

The acoustic Lagrangian density and the full waveform inversion gradient

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ABSTRACT

The Euler-Lagrange equations relate the Lagrangian density \mathcal{L} for a system of particles or fields with the associated equations of motion or field equations. A central problem of field theory is to postulate an \mathcal{L} from which the correct equations derive. The problem may be posed in reverse also: known equations of motion can be used as a starting point from which to deduce the associated \mathcal{L} . This is useful primarily as a pedagogical exercise. However, the \mathcal{L} for acoustic continua is proportional to the acoustic Fréchet derivative, a crucial quantity in seismic full waveform inversion which often must be laboriously calculated. If Fréchet derivatives and thereby FWI gradients are derivable directly from the appropriate continuum mechanical Lagrangian densities, in addition to opening an avenue for physical interpretation of inversion iterates, a considerable savings in calculation would likely be available.

INTRODUCTION

Full waveform inversion (Virieux and Operto, 2009) involves the calculation of Fréchet derivatives (McGillivray and Oldenburg, 1990), or sensitivities, which determine the gradient directions in Newton and quasi-Newton solutions. Much of this development can occur within the framework of adjoint state methods, in which an objective function, constructed with the wave equation as a constraint term, is minimized.

Constraints are incorporated through the use of Lagrange multipliers, which were originally developed for use in Lagrangian dynamics, to help determine the equations of motion when particles were to move not with total freedom but rather on known surfaces. It can be very difficult to express such problems directly in terms of the forces such surfaces exert on the particles in question. Therefore, straight Newtonian accounting of forces was far from optimal in these situations and the method of Lagrange multipliers was a powerful and welcome innovation.

In the Lagrangian formulation, the quantity analogous to the FWI objective function is the action, whose stationary points correspond to actual states the system can access. Not suprisingly, therefore, discussions of adjoint state methods often involve the words “Lagrange”, “Lagrange multiplier”, and even “Lagrangian”. The review papers of Plessix (2006) and Virieux and Operto (2009) are examples.

However, in the range of concepts associated with the Lagrangian formulation of classical mechanics (Goldstein, 1980), there is one which deserves some discussion, that has not yet gotten it (as far as the author can determine). That is the *Lagrangian density*, which is central to the development of the action and the derivation of the equations of motion appropriate to discrete and continuous classical systems.

THE ACOUSTIC FWI GRADIENT

In Appendix A we show using standard methods (see the schematic diagram in Figure 1) that if the waves we measure in our seismic experiment, P , obey the equation

$$\left[\nabla \cdot \left(\frac{1}{\rho(\mathbf{r}_g)} \right) \nabla + \frac{\omega^2}{\kappa(\mathbf{r}_g)} \right] P(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s), \quad (1)$$

where $\rho(\mathbf{r})$ and $\kappa(\mathbf{r})$ are the density and bulk modulus respectively, whose respective distributions are solved for in terms of the quantities

$$s_\kappa(\mathbf{r}) = \frac{1}{\kappa(\mathbf{r})}, \quad s_\rho(\mathbf{r}) = \frac{1}{\rho(\mathbf{r})}, \quad (2)$$

which are adjusted by adding the changes $\delta s_\kappa(\mathbf{r})$ and $\delta s_\rho(\mathbf{r})$, then those changes are proportional to a gradient direction g of the form

$$g(\mathbf{r}) = - \sum_{\mathbf{r}_s, \mathbf{r}_g} \int d\omega [\omega^2 G(\mathbf{r}_g, \mathbf{r}, \omega) G(\mathbf{r}, \mathbf{r}_s, \omega) - \nabla G(\mathbf{r}_g, \mathbf{r}, \omega) \cdot \nabla G(\mathbf{r}, \mathbf{r}_s, \omega)] \delta P^*(\mathbf{r}_g, \mathbf{r}_s, \omega). \quad (3)$$

Although it is a subjective statement, the reader who moves through that derivation step by step would probably agree that it is a bit laborious. The purpose of this paper is to present an observation, rooted in Lagrangian mechanics, which may provide a way around a good portion of this labour.

