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# Accelerating target-oriented elastic full-waveform uncertainty estimation by reciprocity

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# Summary

The accuracy of a model obtained by full-waveform inversion can be estimated by analysing the sensitivity of the data to perturbations of the model parameters in selected subsurface points. Each perturbation requires the computation of the seismic response in the form of Born scattering data for a typically very large number of shots, making the method time consuming. The computational cost can be significantly reduced by considering the point where the subsurface parameters are perturbed as a Born scatterer. Instead of modelling each shot separately, reciprocity relations provide the Green functions from the sources to the scatterer in terms of Green's functions from the scatterer to the sources. In this way, the Born scattering data from a single point in the isotropic elastic case for a marine acquisition with pressure sources and receivers can be expressed in terms of the Green functions for force and moment tensor sources located at the scatterer and only a small number of forward runs are required. A 2-D example illustrates how the result can be used to determine the hessian and local covariance matrix for the model parameters at the scatterer at the cost of 5 forward simulation.



### Accelerating target-oriented elastic full-waveform uncertainty estimation by reciprocity

### Introduction

Proper characterization of the underground conditions including uncertainty quantification is required in applications such as seismic exploration, monitoring of exiting hydrocarbon reservoirs, storage of  $CO_2$  or  $H_2$ , and geothermal energy. The subsurface is described by a set of model parameters which are reconstructed by minimising the misfit between the observed and the simulated data. The accuracy of the reconstruction depends on the sensitivity of the data to perturbations of the model parameters, commonly characterized by the second derivatives, or hessian, of the misfit function at the global minimum. The pseudo-inverse of the hessian is proportional to the covariance matrix of the model parameters in the maximum likelihood estimator (Backus and Gilbert, 1970; Tarantola, 2005).

One cost-effective way to estimate the hessian in a finite-difference code is to put perturbations in the model parameters on a sparse set of grid points and treat them all at once by de-migration or modelling followed by migration (Rickett, 2003). In the acoustic case with a diagonally dominant hessian, the resulting point-spread functions can be cut out of the migration image and interpolated to all grid points as an approximation to the hessian. In the elastic case, however, we observed severe cross talk caused by the difference between P- and S-wave velocities and mixing of events. An alternative approach is to treat one model perturbation at the time, but simultaneously for a collection of points instead of single points to reduce cost. With the same relative perturbation for a region or geological unit, this provides an estimate of the hessian and at the same time suppresses null-space components (Mulder and Kuvshinov, 2023).

In target-oriented applications, we can treat one model perturbation at the time for a limited number of points, which are considered as Born scatterers. For each perturbation, we compute the Born scattering data for an entire survey without modelling the actual shots. Instead, we simulate only a few shots with different source characteristics at each position of a Born scatterer. Seismic data for the full survey and for each parameter are synthesized by applying reciprocity. Ikelle and Amundsen (2000) used a similar approach, but in our formulation, we model water as an elastic solid with zero shear-wave velocity and adopt the second- instead of first-order form of the equations, leading to different, simpler expressions for the Born data. The results enable the construction of a local subset of the hessian, describing the conditional uncertainty for the model parameters at the selected set of subsurface points.

Figure 1 sketches the idea in 2D. A source at  $(x_s, z_s)$  generates the incoming field, indicated by the red arrow, which is scattered at (x, y) towards a receiver at  $(x_r, z_r)$ , indicated by the green arrow. Reciprocity enables the replacement of a Green function from source to scatterer (red arrow) by another Green function from scatterer to





source, indicated by the blue arrow. In this way, a source at the scatter point can generate the Green functions for all shots and receivers at once. In the constant-density acoustic case, this can be accomplished by a single shot. In the elastic case, several shots with different source characteristics are required. Next, the method will be described for the isotropic elastic case with an explosive source and pressure data, followed by a 2D marine example.

