A stochastic approach to mixed linear and nonlinear inverse problems with applications to seismology

Darko Volkov *

July 17, 2020

Abstract

We derive an efficient stochastic algorithm for computational inverse problems that present an unknown linear forcing term and a set of nonlinear parameters to be recovered. It is assumed that the data is noisy and that the linear part of the problem is ill-posed. The vector of nonlinear parameters to be recovered is modeled as a random variable. This random vector is augmented by a random regularization parameter for the linear part. A probability distribution function for this augmented random vector knowing the measurements is derived. We explain how this derivation is related to the maximum likelihood regularization parameter selection [Galatsanos and Katsaggelos, 1992], which we generalize to the case where the underlying linear operator is rectangular and depends on a nonlinear parameter. A major difference in our approach is that, unlike in [Galatsanos and Katsaggelos, 1992], we do not limit ourselves to the most likely regularization parameter, instead we show that due to the dependence of the problem on the nonlinear parameter, there is a great advantage in exploring all positive values of the regularization parameter.

Based on our new probability distribution function, we construct a choice sampling algorithm to compute the posterior expected value and covariance of the nonlinear parameter. This algorithm is greatly accelerated by using a parallel platform where we alternate computing proposals in parallel and combining proposals to accept or reject them as in [Calderhead, 2014].

Finally, our new algorithm is illustrated by solving an inverse problem in seismology. We show how our algorithm performs in that example and how it is able to compute marginal posterior probability functions even in the presence of strong noise. We discuss why this problem can not be approached by using the Generalized Cross Validation method or the discrepancy principle.

Keywords: Regularization, Linear and nonlinear inverse problems, Markov chains, Parallel computing, Elasticity equations in unbounded domains.

1 Introduction

Many physical phenomena are modeled by governing equations which depend linearly on some terms and non-linearly on other terms. For example, the wave equation may depend

*Department of Mathematical Sciences, Worcester Polytechnic Institute, Worcester, MA 01609.
linearly on a forcing term and non-linearly on the medium velocity. This paper is on inverse problems where both a linear part and a nonlinear part are unknown. Such inverse problems occur in passive radar imaging, or in seismology where the source of an earthquake has to be determined (the source could be a point, or a fault) and a forcing term supported on that source is also unknown. This inverse problem is then linear in the unknown forcing term and nonlinear in the location of the source. In the last section of this paper, we show a simulation in seismology where a fault can be reconstructed thanks to our stochastic algorithm for mixed problems, while classic deterministic algorithms fail. There is also another example where mixed linear and nonlinear inverse problems occur: the training phase of neural networks. As most neural networks are based on linear combinations of basis functions depending on a few parameters, these parameters have to be determined by “training” the network on data, in other words by solving a mixed linear and nonlinear optimization problem where the nonlinear part represents the parameters to be determined, [Bishop et al., 1995].

Let us now formulate the mixed linear and nonlinear problem studied in this paper. Assume that after discretization a forward model which is linear in $g$ and nonlinear in $m$ is given by the relation

$$u = A_m g + \mathcal{E},$$  

(1.1)

where $g$ in $\mathbb{R}^p$ is the forcing term, $m$ in $\mathcal{B} \subset \mathbb{R}^q$ is the nonlinear parameter, $A_m$ is an $n \times p$ matrix depending continuously on the parameter $m$, $\mathcal{E}$ is an $n$ dimensional Gaussian random variable assumed to have zero mean and covariance $\sigma^2 I$ with $\sigma > 0$, and $u$ is the resulting data for the inverse problem. Depending on the problem, $m$ may represent a constitutive coefficient in a PDE, or the location of a point source if $A_m$ is derived from a Green function, or the geometry of a support if $A_m$ is derived from the convolution with a Green function. In practice the mapping $m \rightarrow A_m$ is assumed to be known, in other words a model is known. We are interested in challenging cases where the following difficulties arise simultaneously:

(i) the size $n \times p$ of the matrix $A_m$ is such that $p \gg n$ (sparse data),

(ii) the ordered singular values of $A_m$, $t_1 \geq \ldots \geq t_n$ are such that $t_1 \gg t_n$ (even $A_m A_m'$ is ill conditioned),

(iii) the covariance $\sigma^2$ is unknown and not even an estimate of $\sigma$ is available, thus choosing a regularization parameter by the discrepancy principle is impractical (unknown noise level),

(iv) due to the singularity and rectangular shape of $A_m$, for all parameters $m$ in the search set, $\|A_m g - u\|$ can be made arbitrarily small for some $g$ in $\mathbb{R}^p$, thus the Variable Projection (VP) functional as defined in [Golub and Pereyra, 2003] can be minimized to numerical zero for all $m$ in the search set, and consequently the variable projection method is inapplicable.

In light of (iv), solving the inverse problem (1.1) is not about minimizing $\|u - A_m g\|$ over all $m$ in the search set, nor any regularized version thereof. Instead, there is a great advantage to formulating this inverse problem in terms of finding probabilistic information about $m$. We propose in this paper an algorithm capable of computing the expected value of $m$, its covariance matrix, and possibly, the posterior marginal probability distribution function of some of the components of $m$. As to the linear part $g$ of inverse problem (1.1), ultimately, we may only be interested in its expected value knowing some particular value of $m$, such
as its expected value, or any value within a standard deviation of its expected value. Instead of using the VP functional, we start from the regularized error functional,

\[ \|A_m g - u\|^2 + C\|R g\|^2, \]

where \( R \) is an invertible \( p \) by \( p \) matrix. Typical choices for \( R \) include the identity matrix and matrices derived from discretizing derivative operators. In all cases \( R \) is assumed to be square, large, sparse, and well-conditioned. In section 3 we relate the functional (1.2) to the probability density of \( u \) knowing \( \sigma, m \) and \( C \) and we use the Maximum Likelihood (ML) assumption to eliminate \( \sigma \). As far as we know, this idea was first introduced (for linear problems only) in [Galatsanos and Katsaggelos, 1992], but unlike as in that reference, we do not eliminate \( C \): we let \( C \) remain a random variable and thanks to Bayes’ theorem we find a formula for the probability density of \((m, C)\) knowing \( u \): this is stated in Theorem 3.1. In section 4.2 this formula is used to build a parallel, adaptive, choice sampling algorithm to simulate the probability density of \((m, C)\) knowing \( u \) and from there the statistics of \( m \) and \( C \) can be computed. Finally we show in section 5 a numerical simulation where this algorithm is applied to a particularly challenging inverse problem in geophysics. In this problem a fault geometry, described by a nonlinear parameter \( m \) in \( \mathbb{R}^6 \), has to be reconstructed from surface displacement data, a vector \( u \) in \( \mathbb{R}^n \). The data is produced by a large slip field \( G \) modeled by a vector \( g \) in \( \mathbb{R}^p \). \( u \) depends linearly on \( g \) and this dependence can be expressed by a matrix \( A_m \). In this simulation, the matrix \( A_m \) is full since it is derived from convolution by a Green function. In addition, the entries of \( A_m \) are particularly expensive to compute, which is a hallmark of problems involving half space elasticity. This application features all the difficulties (i) through (iv) listed above. This contributes to not only making the VP functional method unsuitable, but also rendering other methods such as Generalized Cross Validation and the discrepancy principle ineffective as discussed in section 5.3.

2 The linear part of the inverse problem

In this section we review three classical methods for selecting an adequate value for the regularization constant \( C \) in (1.2), assuming that the nonlinear parameter \( m \) is fixed. The Euclidean norm will be denoted by \( \| \cdot \| \) and the transpose of a matrix \( M \) will be denoted by \( M' \). Since we assumed that the matrix \( A_{m}' A_m \) is ill-conditioned, it is well known that one should not attempt to minimize \( \|A_m g - u\| \) for \( g \) in \( \mathbb{R}^p \) to solve for the linear part of the inverse problem without some kind of regularization. We then consider a Tikhonov type regularization where we seek to minimize over \( \mathbb{R}^p \) the functional (1.2) for some \( C > 0 \). It is well-known that the functional (1.2) has a unique minimum for \( g \) in \( \mathbb{R}^p \). A difficult issue remains: selecting a value for the regularization constant \( C \). Values that are too low may lead to solutions that are too oscillatory, with very large norms, and overly sensitive to noise. Values that are too large may lead to solutions that are too smooth and that lead to large differences between \( A_m g_{\min} \) and \( u \), where \( g_{\min} \) is the minimizer of (1.2). There is a vast amount of literature on methods for selecting an adequate value for the regularization constant \( C \). An account of most commonly used methods, together with error analysis, can be found in [Vogel, 2002]. In this paper we review three such methods, that we subsequently compare to our own algorithm.
2.1 Generalized cross validation (GCV)

