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Bayesian Inversion in Geoscience

Dario Grana[1], Klaus Mosegaard[2] and Henning Omre[3]
[1]Department of Geology and Geophysics, University of Wyoming, Laramie, WY, USA
[2]Niels Bohr Institute, University of Copenhagen, Copenhagen, Denmark
[3]Department of Mathematical Sciences, Norwegian University of Science and Technology, Trondheim, Norway

Definition

Bayesian inversion is a statistical method used in many geoscience applications to assess the probability distribution of the unknown variables conditioned on the available measurements, where the posterior model is uniquely defined by a prior model representing the knowledge of the variable before the data acquisition and a likelihood model linking the target variables and the measured data.

Introduction

Geophysics theories, such as seismology, electromagnetism, and poro-elasticity, include mathematical relations of the physical processes and properties of rock and fluid properties in the subsurface. If the rock and fluid physical properties are known, then it is possible to apply a forward operator to predict the geophysical response of the subsurface. For example, if the volumetric fractions of the mineral and fluid components of porous rocks are known, then their seismic response can be predicting by solving a set of poro-elastic equations. In practice, the petrophysical properties of the porous rocks are unknown, whereas their geophysical response can be measured using geophysical methods, such as seismic acquisition. Therefore, the prediction of the rock and fluid properties from geophysical measurements can be defined as an inverse problem. Bayesian methods are commonly used in geophysical inverse problems (Tarantola 2005).

Geophysical inverse problems are often ill-posed and the solution is generally nonunique. Bayesian inverse theory provides a mathematical framework for these problems since it aims at calculating the posterior probability distribution of the variables of interest conditioned on the measured data by combining the prior distribution of the model variables with the likelihood function of the data. The prior model represent the knowledge of the variables of interest prior to the data acquisition, whereas the likelihood model links the variables of interest and the measured data. The posterior model is then uniquely identified by these two models (Tarantola 2005). The posterior model can be computed analytically for certain classes of likelihood and prior models, but in the general case, the posterior distribution must be assessed numerically, by iteratively approximating the solution. Bayesian methods have been proposed for a variety of geophysical inverse problems (Mosegaard and Tarantola 1995; Scales and Tenorio 2001; Ulrych et al. 2001; Buland and Omre 2003; Tarantola 2005; Rimstad et al. 2012).

The focus of this entry is on seismic inverse problems for the prediction of subsurface properties from seismic measurements (Aki and Richards 1980). The geophysics literature includes a variety of formulations of the seismic inversion problem, which differ for the formulation and parameterization of the physical operator. Indeed, the seismic inverse problem can be formulated in terms of elastic properties (seismic velocity and density or seismic impedance) or petrophysical properties (porosity, mineral volumes, and fluid saturations), and the physics can include the full wave propagation model or linearized approximations. For linear formulations and under Gaussian assumptions, analytical solutions of the Bayesian inverse problem are derived (Buland and Omre 2003; Grana et al. 2017), whereas for nonlinear formulations, Monte Carlo methods must be adopted to approximate the posterior distribution

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(Mosegaard and Tarantola 1995; Sambridge and Mosegaard 2002).

In the following, we review the main principles of Bayesian inverse theory, present analytical solutions for linear inverse problems assuming Gaussian and Gaussian mixture distributions, and present an overview of Markov chain Monte Carlo methods. These methods are illustrated on a one-dimensional synthetic seismic dataset for the prediction of the elastic properties of porous rocks in the subsurface.

Methods

In geophysical inverse problems, the variable of interest is a physical property in the subsurface, defined on a spatial grid, and it is represented here by the vector $\boldsymbol{m}$, whereas the geophysical data, such as seismic amplitudes, are represented here by the vector $\boldsymbol{d}$. The aim of the inverse problem is to assess the variables $\boldsymbol{m}$ given the measured data $\boldsymbol{d}$ associated with the forward model

$$\boldsymbol{d} = \boldsymbol{f}(\boldsymbol{m}) + \boldsymbol{e}, \tag{1}$$

where $\boldsymbol{f}(\cdot)$ is the geophysical forward operator and $\boldsymbol{e}$ represents the measurement errors. For example, the data can be seismic measurements and the model variables can be elastic and petrophysical properties of porous rocks. The forward operator $\boldsymbol{f}(\cdot)$ can be represented by linear or nonlinear physical relations.