#### Method

The least-squares misfit functional for observed data  $\mathbf{d}^{\text{obs}}$ , modelled by an operator  $\mathscr{F}(\mathbf{m})$  with parameters  $\mathbf{m}$ , has the form  $J(\mathbf{m}) = \frac{1}{2} || \mathscr{F}(\mathbf{m}) - \mathbf{d}^{\text{obs}} ||^2$ . The hessian of  $J(\mathbf{m})$  at its minimum equals  $\mathbf{H} = \mathbf{F}^{\mathsf{T}} \mathbf{F}$  with Fréchet derivative  $\mathbf{F} = \nabla_{\mathbf{m}} \mathscr{F}(\mathbf{m})$  and can be computed by perturbing one model parameter  $m_j$  at the time by  $\delta m_j$ , determining the associated scattering data for a full seismic survey, and cross correlating these data. Earlier, we have applied relative perturbations that are constant in large regions or geological units to estimate the hessian for uncertainty quantification (Mulder and Kuvshinov, 2023). Alternatively, for target-oriented applications, model parameters can be perturbed for each grid point in a small subset of the model. Uncertainty analysis involves simulations of all shots in a seismic survey for each perturbation. The computational cost is significantly reduced by using reciprocity and the Born



approximation. This requires simulating a small number of shots with different source characteristics at the location of the perturbation. From the recorded data at the original shot and receiver positions, we synthesize Born data and use those to compute a subset of the hessian.

The elastodynamic equations in the frequency domain, in terms of the displacement  $\mathbf{u}(\mathbf{x}, \boldsymbol{\omega})$  at position  $\mathbf{x}$  and angular frequency  $\boldsymbol{\omega}$ , are

$$-\omega^2 \rho u_i - \sum_{j=1}^3 \partial_{x_j} \left( \sigma_{ji} + T_{ji} \right) - f_i = 0, \quad i = 1, 2, 3,$$
(1)

with density  $\rho(\mathbf{x})$ , force source  $\mathbf{f}(\mathbf{x}, \boldsymbol{\omega})$ , and symmetric moment source tensor  $\mathbf{T}(\mathbf{x}, \boldsymbol{\omega})$ , which may be rewritten as a force source. The components of the stress tensor  $\sigma$  in the isotropic case are  $\sigma_{ji} = \sigma_{ij} = (v_2 - 2v_3)\varphi \delta_{ij} + 2v_3\varepsilon_{ij}$ . Here,  $\varepsilon_{ij} = \frac{1}{2}(\partial_{x_i}u_j + \partial_{x_j}u_i)$  is the strain tensor,  $\varphi(\mathbf{x}, \boldsymbol{\omega}) = \sum_j \varepsilon_{jj} = \nabla \cdot \mathbf{u}$  is the volumetric strain, and  $\delta_{ij}$  is the Kronecker delta. The model parameters are taken as  $v_1 = \rho$ ,  $v_2 = \rho v_p^2$ ,  $v_3 = \rho v_s^2$ , for P- and S-wave velocities  $v_p$  and  $v_s$ , respectively. The Born approximation with incoming fields  $\mathbf{u}$  and scattered fields  $\delta \mathbf{u}$  can be expressed as

$$\omega^{2} \mathbf{v}_{1} \delta u_{i} - \partial_{x_{i}} \left[ (\mathbf{v}_{2} - 2\mathbf{v}_{3}) \delta \varphi \right] - \sum_{j} \partial_{x_{j}} \left( 2\mathbf{v}_{3} \delta \varepsilon_{ij} \right) = \omega^{2} \delta \mathbf{v}_{1} u_{i} + \partial_{x_{i}} \left[ (\delta \mathbf{v}_{2} - 2\delta \mathbf{v}_{3}) \varphi \right] + \sum_{j} \partial_{x_{j}} \left( 2\delta \mathbf{v}_{3} \varepsilon_{ij} \right),$$
<sup>(2)</sup>