We first note that setting $h = Rg$, minimizing $\|A_mR^{-1}h - u\|^2 + C\|h\|^2$ is equivalent to minimizing for $h$ in $\mathbb{R}^p$, 

$$\|A_mR^{-1}h - u\|^2 + C\|h\|^2. \tag{2.1}$$

The GCV method was first introduced and analyzed in [Golub et al., 1979]. The parameter $C$ is selected by minimizing 

$$\|(I - BB^#)u\|^2 \quad \frac{\text{tr} (I - BB^#)}{2}, \tag{2.2}$$

where $B = A_mR^{-1}$, $B^#$ is the pseudo-inverse of $B$ given by, 

$$B^# = (B'B + CI)^{-1}B',$$ \tag{2.3}

and $\text{tr}$ is the trace operator. Note that, 

$$BB^# = A_m(A_m'A_m + CR'R)^{-1}A'_m. \tag{2.4}$$

It is well known that for a fixed $C$, (2.1) as a function of $h$ achieves a unique minimum at $B^#u$. Let $C_{GCV}$ be the value of $C$ which minimizes (2.2). Golub et al. proved in [Golub et al., 1979] that as a function of $C$, the expected value of $\|A_mg - BB^#u\|^2$ which can be thought of as an indicator of fidelity of the pseudo-solution $B^#u$ to the equation $u = Bh + \mathcal{E}$, is approximately minimized at $C = C_{GCV}$ as $n \to \infty$. Although the GCV method enjoys this remarkable asymptotic property and does not require the knowledge of the covariance $\sigma^2$, many authors have noted that determining the minimum of (2.2) in practice can be costly and inaccurate as in practical situations the quantity in (2.2) is flat near its minimum for a wide range of values of $C$ [Thompson et al., 1989, Varah, 1983].

2.2 The discrepancy principle (CLS)

The discrepancy principle [Morozov, 1966, Vogel, 2002] advocates choosing a value for $C$ such that 

$$\|u - BB^#u\|^2 = n\sigma^2. \tag{2.5}$$

This method is also called the constrained least square (CLS), [Galatsanos and Katsaggelos, 1992]. A regularization constant $C$ such that (2.5) is achieved will be denoted by $C_{CLS}$. Clearly, applying this method requires a knowledge of the value of the covariance $\sigma^2$ or at least some reasonable approximation of its value. Even if $\sigma^2$ is known, $C_{CLS}$ leads to solutions that are in general overly smooth, [Galatsanos and Katsaggelos, 1992, Vogel, 2002].

2.3 Maximum likelihood (ML)

Of all three previously known methods that we use in our paper for comparison to our proposed algorithm, this one is of greatest interest since we will show in the next section how a modified and expanded version can be successfully adapted to mixed linear and nonlinear inverse problems. To the best of our knowledge the ML method was first proposed in [Galatsanos and Katsaggelos, 1992]. It relies on maximizing the likelihood of the minimizer
of (1.2) knowing \( \sigma \) and \( C \). As the maximum is computed over all \( \sigma > 0 \), Galatsanos and Katsaggelos obtained in [Galatsanos and Katsaggelos, 1992] an expression that is independent of \( \sigma \), that they then minimize in \( C \). This expression to be minimized in \( C \) is,

\[
\frac{u'(I - BB^\#)u}{(\det(I - BB^\#))^{1/n}},
\]

where \( BB^\# \) is as in (2.4). We will show that the numerator in (2.6) is positive for any non-zero \( u \). We will also indicate how the determinant in the denominator of (2.6) can be efficiently evaluated from \( A_m \) and \( R \). Minimizing (2.6) does not require any knowledge of the covariance \( \sigma^2 \). Interestingly, if \( C \) is set to be \( C_{ML} \), the minimizer of (2.6), Galatsanos and Katsaggelos showed in [Galatsanos and Katsaggelos, 1992] the relation

\[
u'(I - BB^\#)u = n\sigma^2.
\]

In [Galatsanos and Katsaggelos, 1992], formulas (2.6) and (2.7) were only established in the case of square matrices \( A_m \) \((n = p)\). The generalization to rectangular matrices is rather straightforward. In this paper, our main contribution is to generalize the ML method to mixed linear and nonlinear inverse problems as \( m \) becomes variable and to propose an alternative to minimizing the ratio (2.6). In this alternative \( C \) will itself be a random variable. Instead of only retaining the most likely value of \( C \), we will consider all positive values of \( C \). There is a simple intuitive explanation for why this new approach will prove to be fruitful. Since the nonlinear parameter \( m \) is variable, the ‘optimal’ value for \( C \) depends on \( m \). One line of thinking is to compute the optimal value for \( C \) as a function of \( m \) using the GCV or the CLS method. Our numerical simulations show that this leads to highly unstable solutions. This is chiefly due to the fact that for values of \( m \) which are far from its ‘correct’ value, the computed value for \( C \) is low so more irregular solutions for the linear part of the problem are favored. For values of \( m \) which are close to its ‘correct’ value, higher values for \( C \) are selected and accordingly more regular solutions for the linear part of the problem are favored: altogether this leads to a poor way of comparing how well different values of \( m \) will lead to better fitting the data. One way around that hurdle is to find a criterion for selecting a uniform value of \( C \) for all \( m \) as in previous studies [Volkov and Sandiumenge, 2019; Volkov et al., 2017a]. This led to acceptable results on simulated data and on measured data, albeit the nonlinear parameter had to be restricted to be three dimensional for this approach to be fruitful. However, a physical argument can be made against selecting a uniform value of \( C \) for all \( m \): suppose that equation (1.1) models a physical phenomenon such that the nonlinear parameter \( m \) is related to a distance \( r \) to a set of sources. Suppose that the intensity of the induced physical field decays in \( r^{-1} \) or in \( r^{-2} \). Then in order to produce the same intensity of measurement, a faraway source will require a stronger impulse and pushes toward lower values of \( C \). This explains why the selection for a uniform value of \( C \) leads to a bias toward decreasing the distance to reconstructed sources.

### 3 A new Bayesian approach for finding the posterior of the augmented random variable \((m, C)\)

We make the following assumptions:

**H1.** \( u, g, m \) and \( C \) are random variables in \( \mathbb{R}^n, \mathbb{R}^p, B \subset \mathbb{R}^q, (0, \infty) \), respectively,
H2. \((m, C)\) has a known prior distribution denoted by \(\rho_{pr}(m, C)\),

H3. \(A_m\) is an \(n\) by \(p\) matrix which depends continuously on \(m\),

H4. \(\mathcal{E}\) is an \(n\) dimensional Gaussian random variable that we assume to have zero mean and covariance \(\sigma^2 I\), with \(\sigma > 0\),

H5. relation (1.1) holds,

H6. \(R\) is a fixed invertible \(p\) by \(p\) matrix and we set \(B = A_mR^{-1}\),

H7. we set \(g_{\text{min}} = (A_mA_m + CR'R)^{-1}A_mu\), equivalently, \(g_{\text{min}}\) is the minimizer of (1.2),

H8. the ML assumption: the prior of \(C_1^2Rg\) is also a normal random variable with zero mean and covariance \(\sigma^2 I\).

The ML assumption H8 was introduced in Galatsanos and Katsaggelos, 1992 and justified in that paper by a physical argument. Here we give another interpretation. The functional (1.2) may be rewritten as

\[||A_mg - u||^2 + ||C_1^2Rg||^2.\] (3.1)

According to (1.1), we would like the difference \(A_mg - u\) to behave like a normal random variable with zero mean and covariance \(\sigma^2 I\). Assuming that the the prior of \(C_1^2Rg\) is also a normal random variable with zero mean and covariance \(\sigma^2 I\) restores a balance between reconstruction fidelity (first term in (3.1)) and regularity requirements (second term in (3.1)).

**Theorem 3.1** Assume assumptions H1 to H8 hold. Let \(\rho(u|\sigma, m, C)\) be the marginal probability density of \(u\) knowing \(\sigma, m, C\). As a function of \(\sigma > 0\), \(\rho(u|\sigma, m, C)\) achieves a unique maximum at

\[\sigma_{\text{max}}^2 = \frac{1}{n}(C\|Rg_{\text{min}}\|^2 + \|u - A_mg_{\text{min}}\|^2).\] (3.2)

Fixing \(\sigma = \sigma_{\text{max}}\), the probability density of \((m, C)\) knowing \(u\) is then given, up to a multiplicative constant, by the formula

\[\rho(m, C|u) \propto \det(C^{-1}B'B + I)^{-\frac{1}{2}}(C\|Rg_{\text{min}}\|^2 + \|u - A_mg_{\text{min}}\|^2)^{-\frac{1}{2}}\rho_{pr}(m, C).\] (3.3)

**Proof:** According to H4, H5, the probability density of \(u\) knowing \(g, \sigma, m, C\) is, since \(u\) does not depend on \(C\),

\[\rho(u|g, \sigma, m, C) = \rho(u|g, \sigma, m) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{p}{2}} \exp\left(-\frac{1}{2\sigma^2}\|u - A_mg\|^2\right).\] (3.4)