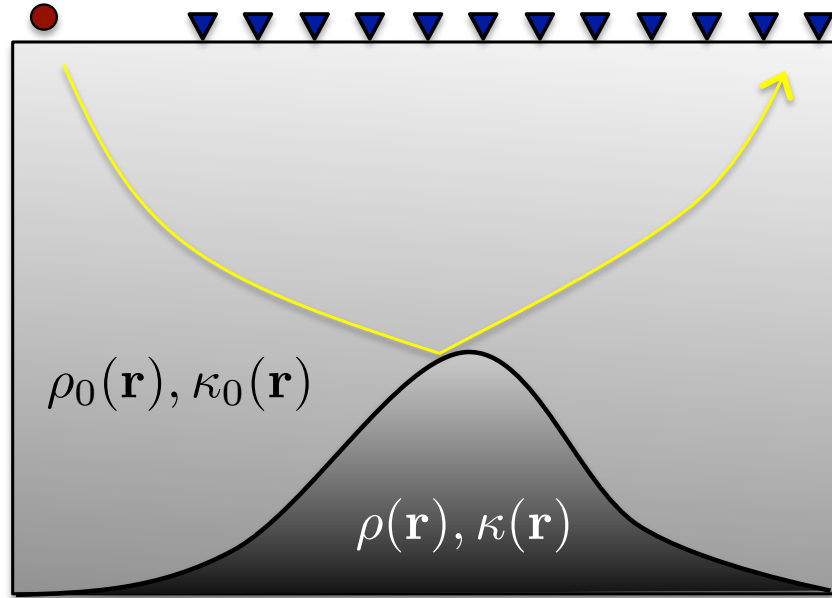


FIG. 1. The acoustic seismic reflection problem.

REVIEW OF LAGRANGIAN METHODS

Lagrangian methods are based on the principle of least action. In a fixed time interval, the path a system actually takes in nature is the one for which the integral of the difference between the kinetic and potential energies over the path is stationary. Field equations, for fields χ , are generally derivable by analyzing the action S

$$S(\chi) = \int dt \int d\mathbf{r} \mathcal{L}(\chi, \nabla\chi, \dot{\chi}), \quad (4)$$

where \mathcal{L} is a suitably chosen Lagrangian density. Realizable states of a field χ are associated with stationary values of this integral:

$$\delta S(\chi) = 0. \quad (5)$$

The integral is over the independent variables of the problem. So, the expression in equation (4) is a 3+1 problem in which there are three independent spatial variables and one time variable.

Example: a particle moving freely and in potentials

In the problem of the motion of single particle moving freely or in a potential, the field being solved for is the position of the particle, $\chi = \mathbf{r}(t)$. The Lagrangian formulation is therefore a 0+1 problem, where time is the only independent variable. The variation in the action can be written as

$$\delta S = \int_{t_1}^{t_2} dt \left[\mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) + \frac{\partial \mathcal{L}}{\partial \mathbf{r}} \cdot \delta \mathbf{r} + \frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}} \cdot \delta \dot{\mathbf{r}} - \mathcal{L}(\mathbf{r}, \dot{\mathbf{r}}) \right], \quad (6)$$

whereby condition (5) leads to the Euler-Lagrange equations:

$$\frac{d}{dt} \left(\frac{\partial \mathcal{L}}{\partial \dot{\mathbf{r}}} \right) = \frac{\partial \mathcal{L}}{\partial \mathbf{r}} \quad (7)$$

The Lagrangian density for this single particle of mass m , if it is moving in a potential V , is the difference between its kinetic energy and this potential:

$$\mathcal{L} = \frac{1}{2} m \dot{\mathbf{r}}^2 - V(\mathbf{r}). \quad (8)$$

Substituting equation (8) into (7) we obtain

$$\frac{d}{dt} m \dot{\mathbf{r}} = -\nabla_{\mathbf{r}} V, \quad (9)$$

where $\nabla_{\mathbf{r}} = \partial/\partial \mathbf{r}$. The three components of equation (9) are the equations of motion for the particle, which would otherwise be determined through the standard Newtonian accounting of the forces. Setting $V = 0$ recovers the equations for a free particle.