with  $\delta \varphi = \sum_{j} \delta \varepsilon_{jj}$  and  $\delta \varepsilon_{ij} = \frac{1}{2} (\partial_{x_j} \delta u_i + \partial_{x_i} \delta u_j)$  for i, j = 1, 2, 3. The scattered data follow either from solving the two coupled systems (1) and (2) or by a Taylor-series approximation (Fichtner, 2011, e.g.). In the last case, the background data are determined once for the system (1) and only one similar system has to be solved for each perturbation, reducing the cost by almost a half if many perturbations are considered, but at the expense of robustness. The data will be noisy if the scale of the perturbation is too small and will be contaminated by multiple scattering and nonlinear effects if the scale is too large.

We consider three types of delta-functional forces with components  $f_j^{(0)}(\mathbf{x}, \mathbf{x}_s) = \partial_{x_j} \delta(\mathbf{x} - \mathbf{x}_s), f_j^{(\alpha)}(\mathbf{x}, \mathbf{x}_s) = \partial_{x_j} \delta(\mathbf{x} - \mathbf{x}_s), f_j^{(\alpha)}(\mathbf{x} - \mathbf{x}_s)$  $\delta_{j\alpha}\delta(\mathbf{x}-\mathbf{x}_s)$ , and  $f_i^{(\alpha\beta)}(\mathbf{x},\mathbf{x}_s) = \delta_{j\alpha}\partial_{x_\beta}\delta(\mathbf{x}-\mathbf{x}_s) + \delta_{j\beta}\partial_{x_\alpha}\delta(\mathbf{x}-\mathbf{x}_s)$ . Here,  $\mathbf{f}^{(0)}$  is the force due to the pressure gradient, a force in the  $\alpha$ -direction is denoted by  $\mathbf{f}^{(\alpha)}$ , and  $\mathbf{f}^{(\alpha\beta)}$  is the momentum force caused by a stress tensor with two non-diagonal components  $T_{\alpha\beta} = T_{\beta\alpha} = \delta(\mathbf{x} - \mathbf{x}_s)$  or with a single diagonal component  $T_{\alpha\alpha} = 2\delta(\mathbf{x} - \mathbf{x}_s)$ . An explosive source  $\mathbf{f}^{(0)} = \frac{1}{2}\sum_{\alpha} \mathbf{f}^{(\alpha\alpha)}$ . The related Green functions are labelled in the following way: the superscript denotes the physical field, the subscript before the semicolon denotes the field component(s) or is empty if the field is scalar, and the subscript after the semicolon is the label of the force that the Green function represents. For example, the Green functions  $G_{i;\alpha}^{u}(\mathbf{x},\mathbf{x}_{s}), G_{\alpha}^{\varphi}(\mathbf{x},\mathbf{x}_{s})$ , and  $G_{ij;\alpha}^{\varepsilon}(\mathbf{x},\mathbf{x}_{s})$  define the displacement  $u_{i}(\mathbf{x})$ , the volumetric strain  $\varphi(\mathbf{x})$ , and the strain tensor  $\varepsilon_{ij}(\mathbf{x})$  for a delta-function force source  $\mathbf{f}^{(\alpha)}$ . Reciprocity hinges on the symmetry properties of the spatial operator together with Green's second identity that relates volume integrals with divergence operators to surface integrals with normal derivatives. The symmetry of the elasticity tensor implies  $\sum_{ij} (\sigma_{ii} \varepsilon'_{ji} - \sigma'_{ii} \varepsilon_{ji}) = 0$ , given two states **u** and **u'** driven by forces **f** and **f'**, respectively. With zero initial values for the displacements and their time derivatives, this gives (Achenbach, 1975, Theorem 3.2)  $\int_{\Omega} (\mathbf{f} \cdot \mathbf{u}' - \mathbf{f}' \cdot \mathbf{u}) d\mathbf{x} = 0$ , either for zero traction at one part of the boundary of a domain  $\Omega$ , or, if another part of the boundary is located at infinity, for wavefield decays sufficiently fast. Substituting  $f_j = f_i^{(0)} = \partial_{x_j} \delta(\mathbf{x} - \mathbf{x}_s)$  in the above equation, we obtain