Due to assumption H8,

\[\rho(g|\sigma, m, C) = \rho(g|\sigma, C) = \left(\frac{1}{2\pi\sigma^2}\right)^{\frac{1}{2}}(\det(CR'R))^{\frac{1}{2}} \exp\left(-\frac{C}{2\sigma^2}\|Rg\|^2\right),\] (3.5)

since this prior is independent of \(m\). The joint distribution of \(u, g\) knowing \(\sigma, m, C\) is related to the distribution of \(u\) knowing \(g, \sigma, m, C\) by

\[\rho(u, g|\sigma, m, C) = \rho(u|g, \sigma, m, C)(\int \rho(u, g|\sigma, m, C)du).\] (3.6)
Now, \( \int \rho(\mathbf{u}, \mathbf{g}|\sigma, \mathbf{m}, C)d\mathbf{u} \) is the prior probability distribution of \( \mathbf{g} \) [Kaipio and Somersalo, 2006], which we said was given by (3.5). Combining (3.4) and (3.5) we obtain
\[
\rho(\mathbf{u}|\sigma, \mathbf{m}, C) = \int \rho(\mathbf{u}, \mathbf{g}|\sigma, \mathbf{m}, C)d\mathbf{g}
\]
\[
= (\frac{1}{2\pi\sigma^2})^{\frac{n+n}{2}}\pi^\frac{n}{2} (\det(\mathbf{CR}'\mathbf{R}))^{\frac{1}{2}} \int \exp(-\frac{C}{2\sigma^2} \|\mathbf{Rg}\|^2 - \frac{1}{2\sigma^2} \|\mathbf{u} - \mathbf{Amg}\|^2) d\mathbf{g}. \tag{3.7}
\]
This last integral can be computed explicitly [Volkov and Sandiumenge, 2019] to find
\[
\int \exp(-\frac{C}{2\sigma^2} \|\mathbf{Rg}\|^2 - \frac{1}{2\sigma^2} \|\mathbf{u} - \mathbf{Amg}\|^2) d\mathbf{g}
\]
\[
= \exp(-\frac{C}{2\sigma^2} \|\mathbf{Rg}_{\min}\|^2 - \frac{1}{2\sigma^2} \|\mathbf{u} - \mathbf{Amg}_{\min}\|^2) (\det(\frac{1}{2\pi}(\frac{1}{\sigma^2}\mathbf{A}'\mathbf{Am} + \frac{C}{\sigma^2}\mathbf{CR}'))^{-\frac{1}{2}}, \tag{3.8}
\]
where \( \mathbf{g}_{\min} \) is as stated in H7. The determinant in (3.8) is of order \( p \) so the terms in \( \sigma \) in (3.8) and (3.7) simplify to obtain,
\[
(\frac{1}{2\pi\sigma^2})^{\frac{n+n}{2}}\pi^\frac{n}{2} (\det(\mathbf{CR}'\mathbf{R}))^{\frac{1}{2}} \exp(-\frac{C}{2\sigma^2} \|\mathbf{Rg}_{\min}\|^2 - \frac{1}{2\sigma^2} \|\mathbf{u} - \mathbf{Amg}_{\min}\|^2) (\det(\frac{1}{2\pi}(\frac{1}{\sigma^2}\mathbf{A}'\mathbf{Am} + \frac{C}{\sigma^2}\mathbf{CR}'))^{-\frac{1}{2}}, \tag{3.9}
\]
which we now maximize for \( \sigma \) in \( (0, \infty) \). Note that \( \mathbf{g}_{\min} \) does not depend on \( \sigma \). As \( \sigma \) tends to infinity, the limit of (3.9) is clearly zero. As \( \sigma \) tends to zero, as long as \( \mathbf{u} \) is non-zero, \( \|\mathbf{Rg}_{\min}\| \neq 0 \), so the limit of (3.9) is again zero. We then take the derivative of (3.9) in \( \sigma \) and set it to equal to zero to find the equation
\[
-n\sigma^{-n-1} + \sigma^{-n}(\frac{C}{2\sigma^2} \|\mathbf{Rg}_{\min}\|^2 - \frac{1}{2\sigma^2} \|\mathbf{u} - \mathbf{Amg}_{\min}\|^2) = 0,
\]
thus the value
\[
\sigma_{\max}^2 = \frac{1}{n}(\frac{C}{2} \|\mathbf{Rg}_{\min}\|^2 + \|\mathbf{u} - \mathbf{Amg}_{\min}\|^2)
\]
maximizes the density \( \rho(\mathbf{u}|\sigma, \mathbf{m}, C) \). Substituting (3.2) in (3.9) and recalling that we set \( B = \mathbf{AmR}^{-1} \), we find for this particular value of \( \sigma^2 \),
\[
\rho(\mathbf{u}|\mathbf{m}, C) \propto \det(\mathbf{C}^{-1}\mathbf{B}'\mathbf{B} + \mathbf{I})^{-\frac{1}{2}} (\|\mathbf{Rg}_{\min}\|^2 + \|\mathbf{u} - \mathbf{Amg}_{\min}\|^2)^{-\frac{1}{2}},
\]
where \( \propto \) means 'equal to some constant times'. Since our goal is to reconstruct \( \mathbf{m} \) and \( C \) knowing \( \mathbf{u} \) we apply Bayes’ law
\[
\rho(\mathbf{m}, C|\mathbf{u}) \propto \rho(\mathbf{u}|\mathbf{m}, C)\rho_{pr}(\mathbf{m}, C),
\]
to obtain (3.3). \( \square \)

We now compare formulas (3.2) and (3.3) from Theorem 3.1 to formulas (28) and (29) found in [Galatsanos and Katsaggelos, 1992]. Let us first emphasize a major difference in our approach. In [Galatsanos and Katsaggelos, 1992], the ratio (28) is optimized in the regularization parameter (\( \lambda \) in their paper), so eventually only one regularization parameter is considered. Instead, formula (3.3) uses a prior on the regularization parameter \( C \), so all values of \( C > 0 \) can be considered.
In order to show the connection between the numerator of (28) in [Galatsanos and Katsaggelos, 1992] and the term \((C\|R_{gm}\|^2 + \|u - A_m g_{min}\|^2)\) in (3.3), we note that since \(g_{min}\) satisfies assumption H7,

\[
\|u - A_m g_{min}\|^2 + C\|R_{gm}\|^2 = \|u\|^2 - 2\langle g_{min}, A'_m u \rangle + C\langle g_{min}, R'R_{gm}\rangle = \|u\|^2 - 2\langle g_{min}, A'_{gm} A_m g_{min} \rangle + C\langle g_{min}, R'R_{gm}\rangle + C\langle g_{min}, R'R_{gm}\rangle - C\langle g_{min}, A'_{gm} A_m g_{min} \rangle,
\]

which is the analog of the numerator in formula (28) in [Galatsanos and Katsaggelos, 1992].

To relate the determinant in (3.3) to the determinant in formula (28) in [Galatsanos and Katsaggelos, 1992], we need the following lemma.

**Lemma 3.1** For any \(C > 0\),

\[
\det(C^{-1}B'B + I) = \det(I - B'B(B'B + CI)^{-1}B') = \det(I - B(B'B + CI)^{-1}B')
\]

**Proof:** We first notice that

\[
I - B'B(B'B + CI)^{-1} = I - B'B + CI - CI(B'B + CI)^{-1} = (C^{-1}B'B + I)^{-1},
\]

so the first two terms in (3.10) are equal. Note that \((C^{-1}B'B + I)^{-1} = C(B'B + CI)^{-1}\).

Let \(\lambda\) be an eigenvalue of \(C(B'B + CI)^{-1}\) which is different from 1. There is an \(x \neq 0\) in \(\mathbb{R}^p\) such that \(C(B'B + CI)^{-1}x = \lambda x\). This implies that

\[
B'Bx = \left(\frac{C}{\lambda} - C\right)x
\]

and in particular \(Bx \neq 0\). From (3.12),

\[
(B'B + CI)^{-1}B'x = \left(\frac{C}{\lambda} - C\right)(B'B + CI)^{-1}x = (1 - \lambda)x,
\]

Thus

\[
B(B'B + CI)^{-1}B'x = (1 - \lambda)Bx,
\]

and

\[
(I - B(B'B + CI)^{-1}B')Bx = \lambda Bx,
\]

which shows that \(\lambda\) is also an eigenvalue of \(I - B(B'B + CI)^{-1}B'\) since \(Bx \neq 0\). The same calculation can be used to show that if \(x_1, \ldots, x_r\) are \(r\) independent eigenvectors of
Conversely, let $\mu$ be an eigenvalue of $I - B(B'B + CI)^{-1}B'$ which is different from 1. Then there is a non-zero $y$ in $\mathbb{R}^n$ such that
\[(I - B(B'B + CI)^{-1}B')y = \mu y.\] 
(3.13)