In a deterministic setting, the least square solution $\hat{\boldsymbol{m}}$ can be obtained by minimizing the L2 norm of the residuals $\boldsymbol{r} = \boldsymbol{d} - \boldsymbol{f}(\boldsymbol{m})$, i.e., difference between measured and predicted data:

$$\hat{\boldsymbol{m}} = \arg\min_{\boldsymbol{m}} \|\boldsymbol{d} - \boldsymbol{f}(\boldsymbol{m})\|_2. \tag{2}$$

For ill-conditioned and rank-deficient systems, singular value decomposition or regularization methods, such as Tikhonov regularization, are generally applied.

In a probabilistic setting, the solution of the inverse problem is expressed as the posterior probability distribution $p(\boldsymbol{m}|\boldsymbol{d})$ of the variables given the measured data, which can be assessed using Bayes' theorem

$$p(\boldsymbol{m}|\boldsymbol{d}) = \frac{p(\boldsymbol{d}|\boldsymbol{m})p(\boldsymbol{m})}{p(\boldsymbol{d})} = \text{const} \times p(\boldsymbol{d}|\boldsymbol{m})p(\boldsymbol{m}) \tag{3}$$

where $p(\boldsymbol{m})$ is the prior distribution of the variables, $p(\boldsymbol{d}|\boldsymbol{m})$ is the data likelihood function, and $p(\boldsymbol{d})$ is a normalizing constant to guarantee that the posterior distribution $p(\boldsymbol{m}|\boldsymbol{d})$ is a valid probability distribution.

The Bayesian inversion concept is graphically displayed in Fig. 1. The goal is to assess the variable of interest $\boldsymbol{m}$ given a value $\boldsymbol{d}^0$ of the measured data $\boldsymbol{d}$. Figure 1a displays the likelihood model $p(\boldsymbol{d}|\boldsymbol{m})$ and the prior model $p(\boldsymbol{m})$. The Bayesian inversion operates in the $[\boldsymbol{m} \times \boldsymbol{d}]$- space. The forward operator $\boldsymbol{f}(\boldsymbol{m})$ and the associated random error $\boldsymbol{e}$ define the likelihood model $p(\boldsymbol{d}|\boldsymbol{m})$, whereas the prior model $p(\boldsymbol{m})$ with prior expectation $\boldsymbol{\mu}_m$ is specified based on the prior knowledge of the variable $\boldsymbol{m}$. Figure 1b displays the joint distribution $p(\boldsymbol{m}, \boldsymbol{d}) = p(\boldsymbol{d}|\boldsymbol{m})p(\boldsymbol{m})$ as a contour map. The joint model fully defines the interaction between $\boldsymbol{m}$ and $\boldsymbol{d}$. The marginal distribution $p(\boldsymbol{d})$ is obtained by integrating $p(\boldsymbol{m}, \boldsymbol{d})$ over the values of the variable $\boldsymbol{m}$. The normalizing constant $p(\boldsymbol{d}^0)$ is obtained by evaluating the marginal distribution in the data value $\boldsymbol{d}^0$.

Figure 1c displays the posterior distribution $p(\boldsymbol{m}|\boldsymbol{d}^0) = p(\boldsymbol{m}, \boldsymbol{d}^0)/p(\boldsymbol{d}^0)$ in Eq. 3 and its posterior expectation $\boldsymbol{\mu}_{m|d^0}$ for the data value $\boldsymbol{d}^0$. In the general case, the prior and posterior models might not be Gaussian. For highly skewed or multimodal distributions, the variable values associated with the maximum of the prior and posterior models are generally more informative than the prior and posterior expectations.

Bayesian Linear Inversion

In the case of linear operators, the forward model in Eq. 1 is rewritten as a linear system of equations

$$\boldsymbol{d} = \mathbf{F}\boldsymbol{m} + \boldsymbol{e}, \tag{4}$$

where $\mathbf{F}$ is the matrix defined by the linear operator $\boldsymbol{f}(\cdot)$. If the random error $\boldsymbol{e}$ is assumed to be Gaussian with $\mathbf{0}$-mean and covariance matrix equal to $\boldsymbol{\Sigma}_e$, then the likelihood model $p(\boldsymbol{d}|\boldsymbol{m})$ is Gaussian

$$p(\boldsymbol{d}|\boldsymbol{m}) = \mathcal{N}(\boldsymbol{d}; \mathbf{F}\boldsymbol{m}, \boldsymbol{\Sigma}_e) \tag{5}$$

with expectation $\mathbf{F}\boldsymbol{m}$ linear in $\boldsymbol{m}$ and covariance matrix $\boldsymbol{\Sigma}_e$.