$$\int_{\Omega} \mathbf{f}' \cdot \mathbf{u} \, \mathrm{d}\mathbf{x} = -\boldsymbol{\varphi}'(\mathbf{x}_s),\tag{3}$$

where  $\varphi'$  is the volumetric strain generated by force  $\mathbf{f}'$ . The reciprocity relations are obtained by setting in eq. (3)  $\mathbf{f}' = \mathbf{f}^{(0)}(\mathbf{x}, \mathbf{x}'), \mathbf{f}' = \mathbf{f}^{(\alpha)}(\mathbf{x}, \mathbf{x}'), \text{ and } \mathbf{f}' = \mathbf{f}^{(\alpha\beta)}(\mathbf{x}, \mathbf{x}')$ :

$$G_{;0}^{\varphi}(\mathbf{x}',\mathbf{x}_{s}) = G_{;0}^{\varphi}(\mathbf{x}_{s},\mathbf{x}'), \quad G_{\alpha;0}^{u}(\mathbf{x}',\mathbf{x}_{s}) = -G_{;\alpha}^{\varphi}(\mathbf{x}_{s},\mathbf{x}'), \quad G_{\alpha\beta;0}^{\varepsilon}(\mathbf{x}',\mathbf{x}_{s}) = \frac{1}{2}G_{;\alpha\beta}^{\varphi}(\mathbf{x}_{s},\mathbf{x}').$$
(4)

The last expression is slightly different from eq. (A-27) of Arntsen and Carcione (2000) because we combine the stress components  $T_{\alpha\beta}$  and  $T_{\beta\alpha}$  for  $\alpha \neq \beta$  in a single force  $\mathbf{f}^{(\alpha\beta)}$ .



In the example later on, we will consider explosive sources at  $\mathbf{x}_s$  and volumetric-strain or 'pressure' data  $\varphi$  at  $\mathbf{x}_r$ . According to eq. (2), the Born data can be expressed as

$$\varphi(\mathbf{x}_r;\mathbf{x}_s) = \int d\mathbf{x} \left\{ \delta v_1(\mathbf{x}) \varphi^{(1)}(\mathbf{x}_r;\mathbf{x};\mathbf{x}_s) + [\delta v_2(\mathbf{x}) - 2\delta v_3(\mathbf{x})] \varphi^{(2)}(\mathbf{x}_r;\mathbf{x};\mathbf{x}_s) + 2\delta v_3(\mathbf{x}) \varphi^{(3)}(\mathbf{x}_r;\mathbf{x};\mathbf{x}_s) \right\}, \quad (5)$$

with the scattering Green functions

$$\varphi^{(1)}(\mathbf{x}_{r};\mathbf{x};\mathbf{x}_{s}) = \omega^{2} \sum_{i} G^{\varphi}_{;i}(\mathbf{x}_{r},\mathbf{x}) G^{u}_{i;0}(\mathbf{x},\mathbf{x}_{s}) = -\omega^{2} \sum_{i} G^{\varphi}_{;i}(\mathbf{x}_{r},\mathbf{x}) G^{\varphi}_{;i}(\mathbf{x}_{s},\mathbf{x}),$$
(6a)

$$\varphi^{(2)}(\mathbf{x}_r; \mathbf{x}; \mathbf{x}_s) = G^{\varphi}_{;0}(\mathbf{x}_r, \mathbf{x}) G^{\varphi}_{;0}(\mathbf{x}, \mathbf{x}_s) = G^{\varphi}_{;0}(\mathbf{x}_r, \mathbf{x}) G^{\varphi}_{;0}(\mathbf{x}_s, \mathbf{x}),$$
(6b)