As $y \neq 0$ and $\mu \neq 1$, we infer from (3.13) that $B'y \neq 0$. It also follows from (3.13)
\[(I - B'B(B'B + CI)^{-1})(B'y) = \mu(B'y)\]
and due to (3.11)
\[(C^{-1}B'B + I)^{-1}(B'y) = \mu(B'y),\]

thus $\mu$ is an eigenvalue of $(C^{-1}B'B + I)^{-1}$ as $B'y \neq 0$. The same calculation can be used to show that if $y_1, ..., y_r$ are $r$ independent eigenvectors of $(I - B(B'B + CI)^{-1}B')$ for the eigenvalue $\mu \neq 1$, then $B'y_1, ..., B'y_r$ are $r$ independent eigenvectors of $C(B'B + CI)^{-1}$ for the eigenvalue $\mu$. In conclusion we have shown that the symmetric matrices $(C^{-1}B'B + I)^{-1}$ and $I - B(B'B + CI)^{-1}B'$ have the same eigenvalues with same multiplicity, except possibly for the eigenvalue 1. It follows that they have same determinant. \(\square\)

The determinants in (3.10) can be evaluated efficiently. In many applications the matrix $A_m$ is rectangular. In the particular application shown later in this paper, $n << p$. We recall that the matrix $R$ is sparse and well-conditioned, so $B = A_mR^{-1}$ can be efficiently evaluated. Let $s_1, ..., s_r$ be the non-zero singular values of $B$ counted with multiplicity. Note that $r \leq \min\{n, p\}$. In practice, if both $n$ and $p$ are large, since we assumed that the singular values of $A_m$ are rapidly decaying, computing just the largest singular values of $B$ is sufficient. The eigenvalues of $I + C^{-1}B'B$ that are different from 1 are $1 + C^{-1}s_1^2, ..., 1 + C^{-1}s_r^2$, and accordingly
\[
(det(C^{-1}B'B + I))^{-1} = \prod_{j=1}^{r}(1 + C^{-1}s_j^2)^{-1}.
\] 
(3.14)

4 Proposed algorithm

We first present in section 4.1 a single-processor version of our adaptive choice sampling algorithm derived from formula (3.3). A reader familiar with this kind of algorithms can just focus on the notations introduced in section 4.1 and the sub-algorithm for computing the relative probability densities of proposals, and then move to section 4.2 where we explain how this algorithm can be adjusted to multi-processor platforms. The adjustment is based on Calderhead, 2014, where it is shown that astute combinations between proposals computed in parallel result in better mixing and faster convergence properties.

4.1 Single processor algorithm

Based on (3.3), we define the non-normalized distribution
\[
\mathcal{R}(m, C) = \det(C^{-1}B'B + I)^{-\frac{1}{2}}(C\|Rg_{min}\|^2 + \|u - A_m g_{min}\|^2)^{-\frac{1}{2}}\rho_{pr}(m, C).
\] 
(4.1)
Our proposed algorithm will call a sub-algorithm which computes $\mathcal{R}(m, C)$ for a given $(m, C)$. We use the following notations: $E$ for expected value, $\text{cov}$ for covariance matrix, $\mathcal{N}(\mu, \Sigma)$ for a normal distribution with mean $\mu$ and covariance $\Sigma$, $U(0, 1)$ for a uniform distribution in the interval $(0, 1)$. The random walk algorithm starts from a point $(m_1, C_1)$ in $\mathbb{R}^{q+1}$ such that $\rho_{pr}(m_1, C_1) > 0$ and an initial covariance matrix $\Sigma_0$ obtained from the prior distribution. A good choice of the initial point $(m_1, C_1)$ may have a strong impact on how many sampling steps are necessary in our algorithm. A poor choice may result in a very long "burn in" phase where the random walk is lost in a low probability region. How to find a good starting point $(m_1, C_1)$ depends greatly on the application, so we will discuss that issue in a later section where we cover a specific example. Our basic single processor algorithm follows the well established adaptive MCMC propose/accept/reject algorithm [Roberts and Rosenthal, 2009]. Let $\beta_k$ be a decreasing sequence in $(0, 1)$ which converges to 0. This sequence is used to weigh a convex combination between the initial covariance $\Sigma_0$ and the covariance $\Sigma$ learned from sampling. The updating of $\Sigma$ need not occur at every step. Let $N$ be the total number of steps and $N'$ the number of steps between updates of $\Sigma$. We require that $1 < N' < N$. Finally the covariance for the proposals is adjusted by a factor of $(2.38)^2(q + 1)^{-1}$ as recommended in [Roberts et al., 2001] [Roberts and Rosenthal, 2009]. It was shown in [Roberts et al., 2001] that this scaling leads to an optimal acceptance rate.

Propose/accept/reject samples with an adaptive covariance for the proposal density

1. Start from a point $(m_1, C_1)$ in $\mathbb{R}^{q+1}$ and set $\Sigma = \Sigma_0$.
2. for $j = 2$ to $N$ do:
   2.1. if $j$ is a multiple of $N'$ update the covariance $\Sigma$ by using the points $(m_k, C_k), 1 \leq k \leq j - 1$,
   2.2. draw $(m^*, C^*)$ from $(m_{j-1}, C_{j-1}) + (1 - \beta_j)\mathcal{N}(0, (2.38)^2(q + 1)^{-1}\Sigma) + \beta N(0, (2.38)^2(q + 1)^{-1}\Sigma_0)$,
   2.3. use the sub-algorithm for computing $\mathcal{R}(m^*, C^*)$,
   2.4. draw $u$ from $U(0, 1)$,
   2.5. if $u < \frac{\mathcal{R}(m^*, C^*)}{\mathcal{R}(m_{j-1}, C_{j-1})}$ set $(m_j, C_j) = (m^*, C^*)$, else set $(m_j, C_j) = (m_{j-1}, C_{j-1})$.

The sub-algorithm for computing $\mathcal{R}(m, C)$ depends on the application. We present in the last section an application where $A_m$ is derived from an integral operator with an integration kernel which is very expensive to compute. In that case the matrix $A_m$ is full and it is advantageous to use array operations to compute the entries of $A_m$ in aggregate. Typically, the regularization matrix $R$ could be the identity or a matrix derived from the evaluation of discrete derivatives, plus a few entries to make $R$ well conditioned. In the application shown in the last section, $R$ is in the latter form. Note that $R' R$ is sparse too and does nor depend on $m$, so it should be evaluated only once and stored. In any case, it is important to take advantage of the sparsity of $R$. Computing $\text{det}(C^{-1}B' B + I)^{-1}$ should take advantage of formula (3.14). As discussed after the proof of lemma 3.1 only the first
non-zero singular values of $B$ are needed. If the size of $B$ is large, one can take advantage of randomized SVD techniques. Finally, for larger problems, an iterative solver should be used to evaluate $g_{\text{min}} = (A_m'A_m + CR'R)^{-1}A_m'\mathbf{u}$, the minimizer of (1.2). For efficiency, one should make sure to code the function $g \rightarrow (A_m'A_m + CR'R)g$ without evaluating the matrix product $A_m'A_m$.

### 4.2 Parallel algorithm

Let $N_{\text{par}}$ be the number of processing units. A straightforward way of taking advantage of multiple processors is to generate $N_{\text{par}}$ separate chains of samples using the single processor algorithm described in section 4.1 and then concatenate them. However, computations can be greatly accelerated by analyzing the proposals produced by the chains in aggregate, as indicated above, while in section 4.1 ($m, C_j$) was a $q+1$ dimensional vector, here we set $M_j$ to be a $q+1$ by $N_{\text{par}}$ matrix where the $k$-th column will be denoted by $M_j(k)$ and is a sample of the random variable $(m, C)$, $k = 1, ..., N_{\text{par}}$. Next, if $j \geq 2$, we assemble an $N_{\text{par}} + 1$ by $N_{\text{par}} + 1$ transition matrix $T$ from the computed non-normalized densities $\mathcal{R}(M_j-1(N_{\text{par}}))$ and $\mathcal{R}(M^*(k))$, $k = 1, ..., N_{\text{par}}$, where $M^*$ is the proposal. Let $w$ be the vector in $\mathbb{R}^{N_{\text{par}}+1}$ with coordinates

$$w = (\mathcal{R}(M_{j-1}(N_{\text{par}})), \mathcal{R}(M^*(1)), ..., \mathcal{R}(M^*(N_{\text{par}}))).$$

The entries of the transition matrix $T$ are given by the following formula [Calderhead, 2014].

$$T_{k,l} = \begin{cases} \frac{1}{N_{\text{par}}} \min\{1, \frac{w_l}{w_k}\}, & \text{if } k \neq l, \\ 1 - \sum_{1 \leq i \leq N_{\text{par}} + 1, i \neq k} T_{k,i}, & \text{if } k = l. \end{cases} \quad (4.2)$$

Note that for $k = 1, ..., N_{\text{par}} + 1$ the row $T_{k,1}, ..., T_{k,N_{\text{par}}+1}$ defines a discrete probability distribution on $\{1, ..., N_{\text{par}} + 1\}$.