THE LAGRANGIAN DENSITY FOR ACOUSTIC MEDIA

The Euler-Lagrange equations, we note, involve derivatives of the Lagrangian density with respect to the *field variables* of the problem. In the case of the single particle, the position \mathbf{r} was the field. It is important to bear that in mind so that the extension of the Lagrangian approach to continuous media makes intuitive sense.

We consider a seismic inverse problem involving acoustic wave fields p :

$$p(\mathbf{r}, \mathbf{r}', t) = P(\mathbf{r}, \mathbf{r}', \omega)e^{i\omega t}, \quad (10)$$

focusing in particular on frequency domain amplitudes P . This is the new field. It will be the variable with respect to which the appropriate Lagrangian density has its derivatives taken.

Equations for the motion of particles and fields (the acoustic wave equation being one example) are generally derivable by analyzing the action S

$$S(p) = \int dt \int d\mathbf{r} \mathcal{L}(p, \nabla p, \dot{p}), \quad (11)$$

where \mathcal{L} is a suitably chosen Lagrangian density. Realizable states of a field p are associated with stationary values of this integral:

$$\delta S(p) = 0. \quad (12)$$

The Euler-Lagrange equations, which are satisfied when equation (12) is satisfied, are, for a scalar non relativistic field p , of the form

$$\nabla \cdot \left[\frac{\partial \mathcal{L}}{\partial(\nabla p)} \right] + \frac{\partial}{\partial t} \left(\frac{\partial \mathcal{L}}{\partial \dot{p}} \right) = \frac{\partial \mathcal{L}}{\partial p}. \quad (13)$$

For P we may instead write

$$\nabla \cdot \left[\frac{\partial \mathcal{L}}{\partial(\nabla P)} \right] + (i\omega) \left(\frac{\partial \mathcal{L}}{\partial(i\omega P)} \right) = \frac{\partial \mathcal{L}}{\partial P}. \quad (14)$$

From the EL equations the field/motion equations are quickly derived. Notice now that if we expect the acoustic wave equation in the temporal frequency domain, i.e.,

$$\nabla \cdot \left(\frac{1}{\rho(\mathbf{r})} \nabla P(\mathbf{r}, \mathbf{r}', \omega) \right) + \frac{\omega^2}{\kappa(\mathbf{r})} P(\mathbf{r}, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}'), \quad (15)$$

to result from (14), almost without any further calculation we see by comparing (14) and (15) that the Lagrangian density must be

$$\mathcal{L} = \mathcal{L}_\rho + \mathcal{L}_\kappa + \mathcal{L}_{\text{source}}, \quad (16)$$

where

$$\mathcal{L}_\rho = \frac{1}{2\rho(\mathbf{r})} \nabla P(\mathbf{r}, \mathbf{r}', \omega) \cdot \nabla P(\mathbf{r}, \mathbf{r}', \omega), \quad (17)$$

and

$$\mathcal{L}_\kappa = \frac{1}{2\kappa(\mathbf{r})} \omega^2 P(\mathbf{r}, \mathbf{r}', \omega) P(\mathbf{r}, \mathbf{r}', \omega), \quad (18)$$

and

$$\mathcal{L}_{\text{source}} = \delta(\mathbf{r} - \mathbf{r}') P(\mathbf{r}, \mathbf{r}', \omega). \quad (19)$$

This is easily confirmed by checking a range of references (Goldstein, 1980, equation (12-30), pg. 553)

THE LAGRANGIAN DENSITY AND THE FWI GRADIENT

Compare equations (17)–(18) with equation (3). Evidently

$$\mathcal{L}_\rho \propto \frac{\partial P(\mathbf{r}', \omega)}{\partial s_\rho(\mathbf{r})}, \quad (20)$$

and

$$\mathcal{L}_\kappa \propto \frac{\partial P(\mathbf{r}', \omega)}{\partial s_\kappa(\mathbf{r})}. \quad (21)$$