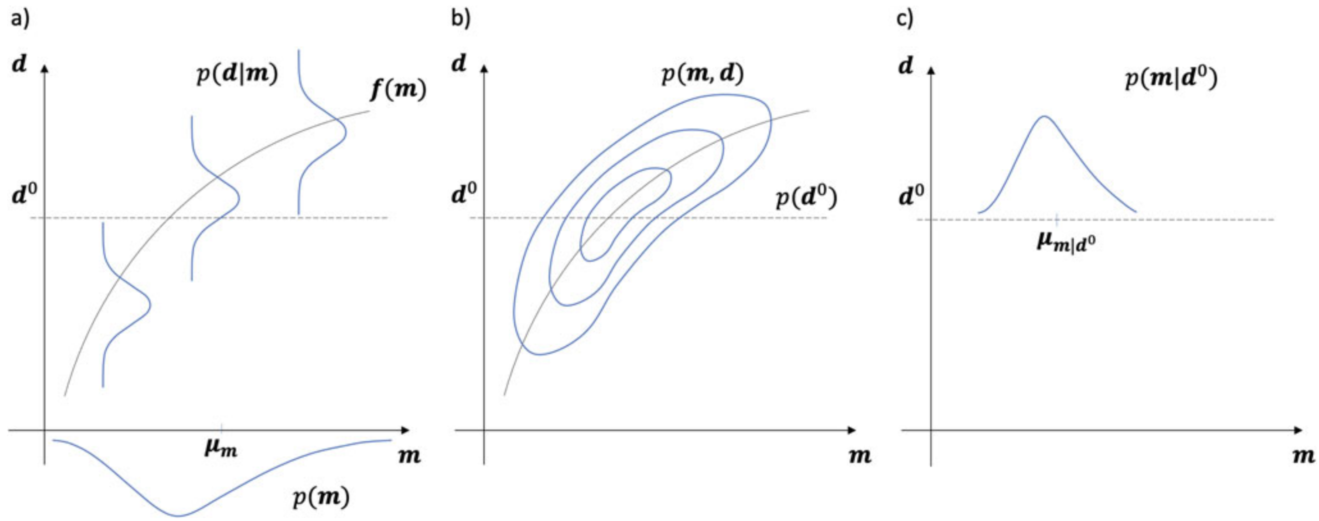
If the prior model of the variables $p(\boldsymbol{m})$ is Gaussian, then the posterior model of the variables given the measured data $p(\boldsymbol{m}|\boldsymbol{d})$ is also Gaussian. Hence, the prior and posterior models are conjugate distributions with respect to the likelihood model $p(\boldsymbol{d}|\boldsymbol{m})$. For a Gaussian prior model $p(\boldsymbol{m}) = \mathcal{N}(\boldsymbol{m}; \boldsymbol{\mu}_m, \boldsymbol{\Sigma}_m)$ with expectation $\boldsymbol{\mu}_m$ and covariance matrix $\boldsymbol{\Sigma}_m$, the posterior distribution of the variable $[\boldsymbol{m}|\boldsymbol{d}]$ is also Gaussian

$$p(\boldsymbol{m}|\boldsymbol{d}) = \mathcal{N}\left(\boldsymbol{m}; \boldsymbol{\mu}_{m|d}, \boldsymbol{\Sigma}_{m|d}\right) \tag{6}$$

with conditional expectation $\boldsymbol{\mu}_{m|d}$ and conditional covariance matrix $\boldsymbol{\Sigma}_{m|d}$ given by

$$\boldsymbol{\mu}_{m|d} = \boldsymbol{\mu}_m + \boldsymbol{\Sigma}_m\mathbf{F}^T\left[\mathbf{F}\boldsymbol{\Sigma}_m\mathbf{F}^T + \boldsymbol{\Sigma}_e\right]^{-1}(\boldsymbol{d} - \mathbf{F}\boldsymbol{\mu}_m), \tag{7}$$

and



Bayesian Inversion in Geoscience, Fig. 1 Graphical representation of Bayesian inversion: (**a**) prior and likelihood models, (**b**) joint model, and (**c**) posterior model

$$\boldsymbol{\Sigma}_{m|d} = \boldsymbol{\Sigma}_m - \boldsymbol{\Sigma}_m \mathbf{F}^T \left[\mathbf{F}\boldsymbol{\Sigma}_m \mathbf{F}^T + \boldsymbol{\Sigma}_e\right]^{-1} \mathbf{F}\boldsymbol{\Sigma}_m, \tag{8}$$

respectively. The posterior variances of the marginal distributions are independent of the measurement values and only depends on the parameters of prior model and measurement errors. The derivation can be found in Tarantola (2005).