#### Parallel propose/accept/reject samples with an adaptive covariance for the proposal density

1. Start from a point $(m_1, C_1)$ in $\mathbb{R}^{q+1}$ and set $\Sigma = \Sigma_0$. Set the $N_{\text{par}}$ columns of $M_1$ to be equal to $(m_1, C_1)$.

2. for $j = 2$ to $N$ do:

   2.1. if $j$ is a multiple of $N^*$ update the covariance $\Sigma$ by using the points $M_k(l)$, $1 \leq k \leq j - 1, 1 \leq l \leq N_{\text{par}}$.

   2.2. for $k = 1$ to $N_{\text{par}}$, draw the proposals $M^*(k)$ from $M_{j-1}(N_{\text{par}}) + (1 - \beta_k)\mathcal{N}(0, (2.38)^2(q + 1)^{-1}\Sigma) + \beta_k\mathcal{N}(0, (2.38)^2(q + 1)^{-1}\Sigma_0)$.

   2.3. use the sub-algorithm for computing in parallel $\mathcal{R}(M^*(k))$, $k = 1, ..., N_{\text{par}}$.

   2.4. assemble the $N_{\text{par}} + 1$ by $N_{\text{par}} + 1$ transition matrix $T$ as indicated above.

   2.5. for $k = 2, ..., N_{\text{par}} + 1$ draw an integer $p$ in $\{1, ..., N_{\text{par}} + 1\}$ using the probability distribution $T_{k,1}, ..., T_{k,N_{\text{par}}+1}$; if $p = 1$ set $M_j(k - 1) = M_{j-1}(N_{\text{par}})$ (reject), otherwise set $M_j(k - 1) = M^*(p - 1)$ (accept).
Note that this parallel algorithm is especially well suited to applications where computing the non-normalized density \( R(m, C) \) is particularly expensive. In that case, even the naive parallel algorithm where \( N_{\text{par}} \) separate chains are computed in parallel will be about \( N_{\text{par}} \) times more efficient than the single processor algorithm. The parallel algorithm presented in this section is in fact even more efficient due to superior mixing properties and sampling performance: the performance is not overly sensitive to tuning of proposal parameters [Calderhead, 2014].

5 Application to the fault inverse problem in seismology and numerical simulations

We now formulate a fault inverse problem in seismology that we will solve using the algorithm introduced in section 4.2. Using standard rectangular coordinates, denote \( x = (x_1, x_2, x_3) \) elements of \( \mathbb{R}^3 \). We define \( \mathbb{R}^3^- \) to be the open half space \( x_3 < 0 \). We use the equations of linear elasticity with Lamé constants \( \lambda \) and \( \mu \) such that \( \lambda > 0 \) and \( \lambda + \mu > 0 \). For a vector field \( \mathbf{V} = (V_1, V_2, V_3) \) the stress and strain tensors will be denoted as follows,

\[
\sigma_{ij}(\mathbf{V}) = \lambda \text{div} \mathbf{V} \delta_{ij} + \mu (\partial_i V_j + \partial_j V_i),
\]

\[
\epsilon_{ij}(\mathbf{V}) = \frac{1}{2} (\partial_i V_j + \partial_j V_i),
\]

and the stress vector in the direction \( \mathbf{e} \in \mathbb{R}^3 \) will be denoted by

\[ T_e \mathbf{V} = \sigma(\mathbf{V}) \mathbf{e}. \]

Let \( \Gamma \) be a Lipschitz open surface which is strictly included in \( \mathbb{R}^3^- \), with normal vector \( \mathbf{n} \). We define the jump \([\mathbf{V}]\) of the vector field \( \mathbf{V} \) across \( \Gamma \) to be

\[ [\mathbf{V}](x) = \lim_{h \to 0^+} \mathbf{V}(x + h\mathbf{n}) - \mathbf{V}(x - h\mathbf{n}), \]

for \( x \) in \( \Gamma \), if this limit exists. Let \( \mathbf{U} \) be the displacement field solving

\[
\begin{align*}
\mu \Delta \mathbf{U} + (\lambda + \mu) \nabla \text{div} \mathbf{U} &= 0 \text{ in } \mathbb{R}^3^- \setminus \Gamma, \\
T_{e_3} \mathbf{U} &= 0 \text{ on the surface } x_3 = 0, \\
T_n \mathbf{U} &= 0 \text{ is continuous across } \Gamma, \\
[\mathbf{U}] &= G \text{ is a given jump across } \Gamma,
\end{align*}
\]

(5.1)\hspace{1cm} (5.2)\hspace{1cm} (5.3)\hspace{1cm} (5.4)

\[
\mathbf{U}(x) = O(\frac{1}{|x|^2}), \nabla \mathbf{U}(x) = O(\frac{1}{|x|^3}), \text{ uniformly as } |x| \to \infty,
\]

(5.5)

where \( e_3 \) is the vector \((0, 0, 1)\).

Let \( D \) be a bounded domain in \( \mathbb{R}^3^- \) with Lipschitz boundary \( \partial D \) containing \( \Gamma \). Let \( H^1(\Gamma) \) be the space of restrictions to \( \Gamma \) of vector fields in \( H^1(\partial D) \) supported in \( \Gamma \). In [Volkov et al., 2017a], we defined the functional space \( \mathbf{S} \) of vector fields \( \mathbf{V} \) defined in \( \mathbb{R}^3^- \setminus \Gamma \) such that \( \nabla \mathbf{V} \) and \( (1 + \mathbf{V} \cdot \mathbf{e})^{\frac{1}{2}} \) are in \( L^2(\mathbb{R}^3^- \setminus \Gamma) \) and we proved the following existence and uniqueness result.
Theorem 5.1 Let $\mathcal{G}$ be in $\tilde{H}^{1/2}(\Gamma)^2$. The problem (5.1-5.4) has a unique solution in $\mathbf{S}$. In addition, the solution $\mathcal{U}$ satisfies the decay conditions (5.5).

Can both $\mathcal{G}$ and $\Gamma$ be determined from the data $\mathcal{U}$ given only on the plane $x_3 = 0$? The following Theorem shown in [Volkov et al., 2017a] asserts that this is possible if the data is known on a relatively open set of the plane $x_3 = 0$.

Theorem 5.2 Let $\Gamma_1$ and $\Gamma_2$ be two connected open surfaces that are finite unions of polygons. For $i$ in $\{1, 2\}$, assume that $\mathcal{U}^i$ solves (5.1-5.4) for $\Gamma_i$ in place of $\Gamma$ and $\mathcal{G}^i$, a tangential field in $\tilde{H}^{1/2}(\Gamma_i)^2$, in place of $\mathcal{G}$. Assume that $\mathcal{G}^i$ has full support in $\Gamma_i$, that is, $\text{supp } \mathcal{G}^i = \Gamma_i$. Let $V$ be a non empty open subset in $\{x_3 = 0\}$. If $\mathcal{U}^1$ and $\mathcal{U}^2$ are equal in $V$, then $\Gamma_1 = \Gamma_2$ and $\mathcal{G}^1 = \mathcal{G}^2$.

Theorems 5.1 and 5.2 were proved in [Volkov et al., 2017a] for media with constant Lamé coefficients. Later, in [Aspri et al., 2020b], the direct problem (5.1-5.4) was analyzed under weaker conditions for the regularity of the displacement field $\mathcal{U}$ and the slip field $\mathcal{G}$. In [Aspri et al., 2020a], the direct problem (5.1-5.4) was proved to be uniquely solvable in case of piecewise Lipschitz coefficients and general elasticity tensors. Both [Aspri et al., 2020b] and [Aspri et al., 2020a] include a proof of uniqueness for the fault inverse problem under appropriate assumptions. In our case, the solution $\mathcal{U}$ to problem (5.1-5.4) can also be written out as the convolution on $\Gamma$

$$\mathcal{U}(x) = \int_{\Gamma} \mathbf{H}(x, y, \mathbf{n}) \mathcal{G}(y) \, d\sigma(y),$$

(5.6)

where $\mathbf{H}$ is the Green’s tensor associated to the system (5.1-5.5), and $\mathbf{n}$ is the normal to $\Gamma$. The practical determination of this adequate half space Green’s tensor $\mathbf{H}$ was first studied in [Okada, 1992], and later, more rigorously, in [Volkov, 2009]. Due to formula (5.6), we can define a continuous mapping $\mathcal{M}$ from tangential fields $\mathcal{G}$ in $H^1(\Gamma)^2$ to surface displacement fields $\mathcal{U}(x_1, x_2, 0)$ in $L^2(V)$ where $\mathcal{U}$ and $\mathcal{G}$ are related by (5.1-5.5). Theorem 5.2 asserts that this mapping is injective, so an inverse operator can be defined. It is well known, however, that such an operator $\mathcal{M}$ is compact, therefore its inverse is unbounded. It is thus clear that any stable numerical method for reconstructing $\mathcal{G}$ from $\mathcal{U}(x_1, x_2, 0)$ will have to use some regularization process.