There is an equivalence between the acoustic Lagrangian density (i.e., the integrand of the action which, when minimized, leads to the acoustic equations of motion) and the acoustic Fréchet derivatives involved in the gradient calculation. “Reverse engineering” a Lagrangian density from its associated equations of motion is an almost calculation-free task, normally useful only for pedagogy in physics. If this equivalence holds for all acoustic and elastic fields, much laborious calculation in posing full waveform inversion problems (see Appendix A below) may be avoided this way.

CONCLUSIONS

Although connections between energy methods in mechanics and adjoint-state methods for deriving full waveform inversion methods have been extensively drawn, little specific comment appears about the connection between the *Lagrangian density* and the *full waveform inversion gradient*. The two acoustic sensitivities, which are a key component of the gradient calculations, appear to each be proportional to one of the three components of the acoustic Lagrangian density. If this is pattern persists over all type of wave inverse problem, then it may represent a considerable savings in computational effort, and it may also lead to lines of inquiry between the energy of an acoustic wave and the solution of Earth property estimation problems.

ACKNOWLEDGMENTS

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APPENDIX A: DERIVATION OF THE ACOUSTIC FWI GRADIENT

Our purpose in this paper is to show how the rather laborious derivation of multi-parameter acoustic FWI gradients can evidently be circumvented by considering Lagrangian densities. In this section we will derive the acoustic FWI gradient the standard way, partly to have a form for the gradient to compare our other results to, and partly to illustrate its laboriousness.

Wave equations

We will require two wave equations to derive the forms of the sensitivities and gradient, a perturbed equation and a reference or unperturbed equation. The perturbed wave equation is

$$\left[\nabla \cdot \left(\frac{1}{\rho(\mathbf{r}_g)} \right) \nabla + \frac{\omega^2}{\kappa(\mathbf{r}_g)} \right] G_P(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s) \quad (22)$$

where $\rho(\mathbf{r})$ and $\kappa(\mathbf{r})$ are the density and bulk modulus of the perturbed medium respectively, and the unperturbed or background equation is

$$\left[\nabla \cdot \left(\frac{1}{\rho_0(\mathbf{r}_g)} \right) \nabla + \frac{\omega^2}{\kappa_0(\mathbf{r}_g)} \right] G(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s). \quad (23)$$

The model parameter s is likewise generalized to accommodate both parameters. We introduce perturbed and unperturbed models

$$\begin{aligned} s_\kappa(\mathbf{r}) &= \frac{1}{\kappa(\mathbf{r})}, & s_{\kappa_0}(\mathbf{r}) &= \frac{1}{\kappa_0(\mathbf{r})}, \\ s_\rho(\mathbf{r}) &= \frac{1}{\rho(\mathbf{r})}, & s_{\rho_0}(\mathbf{r}) &= \frac{1}{\rho_0(\mathbf{r})}, \end{aligned} \quad (24)$$

and perturbations

$$\begin{aligned} \delta s_\kappa(\mathbf{r}) &= \frac{a_\kappa(\mathbf{r})}{\kappa_0(\mathbf{r})} \\ \delta s_\rho(\mathbf{r}) &= \frac{a_\rho(\mathbf{r})}{\rho_0(\mathbf{r})}, \end{aligned} \quad (25)$$

where

$$\begin{aligned} a_\kappa(\mathbf{r}) &= 1 - \frac{\kappa_0(\mathbf{r})}{\kappa(\mathbf{r})}, \\ a_\rho(\mathbf{r}) &= 1 - \frac{\rho_0(\mathbf{r})}{\rho(\mathbf{r})}. \end{aligned} \quad (26)$$

