involves the prior covariance matrix $\mathbf{C}_{prior}$. In this research, we leave the estimation about $\mathbf{C}_{prior}$ as an open question and set the same standard deviation of 250 m/s everywhere. Thus, the prior model perturbation distributions range between [-1000 m/s, 1000 m/s] under a 2D Gaussian distribution (Tarantola, 2005). Figure 3a shows a 2D standard deviation map from the posterior covariance, and figure 3b the contribution of the first eigenvector in Figure 2a to the map. The standard deviation maps indicate the uncertainties we have on the maximum a posteriori model. The V_P map has more substantial standard deviations than V_S because the V_S sensitivity kernel possesses more low-wavenumber components than the V_P kernel (Tarantola, 1986; Virieux & Operto, 2009; Wu & Aki, 1985). We can see that the first eigenvector dominates the uncertainties in Figure 3. Note that in some very marginal areas (e.g., the PMLs), their uncertainties remain zero. This occurs because we cannot adjust areas where the Fréchet sensitivity kernels remain zero. Similar explanations can be found in Kennett, Sambridge, and Williamson (1988) and Rawlinson, Fichtner, Sambridge, and Young (2014). Based on these facts, we will take the first eigenvector of the inverse data-misfit Hessian to evaluate the robustness and extract non-unique solutions from a tomographic image.

From equation (16) we see that it is possible to investigate the posterior model distributions with 2D Gaussian random fields, as shown in Figure 4a. Also, equation (16) indicates that $\mathbf{v}_1^T \mathbf{n}$ is a scalar whose value is a function regarding $\mathbf{n}$. Figure 4a shows two Gaussian

Figure 2: Eigen-decomposition of the SRVM-based inverse Hessian factorized by randomised SVD. Plotted in (a) is the eigenvalues λ_i up to rank 58 on logarithmic scale. Plotted in the rest are the 1st, 5th, 10th, 20th, and 58th eigenvectors, respectively, $\mathbf{v}_i$ of the inverse Hessian (*Left* panel: V_P , *Right* panel: V_S velocities, in m/s). Each eigenvector integrates to 1 over the spatial domain.

Figure 3: Standard deviation maps. (a) the full uncertainty map from the posterior covariance; (b) the contribution to the uncertainty map from the 1st eigenvector of the inverse Hessian. EV stands for "eigenvector" in figure titles (*Left* panel: V_P , *Right* panel: V_S velocities, in m/s).

random fields (i.e., $\mathbf{n}$). Figure 4b shows a nullspace shuttle generated by $\mathbf{C}_{prior}^{1/2} \mathbf{v}_1 \eta(\mathbf{n})$ from the SRVM-based elastic FWI. Note that with different $\mathbf{n}$, we may generate thousands of different nullspace shuttles. Rather than a path, a shuttle here is a vehicle, which indicates one perturbed model in the null space spanned by $\mathbf{v}_1$. All the shuttles only differ from figures in the top row of Figure 2a in magnitude. Note that in Figure 2, we use a normalized colorbar for all the subfigures, but here in Figure 4b, we set the limits of the colorbar to 90% of its respective absolute maximum. The absolute maximum values for the posterior V_P and V_S perturbations in Figure 4b are around 150 and 114, respectively. Also, in Figure 4b, we shrink the grey-color scope, which connects the blue and red zones on the colorbar, for a better visualization regarding the structures of different magnitudes.