Assume that in practice, these displacements are measured at $n/3$ points on the plane $x_3 = 0$, where $n$ is a multiple of 3. Since $\mathcal{U}$ is a vector field, this gives rise to a measurement vector $\mathbf{u}$ in $\mathbb{R}^n$. In our numerical simulations, we assume that $\Gamma$ is made up of two contiguous quadrilaterals. Let $\mathbf{m}$ be the vector in $\mathbb{R}^6$ that will determine $\Gamma$ as indicated in the next section. We then write the discrete equivalent of the right hand side integral formula (5.6) as the matrix vector product $A_m \mathbf{g}$, where $\mathbf{g}$ in $\mathbb{R}^p$ is the discrete analog of $\mathcal{G}$ and multiplying by the matrix $A_m$ is the discrete analog of applying the convolution product against $\mathbf{H}$ over $\Gamma$. Taking into account measurement errors, we arrive at the formulation (1.1). Let us now point to some particular features of the matrices $A_m$ and $R$ used in the simulations shown in this paper. First, the $n$ by $p$ matrix $A_m$ is rectangular with $n \sim 500$ and $p \sim 1000$. The singular values of $A_m$ decay fast (this is due to the fast decay of the singular values of the compact operator $\mathcal{M}$), so even choosing a coarser grid on $\Gamma$ which would make $p \leq n$ would still result in an ill-conditioned matrix $A_m^\top A_m$. Another practical aspect of the matrix $A_m$ is that it is full (as is usually the case in problems derived from integral operators) and its entries are expensive to compute (this is due to the nature of the half space elastic Green

13
tensor) [Volkov, 2009], however great gains can be achieved by applying array operations thus taking advantage of multithreading. The matrix $R$ used to regularize $g$ is such that $\|Rg\|^2 = \|Dg\|^2 + \|Eg\|^2$ where $D$ and $E$ are derived from first order partial derivatives and are as in [Volkov et al., 2017a, Appendix B].

5.1 Construction of the data

We consider data generated in a configuration closely related to studies involving field data for a particular region and a specific seismic event [Volkov et al., 2017b, Volkov and Sandiumenge, 2019]. In those studies, simulations involved only planar faults, while here we examine the case of fault geometries defined by pairs of contiguous quadrilaterals. Evidently, reconstructing finer geometries as considered here requires many more measurement points than used in [Volkov et al., 2017b, Volkov and Sandiumenge, 2019] (11 points in [Volkov and Sandiumenge, 2019] versus 195 points here). The higher number of measurement points used here allows us to reconstruct $\Gamma$ even if the data is very noisy, at the cost of finding large standard deviations.

In our model, the geometry of $\Gamma$ is determined from $m$ in $\mathbb{R}^6$ in the following way:

- $\Gamma$ is beneath the square $[-100, 200] \times [-100, 200]$
- Let $P_1$ be the point $(-100, -100, m_1)$
- Let $P_2$ be the point $(-100, m_2, m_3)$, such that $-100 < m_2 < 200$
- Let $P_3$ be the point $(200, m_4, m_5)$, such that $-100 < m_4 < 200$
- Let $P_4$ be the point $(200, 200, m_6)$
- Let $Q_1$ be the point in the plane $P_1P_2P_3$ with $x_1, x_2$ coordinates $(200, -100)$
- Let $Q_2$ be the point in the plane $P_2P_3P_4$ with $x_1, x_2$ coordinates $(-100, 200)$
- Form the union of the two quadrilaterals $P_1P_2P_3Q_1$ and $P_2P_3P_4Q_2$ and discard the part where $x_3 \geq 0$ to obtain $\Gamma$

Note that this definition requires $-100 < m_2, m_4 < 200$. For generating forward data we picked the particular values

$$m = (24, 145, -40, 8, -40 - 50).$$

We sketched $\Gamma$ in Figure 1 where we first show the points $P_1, P_2, P_3, P_4, Q_1, Q_2$ viewed from above, and then we sketch $\Gamma$ in three dimensions. In Figure 2 we show a graph of the slip field $\mathcal{G}$ as a function of $(x_1, x_2)$ (recall that this slip field is supported on $\Gamma$ so Figure 2 shows a projection of $\mathcal{G}$ on a horizontal plane). We model a slip of pure thrust type, meaning that slip occurs in the direction of steepest descent, so only the norm of $\mathcal{G}$ is graphed. We used this slip $\mathcal{G}$ to compute resulting surface displacements thanks to formula using (5.6) a fine mesh for discretizing the integral. The data for the inverse problem is the three dimensional displacements at the measurement points shown in Figure 1 to which we added Gaussian noise with covariance $\sigma^2 I$. We consider two scenarios: lower and higher noise. In the lower noise scenario $\sigma$ was set to be equal to 5% of the maximum of the absolute values of the components of $u$ (in other words, 5% of $\|u\|_\infty$). For the particular realization used in solving the inverse problem, this led to a relative error in Euclidean norm of about 7%. In the higher
Figure 1: The piecewise planar connected surface $\Gamma$. Depths are indicated by color bars. Top graph: view of $\Gamma$ from above with the six points $P_1, P_2, P_3, P_4, Q_1, Q_2$ and contour lines of same depth. Bottom graph: a three dimensional rendition of $\Gamma$. The measurement points are on the surface $x_3 = 0$ and are indicated by black dots.
noise case scenario $\sigma$ was set to be equal to 25% of the maximum of the absolute values of the components of $u$ (in other words, 25% of $\|u\|_\infty$). This time, this led to a relative error in Euclidean norm of about 37%. Both realizations are shown in Figure 3 (only the horizontal components are sketched for the sake of brevity). All length scales used in these simulations are in line with the canonical example from geophysics provided by the 2007 Guerrero slow slip event [Volkov et al., 2017b, Volkov and Sandiumenge, 2019]. In particular, $x_1, x_2, x_3$ are thought of as given in kilometers and $g$ and $u$ in meters. The real life noise level is likely to lie somewhere between the low noise scenario and high noise scenario considered here. There is, however, a significant difference between the data considered in [Volkov et al., 2017b, Volkov and Sandiumenge, 2019] and the data in this study: the number of measurement points here is 195 versus 11 in [Volkov et al., 2017b, Volkov and Sandiumenge, 2019]. This difference is due to the fact that we want to illustrate in this paper that it is possible to reconstruct a more complex piecewise geometry and that we can obtain acceptable results even in the presence of high noise. We will show that this is possible thanks to the use of the posterior probability density (3.3) and the parallel choice sampling algorithm introduced in 4.2. In contrast, in [Volkov and Sandiumenge, 2019], the trapezoidal rule could be used to compute the probability density of the geometry parameters for the fault: this was due to the fact that in that study faults were assumed to be planar so the geometry parameter was only in $\mathbb{R}^3$.

5.2 Numerical results from our parallel algorithm

Recall that Theorem 3.1 and the algorithm discussed in section 4.2 requires the knowledge of a prior distribution for the random variable $(m, C)$. Here, we assume that the priors of $m$ and $C$ are independent. The prior of $m$ was chosen to be uniformly distributed on the subset $\mathcal{B}$ of $[-2, 2]^6$ such that the angle $\theta$ between two vectors normal to the quadrilaterals whose union is $\Gamma$ satisfies $\cos \theta \geq 0.8$. That way, the angle between these two quadrilaterals is between 143 and 217 degrees: this can be interpreted as a regularity condition on the slip
Figure 3: Realizations of noisy horizontal surface displacements (blue) at the measurement points obtained by using the slip field shown in Figure 2 occurring on the fault $\Gamma$ shown in Figure 1. Top: low noise scenario. Bottom: high noise scenario. In each graph the unperturbed field is sketched in red.
field $g$ since it was set to point in the direction of steepest descent. As to $C$, we assumed that $\log_{10} C$ follows a uniform prior on $[-5, 0]$.

We now present results obtained by applying the algorithm from section 4.2 to the data shown in Figure 3 for both the low noise and high noise scenario. Computations were performed on a parallel platform that uses $N_{\text{par}} = 20$ processors. After computing the expected value of $m$, we sketched the corresponding geometry of $\Gamma$ shown in Figure 4, first row, by plotting depth contour lines. On the same graph we plotted the magnitude of the reconstructed slip field on $\Gamma$ as a function of $(x_1, x_2)$. This reconstruction was done by using the expected value of $(m, C)$ and solving the linear system $(A'_m A_m + C R' R) g_{\text{min}} = A'_m u$.