Substituting equations (24) into equations (22)–(23) we obtain

$$\begin{aligned} \left[\nabla \cdot s_\rho(\mathbf{r}_g) \nabla + \omega^2 s_\kappa(\mathbf{r}_g) \right] G_P(\mathbf{r}_g, \mathbf{r}_s, \omega) &= \delta(\mathbf{r}_g - \mathbf{r}_s) \\ \left[\nabla \cdot s_{\rho_0}(\mathbf{r}_g) \nabla + \omega^2 s_{\kappa_0}(\mathbf{r}_g) \right] G(\mathbf{r}_g, \mathbf{r}_s, \omega) &= \delta(\mathbf{r}_g - \mathbf{r}_s). \end{aligned} \quad (27)$$

Acoustic sensitivities

Next we calculate the acoustic sensitivities: we jiggle the model (via δs), and measure how much the field G jiggles (δG) in response. We achieve this by focusing on the perturbed field. By breaking $s_\kappa(\mathbf{r})$ and $s_\rho(\mathbf{r})$ up into $s_{\kappa_0}(\mathbf{r})$, $s_{\rho_0}(\mathbf{r})$ and $\delta s_\kappa(\mathbf{r})$, $\delta s_\rho(\mathbf{r})$, we find we can write the perturbed equation using the operator of the unperturbed equation, that is

$$L_0(\mathbf{r}_g, \omega)G_P(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s) - \omega^2 \delta s_\kappa(\mathbf{r}_g)G_P(\mathbf{r}_g, \mathbf{r}_s, \omega) - \nabla \cdot \delta s_\rho(\mathbf{r}_g)\nabla G_P(\mathbf{r}_g, \mathbf{r}_s, \omega), \quad (28)$$

where

$$L_0(\mathbf{r}_g, \omega) = [\nabla \cdot s_{\rho_0}(\mathbf{r}_g)\nabla + \omega^2 s_{\kappa_0}(\mathbf{r}_g)]. \quad (29)$$

Now, for a single parameter, even in 1D, there were an infinite “number” of sensitivities, since the sensitivity matrix is defined for every point in depth where the model can change, and this was chosen to be a continuous quantity. This will be true here too, but in addition to this infinitude, there will now be two “types” of sensitivity, one for density and one for bulk modulus. They are both derived from equation (28).

Bulk modulus sensitivity

Let us begin with the bulk modulus sensitivities. That is, we will test the change in the field that arises due to a change in $s_\kappa(\mathbf{r})$. We achieve this by setting $\delta s_\rho = 0$. Equation (28) becomes

$$L_0(\mathbf{r}_g, \omega)G_P(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s) - \omega^2 \delta s_\kappa(\mathbf{r}_g)G_P(\mathbf{r}_g, \mathbf{r}_s, \omega), \quad (30)$$

provided $|\delta s_\kappa(\mathbf{r}')|$ is small. As ever we isolate G_P by multiplying the right-hand side by the unperturbed Green’s function and integrating over all space. This results in two terms, one G itself and the other involving δs_κ . The difference $\delta G(\mathbf{r}_g, \mathbf{r}_s, \omega) = G_P - G$ is formed by subtracting the first term from both sides of the equation:

$$\delta G(\mathbf{r}_g, \mathbf{r}_s, \omega) \approx -\omega^2 \delta s_\kappa(\mathbf{r}) \int d\mathbf{r}' G(\mathbf{r}_g, \mathbf{r}', \omega) \delta s_\kappa(\mathbf{r}') G(\mathbf{r}', \mathbf{r}_s, \omega). \quad (31)$$