In Buland and Omre (2003), the Bayesian linear formulation is applied to the seismic inversion problem. This approach is referred to as Bayesian linearized amplitude-versus-offset (AVO) inversion. The linear forward operator is obtained by assuming a convolution of a known wavelet and the linearized AVO approximation (Aki and Richards 1980) of the reflectivity coefficients that are function of the time-derivative of the logarithm of the elastic properties. The convolution is a linear operator, hence the forward operator can be expressed by a matrix multiplication, $\mathbf{F} = \mathbf{WAD}$, where $\mathbf{W}$ is the wavelet matrix, $\mathbf{A}$ is the reflectivity coefficient matrix, and $\mathbf{D}$ is a first-order differential matrix. The forward operator is then linear with respect to the logarithm of the elastic properties $\ln(\boldsymbol{m})$ (where $\boldsymbol{m}$ is here a dimensionless representation of the parameters) and the linear expression in Eq. 4 can be written as $\boldsymbol{d} = \mathbf{WAD}\ln(\boldsymbol{m}) + \boldsymbol{e}$. In Buland and Omre (2003), a Gaussian distribution for the logarithm of the elastic properties $\ln(\boldsymbol{m})$ is assumed, which entails a log-Gaussian prior model of the variable $\boldsymbol{m}$. Based on these assumptions, the seismic inversion problem is analytically tractable and the posterior model of $[\ln(\boldsymbol{m})|\boldsymbol{d}]$ is Gaussian, which entails a log-Gaussian posterior model of the variable $[\boldsymbol{m}|\boldsymbol{d}]$ (Buland and Omre 2003).

Gaussian mixture distributions are also conjugate models with respect to the likelihood function $p(\boldsymbol{d}|\boldsymbol{m})$. If the prior model of the variables is a Gaussian mixture distribution $p(\boldsymbol{m}) = \sum_{\boldsymbol{k}} p(\boldsymbol{k})\mathcal{N}(\boldsymbol{m};\, \boldsymbol{\mu}_{m|k},\, \boldsymbol{\Sigma}_{m|k})$, then the posterior model of the variables given the measured data is also a Gaussian mixture distribution

$$p(\boldsymbol{m}|\boldsymbol{d}) = \sum_{\boldsymbol{k}} p(\boldsymbol{k}|\boldsymbol{d})\mathcal{N}\left(\boldsymbol{m}; \boldsymbol{\mu}_{m|d,k}, \boldsymbol{\Sigma}_{m|d,k}\right) \tag{9}$$

with conditional mean $\boldsymbol{\mu}_{m|d,k}$ and conditional covariance matrix $\boldsymbol{\Sigma}_{m|d,k}$, given by

$$\boldsymbol{\mu}_{m|d,k} = \boldsymbol{\mu}_{m|k} + \boldsymbol{\Sigma}_{m|k}\mathbf{F}^T\left[\mathbf{F}\boldsymbol{\Sigma}_{m|k}\mathbf{F}^T + \boldsymbol{\Sigma}_e\right]^{-1}\left(\boldsymbol{d} - \mathbf{F}\boldsymbol{\mu}_{m|k}\right), \tag{10}$$

and

$$\boldsymbol{\Sigma}_{m|d,k} = \boldsymbol{\Sigma}_{m|k} - \boldsymbol{\Sigma}_{m|k}\mathbf{F}^T\left[\mathbf{F}\boldsymbol{\Sigma}_{m|k}\mathbf{F}^T + \boldsymbol{\Sigma}_e\right]^{-1}\mathbf{F}\boldsymbol{\Sigma}_{m|k}, \tag{11}$$

respectively (Grana et al. 2017). Due to the spatial coupling of the likelihood model in many geophysical applications, the posterior probability $p(\boldsymbol{k}|\boldsymbol{d})$

$$p(\boldsymbol{k}|\boldsymbol{d}) = \frac{p(\boldsymbol{d}|\boldsymbol{k})p(\boldsymbol{k})}{p(\boldsymbol{d})} = \text{const} \times p(\boldsymbol{d}|\boldsymbol{k})p(\boldsymbol{k}) \tag{12}$$

cannot be analytically computed. The numerical calculation of $p(\boldsymbol{k}|\boldsymbol{d})$ is computationally demanding, hence it must be numerically approximated (Grana et al. 2017).

In the framework of Bayesian inverse theory, Monte Carlo methods can be used to generate realizations of the posterior distribution of Gaussian linear inverse problems, honoring a covariance function describing the spatial continuity of the variables.