$$\varphi^{(3)}(\mathbf{x}_{r};\mathbf{x};\mathbf{x}_{s}) = \sum_{j\geq i} G^{\varphi}_{;ij}(\mathbf{x}_{r},\mathbf{x}) G^{\varepsilon}_{ij;0}(\mathbf{x},\mathbf{x}_{s}) = \frac{1}{2} \sum_{j\geq i} G^{\varphi}_{;ij}(\mathbf{x}_{r},\mathbf{x}) G^{\varphi}_{;ij}(\mathbf{x}_{s},\mathbf{x}).$$
(6c)

Synthesis of Born data involves several delta-function sources at **x**: force sources in each of *d* coordinate directions and d(d+1)/2 moment sources for each coordinate combination. The Green functions for an explosive source follow from the latter by  $G_{i0}^{\varphi}(\mathbf{x}, \mathbf{x}_s) = \frac{1}{2} \sum_i G_{ii;0}^{\varepsilon}(\mathbf{x}', \mathbf{x}_s)$ . For a single scattering point, this requires d(d+3)/2 isotropic elastic simulations, 5 in 2D and 9 in 3D, followed by data correlations. If the simulations for the Green functions are carried out with a wavelet, a deconvolution is required in the correlation step, combined with two time derivatives in eq. (6a). The computational cost is still substantially lower than that of separately simulating all shots of a seismic survey.

#### Numerical example

To validate the method, we consider an earlier 2-D isotropic elastic marine subsurface model (Mulder and Kuvshinov, 2023). The material properties were defined by an index map, repeated here as Figure 2. The negative values refer to four reservoirs, zero is used for sea water, and positive values for various layers with piecewise constant elastic properties, shown in Figure 1 of the reference. Three Born scattering data sets were generated with a finite-difference code for a unit perturbation of  $v_k$  (k = 1, 2, 3) at the scatter point x = 3280 m,



Figure 2 Model index map.

z = 2460 m, close to the centroid of the reservoir with index -1. From 5 shots at the scatter point,  $3 \times 199$  shots were synthesized with  $x_s$  from -2.9 to 7.0 km at a 50-m spacing at depth  $z_s = 10$  m and with receiver offsets from  $x_r - x_s = 100$  to 6000 m with a 25-m spacing at a depth  $z_r = 8$  m. A direct Born computation would require  $3 \times 199$  shots at twice the cost, or  $(1+3) \times 199$  shots with a series approach.



**Figure 3** (a) Born data for a unit perturbation in one point of  $v_1 = \rho$  clipped at 25% of the maximum amplitude. (b) Difference between synthesized Born data and those of (a) at the same scale. (c) Comparison of the shortest-offset trace with Born scattering data (blue) and synthesized Born data based on reciprocity (red, dashed).

Figures 3–5 display a comparison of Born data for one shot at  $x_s = 0$  and  $z_s = 10$ m computed directly with the two coupled systems, in panels (a), the difference between the Born data synthesized for 5 different source types at the scatter point and the directly computed data (b), and the shortest-offset trace for each approach, with the directly computed and synthesized Born data. There is a good agreement, bearing in mind that reciprocity for the finite-difference solutions only approximately holds. Finally, Figure 6 shows the normalized covariance matrix at the selected scatterer obtained from the hessian based on synthesized Born data for all 199 shots.





*Figure 5* As Figure 3, but for  $v_3 = \rho v_s^2$ .



## The compu

Conclusions

The computational cost of uncertainty estimation based on a hessian obtained from Born scattering data can be significantly reduced in targetoriented applications where the model parameters of only a small number of subsurface points are considered. Instead of simulating Born data for

Figure 6 Scaled covariance.

an entire seismic survey, only those subsurface points have to be taken as new source positions and all shot and receiver positions of the survey as new receiver positions. For each new source positions, several shots with different source characteristics have to be simulated, for each force and moment tensor component.

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