We next pick a location \mathbf{r} at which to let the model vary, and replace the variation under the integral with

$$\delta s_\kappa(\mathbf{r}') = \delta s_\kappa(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'), \quad (32)$$

such that

$$\begin{aligned} \delta G(\mathbf{r}_g, \mathbf{r}_s, \omega) &\approx -\omega^2 \delta s_\kappa(\mathbf{r}) \int d\mathbf{r}' G(\mathbf{r}_g, \mathbf{r}', \omega) \delta(\mathbf{r} - \mathbf{r}') G(\mathbf{r}', \mathbf{r}_s, \omega) \\ &= -\omega^2 \delta s_\kappa(\mathbf{r}) G(\mathbf{r}_g, \mathbf{r}, \omega) G(\mathbf{r}, \mathbf{r}_s, \omega), \end{aligned} \quad (33)$$

and finally

$$\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\kappa(\mathbf{r})} = \lim_{\delta s_\kappa \rightarrow 0} \frac{\delta G}{\delta s_\kappa} = -\omega^2 G(\mathbf{r}_g, \mathbf{r}, \omega) G(\mathbf{r}, \mathbf{r}_s, \omega). \quad (34)$$

We observe that the bulk modulus sensitivity matrix is essentially unchanged from the scalar velocity sensitivity.

Density sensitivity

Next we move to the density sensitivities. This time we let $\delta s_\kappa = 0$, such that equation (28) becomes

$$L_0(\mathbf{r}_g, \omega)G_P(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s) - \nabla \cdot \delta s_\rho(\mathbf{r}_g) \nabla G_P(\mathbf{r}_g, \mathbf{r}_s, \omega). \quad (35)$$

As before, for small $|\delta s_\rho(\mathbf{r}')|$, we may form the variation δG as follows:

$$\delta G(\mathbf{r}_g, \mathbf{r}_s, \omega) \approx - \int d\mathbf{r}' G(\mathbf{r}_g, \mathbf{r}', \omega) \nabla \cdot \delta s_\rho(\mathbf{r}') \nabla G(\mathbf{r}', \mathbf{r}_s, \omega) \quad (36)$$

remembering that the del operators are acting on the integral variable \mathbf{r}' . This allows, upon again choosing \mathbf{r} as a fixed point at which to vary the density via

$$\delta s_\rho(\mathbf{r}') = \delta s_\rho(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}'), \quad (37)$$

the formation of the derivative

$$\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} = \lim_{\delta s_\rho \rightarrow 0} \frac{\delta G}{\delta s_\rho} = - \int d\mathbf{r}' G(\mathbf{r}_g, \mathbf{r}', \omega) \nabla \cdot \delta(\mathbf{r} - \mathbf{r}') \nabla G(\mathbf{r}', \mathbf{r}_s, \omega). \quad (38)$$

This form is not perfectly satisfactory as the action of the del operators under the integral may not be entirely clear. More insight is gained by using the identity

$$\nabla \cdot (s\mathbf{A}) = \nabla s \cdot \mathbf{A} + s \nabla \cdot \mathbf{A}, \quad (39)$$

by which we are able to say

$$\begin{aligned} \nabla \cdot [\delta(\mathbf{r} - \mathbf{r}') \nabla G(\mathbf{r}', \mathbf{r}_s, \omega)] &= \nabla \delta(\mathbf{r} - \mathbf{r}') \cdot \nabla G(\mathbf{r}', \mathbf{r}_s, \omega) \\ &\quad + \delta(\mathbf{r} - \mathbf{r}') \nabla^2 G(\mathbf{r}', \mathbf{r}_s, \omega). \end{aligned} \quad (40)$$

Some may find it more instructive to see how this plays out with an explicit calculation of these derivatives. In a 2D Cartesian system, the substitution of equation (40) into equation (38) results in

$$\begin{aligned} \frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} &= - \int dx' G(x_g, z_g, x', z, \omega) \delta'(x - x') \frac{\partial G}{\partial x'} \\ &\quad - \int dz' G(x_g, z_g, x, z', \omega) \delta'(z - z') \frac{\partial G}{\partial z'} \\ &\quad - G(x_g, z_g, x, z, \omega) \left[\frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 G}{\partial z^2} \right]. \end{aligned} \quad (41)$$