Monte Carlo Methods

For general nonlinear problems in Eq. 1, analytical solutions are generally not available and numerical techniques such as Monte Carlo and Markov chain Monte Carlo (McMC) algorithms must be adopted to approximate the posterior distribution (Mosegaard and Tarantola 1995; Sambridge and Mosegaard 2002). In Monte Carlo acceptance/rejection sampling approaches, the posterior distribution is approximated by sequentially drawing proposals from a prior distribution of the variable and accepting or rejecting the proposal based on its likelihood. In McMC methods, the posterior distribution is approximated by sequentially drawing proposals from a proposal distribution conditioned on the previous realization of the variable.

Markov chain Monte Carlo methods design a random walk in the variable space using a Markov chain, i.e., a random process in which the probability of moving from the previous state to the current state is defined by a transition probability that depends only on the previous state. In applications to inverse problems, this process is used to draw realizations from the posterior distribution. The sequence of samples, i.e., the Markov chain, asymptotically reaches a stationary distribution that is equal to the posterior distribution of the Bayesian inverse problem. There are different Markov chain Monte Carlo algorithms, including Metropolis, Metropolis-Hastings, and Gibbs sampling.

The most general McMC technique is the Metropolis-Hastings algorithm. According to a Metropolis-Hastings approach frequently used in geoscience, an initial realization $\boldsymbol{m}_0$ is generated from the prior distribution $p(\boldsymbol{m})$ and represents the initial state of the chain. Then, at each iteration i, the proposed realization $\boldsymbol{m}_p$ is generated by sampling from a proposal distribution $g(\boldsymbol{m}|\boldsymbol{m}_{i-1})$ conditioned on the state $\boldsymbol{m}_{i-1}$ at the previous iteration. The proposed realization is accepted with probability

$$p^* = \min\left(\frac{p(\boldsymbol{d}|\boldsymbol{m}_p)p(\boldsymbol{m}_p)g(\boldsymbol{m}_{i-1}|\boldsymbol{m}_p)}{p(\boldsymbol{d}|\boldsymbol{m}_{i-1})p(\boldsymbol{m}_{i-1})g(\boldsymbol{m}_p|\boldsymbol{m}_{i-1})}, 1\right) \quad (13)$$

If accepted, the proposed realization is assigned to the current state $\boldsymbol{m}_i = \boldsymbol{m}_p$, otherwise $\boldsymbol{m}_i = \boldsymbol{m}_{i-1}$. The McMC algorithms converges in the sense that the generated states represent realizations from the posterior model, as iterations increase. The Gibbs sampling is a special case of the Metropolis-Hasting algorithm, and it generates proposals from the full conditional distribution of subdimensions of $\boldsymbol{m}_i$, hence $p^* = 1$ in Eq. 14, such that the proposed state is always accepted. However, in many applications, this advantage of the Gibbs sampler is offset by the need to compute full conditional distributions at each iteration.

In the Metropolis approach, the proposal distribution $g(\boldsymbol{m}|\boldsymbol{m}_{i-1})$ is assumed to be symmetric, such that $g(\boldsymbol{m}|\boldsymbol{m}_{i-1}) = g(\boldsymbol{m}_{i-1}|\boldsymbol{m})$ and the acceptance probability becomes

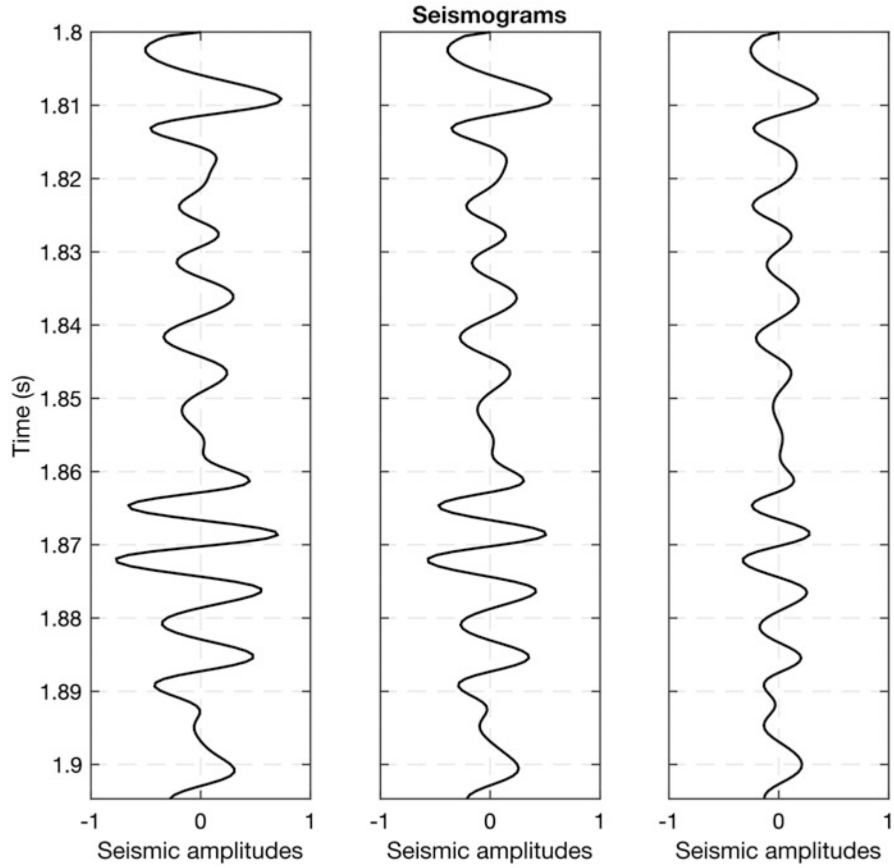
$$p^* = \min\left(\frac{p(\boldsymbol{d}|\boldsymbol{m}_i)p(\boldsymbol{m}_i)}{p(\boldsymbol{d}|\boldsymbol{m}_{i-1})p(\boldsymbol{m}_{i-1})}, 1\right) \quad (14)$$