We use equation (16) to construct different conservatively filtered models. Again, the inverted (maximum a posteriori) model is shown as reference in Figure 5a, with the normalized optimal data misfit value given in the figure title. The other subfigures in Figure 5 show, respectively, the inverted models $\tilde{\mathbf{m}}$ plus $\mathbf{C}_{prior}^{1/2} \mathbf{v}_1 \eta(\mathbf{n})$ amplified by -4 , -2 , $+2$, $+4$, with the corresponding data misfits of the conservative models being displayed on their titles. Each of the data misfits is computed by actually running a forward simulation. With the maximum perturbation in Figure 4b being 150 m/s, from the conservative models we can see that although the structures within the model nullspace perturb between $[-600 \text{ m/s}, 600 \text{ m/s}]$, only slight data-misfit distortions arise. Within a conservative choice of data-misfit tolerance (i.e., 1% of the total data misfit), we can find a broad range of acceptable models, indicating the non-unique solutions in elastic FWI. Because the $\mathbf{C}_{prior}^{1/2} \mathbf{v}_1 \eta(\mathbf{n})$ is implemented a posteriori, we can generate thousands of conservative models in a highly efficient manner. That is also the reason for it being named the "nullspace shuttle". Realizations of the nullspace shuttle show that shallower subsurface structures with better data coverage are robust, the deeper, marginal structures, especially for the high-velocity salt structures, are less robust due to the lack of data coverage. Such observations may help to mitigate the non-uniqueness or uncertainties regarding the tomographic images in future acquisitions.

4 Discussions and Conclusion

Investigating the nullspace shuttle in FWI applications is tantamount to studying the non-uniqueness of the associated inverse problem. Focusing on FWI, The nullspace shuttle allows for a significant change in the tomographic image but only with a slight data-misfit distortion. We construct an SRVM-based nullspace shuttle in elastic FWI, focusing on V_P

Figure 4: Nullspace shuttle. (a) Two 2D Gaussian random fields; (b) the sampled nullspace model perturbations (*Left* panel: V_P , *Right* panel: V_S velocities, in m/s).

Figure 5: Conservative models (i.e., models which conserve the data fit within a small tolerance of 1%). (a) the SRVM-based elastic FWI result, which is the same as Figure 1d but differs in colorbar to better highlight changes in the following nullspace shuttles. Normalized data-misfit values are given in the titles; (b), (c), (d) and (e): the nullspace sampled by conservative filtering. Note that although with significant velocity changes in (b), (c), (d) and (e), the resulting data misfits only slightly differ from the "optimal" data misfit in (a) (*Left panel: V_P , Right panel: V_S velocities, in m/s*).

and V_S velocity model inversions. To this end, we employ a vector-version SRVM algorithm which is memory-efficient and amends to large-scale tomographic problems.

Rather than indirectly determine the nullspace from the effective eigenvectors of the Hessian, we define the first, primary eigenvector of the SRVM-based inverse Hessian through randomised SVD as the generalized nullspace. We put this eigenvector into the posterior model sampling to construct the SRVM-based nullspace shuttle and conservative model-sampling. With the display of the nullspace shuttle, we observe that specific structures in the inverted models are not well resolved by the data assimilation. This means that these subsurface structures are less robust or unique, and should be interpreted with care. For better interpretation of these structures, changes in acquisition geometries or additional informations from well-logs or geological surveys would be recommended.

Because the SRVM method is deeply embedded in the elastic FWI procedure, the demonstrated application can be easily extended to other multi-parameter problems. The construction of the SRVM-based nullspace shuttle is straightforward once the approximated inverse Hessian is constructed. Essentially, our method resembles the Deal and Nolet (1996) nullspace shuttle but illuminates the problem from a complementary direction. Our numerical application highlights that this shuttle as well represents a characterization of the non-uniqueness in elastic FWI.

Acknowledgments

All data analyzed here are openly available. The Marmousi_SRVM model can be found at <https://zenodo.org/badge/latestdoi/125932696>. The Seisflow_SRVM codes can be found at <https://zenodo.org/badge/latestdoi/125918416>. The codes for null-space shuttle can be found at <https://zenodo.org/badge/latestdoi/126001419>. This work was supported by the King Abdullah University of Science & Technology (KAUST) Office of Sponsored Research (OSR) under award No. UAPN#2605-CRG4. Computational resources were provided by the Information Technology Division and Extreme Computing Research Center (ECRC) at KAUST.

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Figure 1.

Accepted Article

(a)

(b)

(c)

(d)

(e)

Figure 2.

Accepted Article

(a)

(b)

(c)

(d)

(e)

(f)

Figure 3.

Accepted Article

(a)

(b)

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Figure 4.

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2D Gaussian random field 1

2D Gaussian random field 2

(a)

Null-space VP Perturbation

Null-space VS Perturbation

(b)

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Figure 5.

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