The reconstructed slip field is very close to the correct one shown in Figure 2. In the second row of Figure 4 we show the error in the reconstruction of the expected depth $x_3$ on $\Gamma$, as a function of $(x_1, x_2)$, and a contour profile of the reconstructed slip $g_{\text{min}}$. We notice that the error is lower where $g_{\text{min}}$ is larger: this is in line with previous theoretical studies [Volkov et al., 2017a, Volkov and Sandiumenge, 2019] where it was proved that fault geometries can only be reconstructed on the support of slip fields. In the third row of Figure 4 we show the absolute value of the depth difference between the geometry obtained by using the expected value of $m$ plus one standard deviation and the expected value of $m$ minus one standard deviation. We note that this difference (close to 2) is very low in the low noise scenario compared to the depth at the center of the support of $g_{\text{min}}$ (close to -40). In the high noise scenario we note that this difference is lower where $g_{\text{min}}$ is larger, in line with the theory. We show in Figure 5 reconstructed posterior marginal distribution functions for the six components of $m$ and for $C$. Interestingly, we notice that the range of high probability for $C$ is much higher in that case (more than 10 times higher, since the graph is that of $\log_{10} C$) in the higher noise scenario. Intuitively, it is clear that stronger noise would require more regularization, as Morozov principle dictates [Vogel, 2002], but the strength of our algorithm is that it automatically selects a good range for $C$, without user input or prior knowledge about $\sigma$. In the low noise scenario, for all six components of $m$, the reconstructed posterior marginal distribution functions peak very close to their correct value, the difference would not actually be visible on the graphs. The picture is quite different in the high noise scenario. The support of the distribution functions are much wider in that case and two peaks are apparent for $m_1$ and for $m_2$. The large width for these distribution functions is related to a much larger number of samples in the random walk for the algorithm to converge as illustrated in Figure 6.

Let us now turn to the issue of choosing a starting point $(m_1, C_1)$. We found it most efficient to draw $N_{\text{burn}} \times N_{\text{par}}$ samples from the prior and use these samples to compute an expected value, which we set to be equal to $(m_1, C_1)$. In fact, we show in section 5.3 that all the deterministic methods that we used to solve inverse problem (1.1) failed, and accordingly a Monte Carlo approach for determining the starting point $(m_1, C_1)$ proved to be more efficient.

To conclude this section, we would like to emphasize that the numerical results that we show in this paper are not so sensitive to the the particular realizations of the noise and the intrinsic randomness of random walks. We conducted a large number of simulations each starting from a different realization of $u$. In the low noise scenario, the differences between final estimates of expected values and covariances were negligible. In the high noise scenario, the differences between final estimates of expected values and covariances were more appreciable, however final errors on the expected value of depth of $\Gamma$ as in row 1 of Figure 4 and the one standard deviation envelope as in row 2 of Figure 4 were comparable.
and the differences were small in the region of high values of the reconstructed slip $g_{\text{min}}$.

5.3 Comparison to methods based on GCV or CLS

5.3.1 The pointwise GCV method

A straightforward idea for solving problem (1.1) using the functional (1.2) in conjunction to the GCV selection criterion for $C$ is to assume that for each $m$ in $B$, $C$ is set to the value $C_{\text{GCV}}(m)$ which minimizes (2.2). After $C_{\text{GCV}}(m)$ is evaluated, the error functional

$$f_{\text{GCV}}(m) = \|A_m g_{\text{min}} - u\|^2 + C_{\text{GCV}}(m) \|R g_{\text{min}}\|^2,$$

(5.8)
is evaluated for a given $m$. Next, $f_{\text{GCV}}$ is minimized for $m$ in $B$. Due to the non-linearity of our problem in the parameter $m$, search algorithms end up trapped in local minima. In fact, even for a fixed $m$, determining $C_{\text{GCV}}(m)$ is problematic due to the lack of a clear numerical minimum as pointed out in [Varah, 1983]. In our simulations, even if we started the search algorithm from a value for $m$ close to the correct value (5.7), the minimization algorithm drifted away from this good starting point to terminate at an unreasonable answer.

5.3.2 The global GCV method

Insights on this method can be found in the celebrated paper [Golub et al., 1979], section 4, and was later more systematically studied in [Andrews, 1991]. In this method, one has to determine the global minimum of the ratio (2.2) for all $m$ in $B$ and $C > 0$. Our numerical simulations showed this led to results that are highly dependent on the starting point for $m$. Again, we observed that even if the search algorithm starts from a value for $m$ close to the correct value (5.7), the minimization terminates at an unreasonable answer.

5.3.3 Pointwise discrepancy principle

Suppose that an approximation to $\sigma$ is known. For each value of the nonlinear parameter $m$ equation (2.5) can be solved for $C$ numerically if $u$ is no further than $\sqrt{n}\sigma$ away from the range of $A_m$. Let $C_{\text{CLS}}(m)$ be the solution to this equation. Next step is to minimize

$$\|A_m g_{\text{min}} - u\|^2 + C_{\text{CLS}}(m) \|R g_{\text{min}}\|^2,$$

to solve for the nonlinear parameter $m$. As previously, this method is plagued by a multitude of local minima and drifts away from a good initial value for $m$.

5.3.4 Global discrepancy principle

Of all alternative methods discussed in this section, this method was the only one that yielded a useful solution, albeit in a much simplified setting. In fact it was effective only if we assumed that $m_1, m_2, m_3$ were known, so that the unknown nonlinear parameter $(m_4, m_5, m_6)$ is in $\mathbb{R}^3$. In practice the exact value of $\sigma$ is not known, but estimates on the range of $\sigma$ can be derived from measurements and from there it is possible to determine a useful range for the regularization constant $C$. To do so, following [Volkov and Sandiumenge, 2019], let $\pi(u)$ be the orthogonal projection of $u$ on the range of $A_m$. Then $\|A_m g_{\text{min}} - \pi(u)\|$ is a continuous
Figure 4: Reconstructed slip field $G$ (discretized by $g_{\text{min}}$) and depth profile for the fault $\Gamma$ (its geometry is modeled by $m$). In all six graphs in this figure, the horizontal axis is for $x_1$, and the vertical axis is for $x_2$. Left column: high noise scenario. Right column: low noise scenario. First row: depth contour lines for $\Gamma$ corresponding to the expected value of $m$ and the slip field modulus (shown in color) given that geometry and the computed expected value of $C$. The slip field was then obtained by applying the formula in H7. Second row: absolute value of the difference between expected depth obtained from the reconstruction and correct depth as a function of $(x_1, x_2)$ shown in color, with contour lines of reconstructed $|G|$. The third row shows the two standard deviation difference between for reconstructed depth, with again contour lines of reconstructed $|G|$. 
Figure 5: Reconstructed posterior marginal distribution functions for the six components of $m$ and for $\log_{10} C$. Blue: high noise scenario. Black: low noise scenario. For $m$, correct values are nearly indistinguishable from the peak of the black curves.
Figure 6: First row: evolution of computed expected values of \( m_1, m_2, m_3 \) (black, blue, and red solid lines) and one standard deviation envelopes. Left: high now scenario. Right: high noise scenario. Second row: evolution of computed expected values of \( m_4, m_5, m_6 \) (black, blue, and red solid lines) and one standard deviation envelopes. Left: high now scenario. Right: high noise scenario.
of function of $C$ in $(0, \infty)$ with range $(\|u - \pi(u)\|, \|u\|)$, see Volkov and Sandiumenge, 2019. Accordingly, let $\text{Err}$ be an estimate of $\sqrt{n}\sigma$. If $\text{Err} \geq \|u_i - \pi(u_i)\|$ we set

$$C_{CLS}(m) = \sup\{C > 0 : \|A_m g_{\min} - \pi(u)\| \leq \text{Err}\},$$

(5.9)

otherwise we set $C_{CLS}(m) = 0$. Finally, we set $C = \sup_{m \in B} C_{CLS}(m)$. Intuitively, this definition amounts to selecting for a given $m$ the value of $C$ that will lead to the most regular solution for a fixed error threshold, and then maximizing these values of $C$ over all $m$ in $B$.

Once a value for $C$ has been selected, we minimize the functional

$$f_C(m) = \|A_m g_{\min} - u_i\|^2 + C\|R g_{\min}\|^2,$$

(5.10)

for $m$ in $B$. Evidently, we have to contend with the non-linearity in $m$ which causes this functional to have many local minima. Consequently, a straightforward Newton’s method is inadequate. An efficient method will have to test a large number of starting points while taking into account the high cost of evaluating $f_C$.