Monte Carlo and Markov chain Monte Carlo approaches are adopted for seismic and petrophysical inversion problems and combined with analytical approximations to sample from the posterior distributions. The methodology is used for litho-fluid classification (Grana et al. 2017) and is also extended to seismic classification problems including categorical variables (de Figueiredo et al. 2019).

Example

We illustrate the application of Bayesian inverse methods to a seismic inversion problem to predict the elastic properties along a one-dimensional profile from a set of seismograms measured with different acquisition geometries. The subsurface variables of interest are: P-wave velocity, S-wave velocity, and density. The measured data include three synthetic seismograms computed from a set of borehole data for incident angles of 12°, 24°, and 36° (Fig. 2). The forward operator is a convolution of a known wavelet and the reflectivity coefficients computed from the elastic properties, according to Aki-Richards approximation for the linearized operator and according to Zoeppritz equations for the nonlinear operator (Aki and Richards 1980).

First, we apply the Bayesian linearized AVO inversion proposed in Buland and Omre (2003) to the seismic dataset in Fig. 3 by using the Aki Richards approximation. The prior distribution model is a trivariate Gaussian distribution of the logarithms of the elastic properties. The prior mean is represented by a low frequency trend of the elastic properties computed by filtering the well log data at a cutoff frequency equal to the lower bound of the seismic bandwidth. The prior covariance matrix is estimated from the difference between the actual well measurements and the prior mean. The prior model includes an exponential spatial correlation function with correlation length of 20 *ms*. The marginal distributions of the prior model are shown in Fig. 3. The measurement error is assumed to be spatially uncorrelated with 0-mean and variance equal to 20% of the variance of the data, corresponding to a signal-to-noise ratio of 5. The posterior distribution of the elastic variables is then the Gaussian distribution of the logarithms of the elastic properties defined in Eq. 6 with parameters given by the analytical expressions in Eqs. 7 and 8. The marginal components of the posterior distribution of the elastic variables are shown in Fig. 4. The



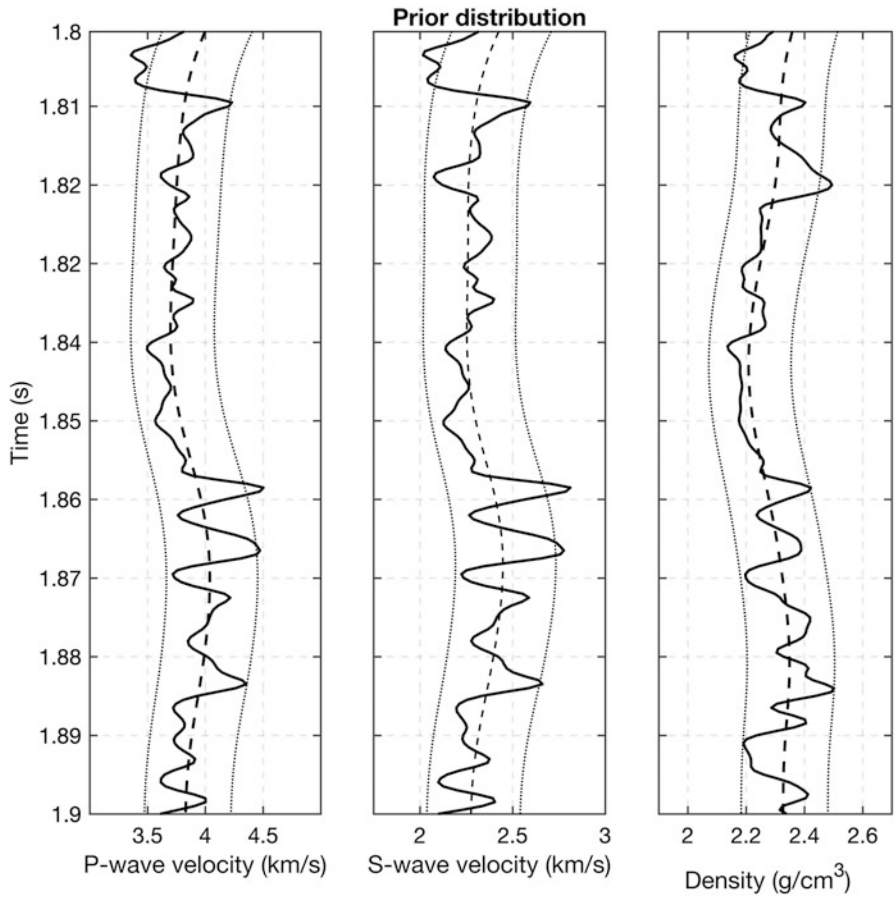
Bayesian Inversion in Geoscience, Fig. 2 Synthetic seismograms representing the seismic measurements: from left to right, seismograms for incident angles of 12°, 24°, and 36°