The general result that

$$\int dx [\delta'(x) f(x)] = - \int dx \left[\delta(x) \frac{\partial f}{\partial x} \right], \quad (42)$$

allows us to replace the derivatives of the delta functions with delta functions which in turn make the evaluation of the integrals straightforward, leaving

$$\begin{aligned} \frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} &= \frac{\partial G}{\partial x}(x_g, z_g, x, z, \omega) \frac{\partial G}{\partial x}(x, z, x_s, z_s, \omega) \\ &+ \frac{\partial G}{\partial z}(x_g, z_g, x, z, \omega) \frac{\partial G}{\partial z}(x, z, x_s, z_s, \omega). \end{aligned} \quad (43)$$

Now this is actually a dot product of gradients:

$$\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} = \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial z} \right] G(x_g, z_g, x, z, \omega) \cdot \left[\frac{\partial}{\partial x}, \frac{\partial}{\partial z} \right] G(x, z, x_s, z_s, \omega), \quad (44)$$

by which we infer that, departing again from the particular coordinate system,

$$\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} = \nabla G(\mathbf{r}_g, \mathbf{r}, \omega) \cdot \nabla G(\mathbf{r}, \mathbf{r}_s, \omega). \quad (45)$$

Acoustic two parameter gradient

In FWI we define an objective function:

$$\phi(s_\kappa, s_\rho) = \frac{1}{2} \sum_{\mathbf{r}_s, \mathbf{r}_g} \int d\omega |\delta P|^2, \quad (46)$$

where

$$\delta P(\mathbf{r}_g, \mathbf{r}_s, \omega) = P(\mathbf{r}_g, \mathbf{r}_s, \omega) - G(\mathbf{r}_g, \mathbf{r}_s, \omega). \quad (47)$$

P are the measurements of the actual field, and G is the modeled field in the current FWI iteration. If we are considering the first iteration, in which the medium is described by our initial guess $\kappa_0(\mathbf{r})$, $\rho_0(\mathbf{r})$, then G satisfies

$$[\nabla \cdot s_{\rho_0}(\mathbf{r}_g) \nabla + \omega^2 s_{\kappa_0}(\mathbf{r}_g)] G(\mathbf{r}_g, \mathbf{r}_s, \omega) = \delta(\mathbf{r}_g - \mathbf{r}_s). \quad (48)$$

We must use a Taylor's series expansion of ϕ in two variables (functions, actually), modulus and density, in analogy to:

$$f(x + \delta x, y + \delta y) = f(x, y) + \frac{\partial f}{\partial x} \delta x + \frac{\partial f}{\partial y} \delta y + \dots, \quad (49)$$

It takes the form

$$\begin{aligned} \phi(s_{\kappa_0} + \delta s_\kappa, s_{\rho_0} + \delta s_\rho) &\approx \phi(s_{\kappa_0}, s_{\rho_0}) + \int d\mathbf{r}' \frac{\partial \phi}{\partial s_\kappa(\mathbf{r}')} \delta s_\kappa(\mathbf{r}') \\ &+ \int d\mathbf{r}' \frac{\partial \phi}{\partial s_\rho(\mathbf{r}')} \delta s_\rho(\mathbf{r}'). \end{aligned} \quad (50)$$

Proceeding as in the single parameter cases, we alter this step so that it represents movement towards a local minimum rather than a local root through a further derivative, this time with respect to first s_κ and then s_ρ :

$$\begin{aligned} \frac{\partial\phi(s_\kappa, s_\rho)}{\partial s_\kappa(\mathbf{r})} &= \frac{\partial\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\kappa(\mathbf{r})} + \int d\mathbf{r}' \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\kappa(\mathbf{r})\partial s_\kappa(\mathbf{r}')} \delta s_\kappa(\mathbf{r}') \\ &+ \int d\mathbf{r}' \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\kappa(\mathbf{r})\partial s_\rho(\mathbf{r}')} \delta s_\rho(\mathbf{r}'), \end{aligned} \quad (51)$$

and

$$\begin{aligned} \frac{\partial\phi(s_\kappa, s_\rho)}{\partial s_\rho(\mathbf{r})} &= \frac{\partial\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\rho(\mathbf{r})} + \int d\mathbf{r}' \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\rho(\mathbf{r})\partial s_\kappa(\mathbf{r}')} \delta s_\kappa(\mathbf{r}') \\ &+ \int d\mathbf{r}' \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\rho(\mathbf{r})\partial s_\rho(\mathbf{r}')} \delta s_\rho(\mathbf{r}'). \end{aligned} \quad (52)$$