Although we did not obtain any meaningful results in the general case where $m$ is in $B \subset \mathbb{R}^6$, we were still able to implement this method in lower dimension. Fix $m_1, m_2, m_3$ to be given by their correct value (5.7) and assume that $(m_4, m_5, m_6)$ is in $\mathbb{R}^3$ with $-100 < m_4 < 200$. We used the Matlab function `surrogateopt` to minimize $f_C$ knowing $(m_1, m_2, m_3)$ for a few values of $C$. The Matlab `surrogateopt` function is based on a minimization algorithm proposed in Gutmann, 2001 which is specifically designed for problems where function evaluations are expensive (in our case it is important to limit the number of times $g_{\min}$ is solved for). This algorithm uses a radial basis function interpolation to determine the next point where the objective function should be evaluated. Computed points where $f_C$ achieves a global minimum are shown in Table 1. Interestingly, in the low noise scenario, we observe that $m_5$ is well reconstructed for all the selected values of $C$, however there is more variability for $m_4$ and $m_6$. The downside of the the global discrepancy method is that there is no objective way to select an optimal value for $f_C$ unless $\sigma$ is known. This is in stark contrast with our proposed algorithm where the range for $C$ is automatically adjusted as the random walk progresses.

| $C$      | Low noise |       |       | High noise |       |       |
|----------|-----------|-------|-------|------------|-------|-------|
| $10^{-5}$| 15.32     | -40.81| -55.49| 10.24      | -39.65| -2.39 |
| $10^{-4.5}$| 21.05     | -40.78| -46.95| 67.71      | -52.24| 6.61  |
| $10^{-4}$ | 23.24     | -41.41| -54.40| 60.36      | -50.27| 5.88  |
| $10^{-3.5}$| 17.13     | -41.25| -50.45| 12.11      | -40.25| -42.73|
| $10^{-3}$ | 3.65      | -39.59| -52.10| 4.90       | -40.37| -49.04|
| $10^{-2.5}$| 6.34      | -39.69| -49.47| 28.07      | -40.40| -45.39|
| $10^{-2}$ | 12.53     | -40.05| -44.40| 16.23      | -39.88| -42.66|

Table 1: Computed values of $m_4, m_5, m_6$ obtained by the global discrepancy method used in conjunction to the global search function `surrogateopt`. The correct values are $m_4 = 8$, $m_5 = -40$, $m_6 = -50$. 

Although we did not obtain any meaningful results in the general case where $m$ is in $B \subset \mathbb{R}^6$, we were still able to implement this method in lower dimension. Fix $m_1, m_2, m_3$ to be given by their correct value (5.7) and assume that $(m_4, m_5, m_6)$ is in $\mathbb{R}^3$ with $-100 < m_4 < 200$. We used the Matlab function `surrogateopt` to minimize $f_C$ knowing $(m_1, m_2, m_3)$ for a few values of $C$. The Matlab `surrogateopt` function is based on a minimization algorithm proposed in Gutmann, 2001 which is specifically designed for problems where function evaluations are expensive (in our case it is important to limit the number of times $g_{\min}$ is solved for). This algorithm uses a radial basis function interpolation to determine the next point where the objective function should be evaluated. Computed points where $f_C$ achieves a global minimum are shown in Table 1. Interestingly, in the low noise scenario, we observe that $m_5$ is well reconstructed for all the selected values of $C$, however there is more variability for $m_4$ and $m_6$. The downside of the the global discrepancy method is that there is no objective way to select an optimal value for $f_C$ unless $\sigma$ is known. This is in stark contrast with our proposed algorithm where the range for $C$ is automatically adjusted as the random walk progresses.
6 Conclusion and perspectives for future work

We have derived in this paper a new probability distribution function for an augmented random vector comprising a set of nonlinear parameters to be inverted and a regularization parameter. Using this probability distribution we built an adaptive and parallel choice sampling algorithm for computing the expected value, the covariance, and marginal probability distributions of this random vector. Our results show that there is a great advantage in exploring all positive values for the regularization parameter and that the expected value of this regularization constant is automatically adjusted by our algorithm to the noise level. This contrasts to uncertainty principle based methods where a threshold based on some estimate of the noise level has to be set subjectively by the user. We have also discussed how GCV methods (pointwise, or global) fail since, as noted by other authors, the minimum of the GCV functional can be unpractical to capture numerically as this functional is often very flat near its minimum. Our algorithm was shown to perform well on an example where the VP functional method is bound to fail due the fact that the underlying linear operator has full numerical range, for all values of the nonlinear parameter.

So far, our numerical simulations have focused on the case \( q << n << p \), where the nonlinear parameter is in \( \mathbb{R}^q \), the measurements are in \( \mathbb{R}^n \), and the unknown forcing term is in \( \mathbb{R}^p \). However, there are applications in geophysical sciences where measurements are nearly continuous in space and time. This often comes at the price of higher error margins. With the notations from this paper, this would correspond to the case where \( n \) and \( p \) are of the same order of magnitude, but \( q \) is larger. We are planning to investigate this new case in future work. Another interesting line of research would be to consider the case where \( q \) is much larger (more nonlinear parameter to be recovered, or an inverse problem that depends non-linearly on a function). In that case we would want to build a method such that the number of times the matrix \( A_m \) has to be assembled and the functional (1.2) has to be minimized does not grow too fast with \( q \).

**Funding**

This work was supported by Simons Foundation Collaboration Grant [351025].

**References**

[Andrews, 1991] Andrews, D. W. (1991). Asymptotic optimality of generalized cl, cross-validation, and generalized cross-validation in regression with heteroskedastic errors. *Journal of Econometrics*, 47(2-3):359–377.

[Aspri et al., 2020a] Aspri, A., Beretta, E., and Mazzucato, A. L. (2020a). Dislocations in a layered elastic medium with applications to fault detection. *preprint arXiv:2004.00321v1.*

[Aspri et al., 2020b] Aspri, A., Beretta, E., Mazzucato, A. L., and Maarten, V. (2020b). Analysis of a model of elastic dislocations in geophysics. *Archive for Rational Mechanics and Analysis*, 236(1):71–111.

[Bishop et al., 1995] Bishop, C. M. et al. (1995). *Neural networks for pattern recognition.* Oxford university press.

24
[Calderhead, 2014] Calderhead, B. (2014). A general construction for parallelizing metropolis- hastings algorithms. Proceedings of the National Academy of Sciences, 111(49):17408–17413.

[Galatsanos and Katsaggelos, 1992] Galatsanos, N. P. and Katsaggelos, A. K. (1992). Methods for choosing the regularization parameter and estimating the noise variance in image restoration and their relation. IEEE Transactions on image processing, 1(3):322–336.

[Golub and Pereyra, 2003] Golub, G. and Pereyra, V. (2003). Separable nonlinear least squares: the variable projection method and its applications. Inverse problems, 19(2):R1.

[Golub et al., 1979] Golub, G. H., Heath, M., and Wahba, G. (1979). Generalized cross-validation as a method for choosing a good ridge parameter. Technometrics, 21(2):215–223.

[Gutmann, 2001] Gutmann, H.-M. (2001). A radial basis function method for global optimization. Journal of global optimization, 19(3):201–227.

[ Jacob et al., 2011] Jacob, P., Robert, C. P., and Smith, M. H. (2011). Using parallel computation to improve independent metropolis–hastings based estimation. Journal of Computational and Graphical Statistics, 20(3):616–635.

[Kaipio and Somersalo, 2006] Kaipio, J. and Somersalo, E. (2006). Statistical and computational inverse problems, volume 160. Springer Science & Business Media.

[Morozov, 1966] Morozov, V. A. (1966). On the solution of functional equations by the method of regularization. In Doklady Akademii Nauk, volume 167, pages 510–512. Russian Academy of Sciences.

[Okada, 1992] Okada, Y. (1992). Internal deformation due to shear and tensile faults in a half-space. Bulletin of the Seismological Society of America, vol. 82 no. 2:1018–1040.

[Roberts and Rosenthal, 2009] Roberts, G. O. and Rosenthal, J. S. (2009). Examples of adaptive mcmc. Journal of Computational and Graphical Statistics, 18(2):349–367.

[Roberts et al., 2001] Roberts, G. O., Rosenthal, J. S., et al. (2001). Optimal scaling for various metropolis-hastings algorithms. Statistical science, 16(4):351–367.

[Thompson et al., 1989] Thompson, A., Kay, J., and Titterington, D. (1989). A cautionary note about crossvalidatory choice. Journal of Statistical Computation and Simulation, 33(4):199–216.

[Varah, 1983] Varah, J. M. (1983). Pitfalls in the numerical solution of linear ill-posed problems. SIAM Journal on Scientific and Statistical Computing, 4(2):164–176.

[Vogel, 2002] Vogel, C. R. (2002). Computational methods for inverse problems, volume 23. Siam.

[Volkov, 2009] Volkov, D. (2009). A double layer surface traction free green’s tensor. SIAM Journal on Applied Mathematics, 69(5):1438–1456.
[Volkov and Sandiumenge, 2019] Volkov, D. and Sandiumenge, J. C. (2019). A stochastic approach to reconstruction of faults in elastic half space. *Inverse Problems & Imaging*, 13(3):479–511.

[Volkov et al., 2017a] Volkov, D., Voisin, C., and Ionescu, I. (2017a). Reconstruction of faults in elastic half space from surface measurements. *Inverse Problems*, 33(5).

[Volkov et al., 2017b] Volkov, D., Voisin, C., and I.R., I. (2017b). Determining fault geometries from surface displacements. *Pure and Applied Geophysics*, 174(4):1659–1678.