maximum posterior predictions of the marginal distribution are in good agreement with the reference data.

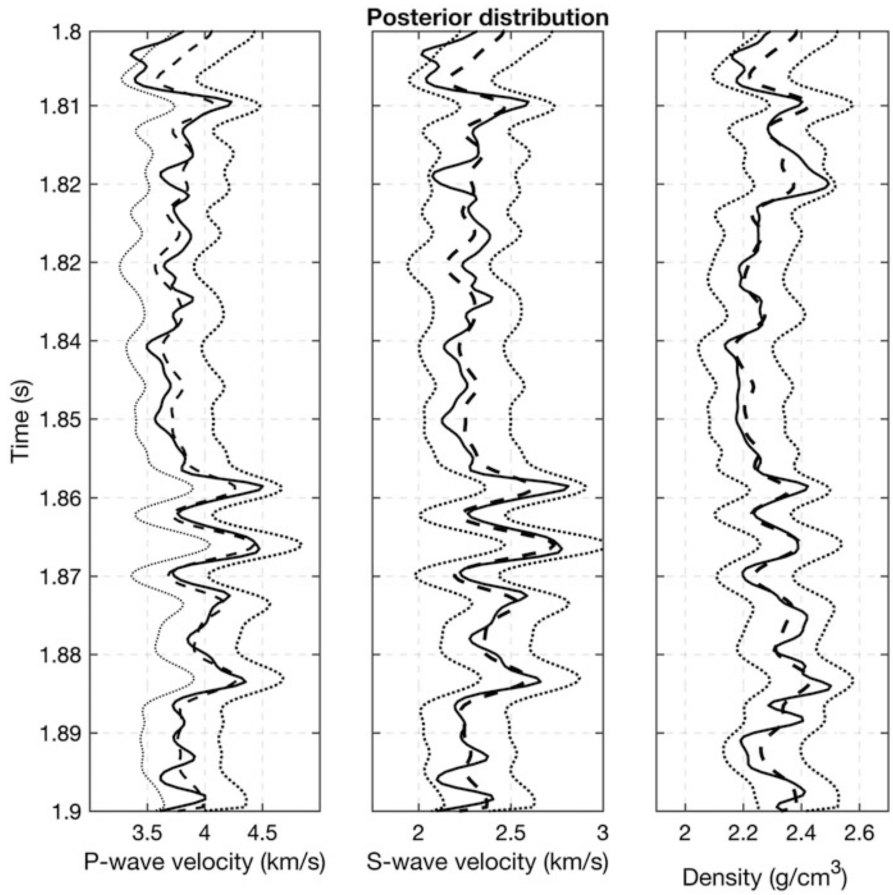
We also apply a Markov chain Monte Carlo method based on the Metropolis-Hastings algorithm to the same seismic dataset using the convolutional operator and the nonlinear Zoeppritz equations. The prior realization of the model variables is generated by sampling from the trivariate prior distribution with exponential spatial correlation function used in the previous example. The proposal distribution is assumed to be Gaussian. In this application, 4000 proposals are drawn from the proposal distribution with an acceptance rate of approximately 24%. Figure 5 shows 500 realizations randomly selected after convergence. The algorithm is repeated 10 times, starting from different states, to avoid that results might be biased by the initial realization of the chain.