Next, we fit a paraboloid to the objective function and step to the minimum of the paraboloid, by forming the sum of these two expressions and setting the result to zero:

$$\frac{\partial\phi(s_\kappa, s_\rho)}{\partial s_\rho(\mathbf{r})} + \frac{\partial\phi(s_\kappa, s_\rho)}{\partial s_\kappa(\mathbf{r})} = 0. \quad (53)$$

This requires

$$g(\mathbf{r}) = g_\kappa(\mathbf{r}) + g_\rho(\mathbf{r}) = - \int d\mathbf{r}' H_\kappa(\mathbf{r}, \mathbf{r}') \delta s_\kappa(\mathbf{r}') - \int d\mathbf{r}' H_\rho(\mathbf{r}, \mathbf{r}') \delta s_\rho(\mathbf{r}'), \quad (54)$$

where

$$H_\kappa(\mathbf{r}, \mathbf{r}') = \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\kappa(\mathbf{r})\partial s_\kappa(\mathbf{r}')} + \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\rho(\mathbf{r})\partial s_\kappa(\mathbf{r}')} \quad (55)$$

and

$$H_\rho(\mathbf{r}, \mathbf{r}') = \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\kappa(\mathbf{r})\partial s_\rho(\mathbf{r}')} + \frac{\partial^2\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\rho(\mathbf{r})\partial s_\rho(\mathbf{r}')}, \quad (56)$$

and

$$g_\kappa(\mathbf{r}) = \frac{\partial\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\kappa(\mathbf{r})}, \quad g_\rho(\mathbf{r}) = \frac{\partial\phi(s_{\kappa_0}, s_{\rho_0})}{\partial s_\rho(\mathbf{r})}. \quad (57)$$

In last year's CREWES report (Margrave et al., 2011), we showed that with an objective function defined as in equation (46), gradients defined as in equations (57)–(58) above are given by:

$$\begin{aligned} g_\kappa(\mathbf{r}) &= - \sum_{\mathbf{r}_s, \mathbf{r}_g} \int d\omega \operatorname{Re} \left[\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\kappa(\mathbf{r})} \delta P^*(\mathbf{r}_g, \mathbf{r}_s, \omega) \right] \\ g_\rho(\mathbf{r}) &= - \sum_{\mathbf{r}_s, \mathbf{r}_g} \int d\omega \operatorname{Re} \left[\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} \delta P^*(\mathbf{r}_g, \mathbf{r}_s, \omega) \right]. \end{aligned} \quad (58)$$

Hence, the total gradient, being the sum of these two quantities is

$$g(\mathbf{r}) = - \sum_{\mathbf{r}_s, \mathbf{r}_g} \int d\omega \operatorname{Re} \left[\frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\kappa(\mathbf{r})} + \frac{\partial G(\mathbf{r}_g, \mathbf{r}_s, \omega)}{\partial s_\rho(\mathbf{r})} \right] \delta P^*(\mathbf{r}_g, \mathbf{r}_s, \omega), \quad (59)$$

and when we substitute the sensitivities we derived in equations (22)–(45), this finally produces the form of the acoustic density and bulk modulus gradient:

$$g(\mathbf{r}) = - \sum_{\mathbf{r}_s, \mathbf{r}_g} \int d\omega \left[\omega^2 G(\mathbf{r}_g, \mathbf{r}, \omega) G(\mathbf{r}, \mathbf{r}_s, \omega) - \nabla G(\mathbf{r}_g, \mathbf{r}, \omega) \cdot \nabla G(\mathbf{r}, \mathbf{r}_s, \omega) \right] \delta P^*(\mathbf{r}_g, \mathbf{r}_s, \omega). \quad (60)$$

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