Conclusions

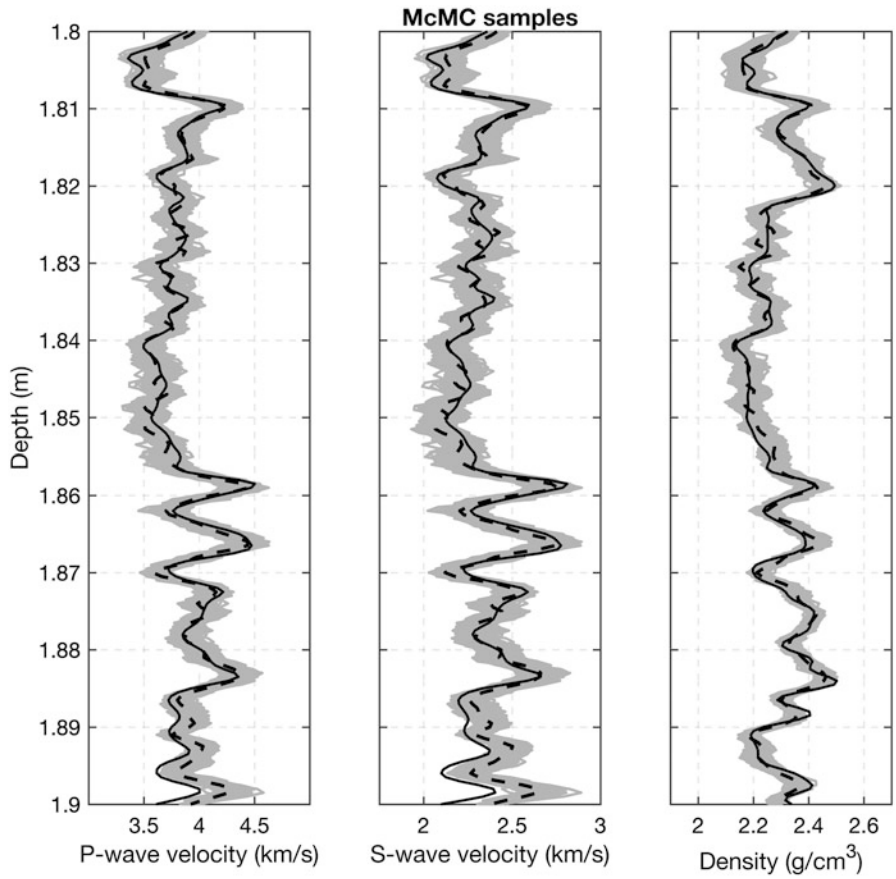
Bayesian inversion methodologies are commonly adopted in geophysical inverse problems for the assessment of the posterior distribution of the subsurface variables conditioned on the available data. The Bayesian approach provides a natural framework to predict the most likely solution and to quantify the associated uncertainty. For linear inverse problems, with Gaussian prior distribution and linear likelihood operators with additive Gaussian errors, the posterior distribution is also Gaussian and the posterior mean and covariance matrix can be analytically assessed. The analytical tractability makes the approach very efficient and easily extendable to three-dimensional studies. For nonlinear problems, the posterior distribution is iteratively approximated using stochastic simulation algorithms such as the Markov chain Monte Carlo method. The need for iterative algorithms makes the approach computationally demanding, especially for large datasets. A demonstration of the two approaches is presented on a seismic inversion problem assessing the posterior distribution of elastic properties of subsurface porous rocks. The Bayesian approach can be extended to other model parameterizations and formulations, to include rock physics models for the prediction of petrophysical properties. Furthermore, categorical variables associated with geological concepts can be included for the classification of litho-fluid classes. Such formulations generally require more complex prior models, combining Gaussian mixture distributions with Markov random fields.



Bayesian Inversion in Geoscience, Fig. 3 Prior distribution of the model variables: from left to right, P-wave velocity, S-wave velocity, and density. Solid black lines represent the true model, dashed black lines represent the mean, and dotted black lines represent the 0.90 confidence interval



Bayesian Inversion in Geoscience, Fig. 4 Posterior distribution of the model variables: from left to right, P-wave velocity, S-wave velocity, and density. Solid black lines represent the true model, dashed black lines represent the mean, and dotted black lines represent the 0.90 confidence interval



Bayesian Inversion in Geoscience, Fig. 5 Markov chain Monte Carlo posterior samples of the model variables: from left to right, P-wave velocity, S-wave velocity, and density. Solid black lines represent the true model, dashed black lines represent the mean, and grey lines represent the posterior samples

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