

# Full Waveform Inversion in Theory

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Short Course on Full Waveform Inversion  
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- 1 Introduction
- 2 Local search
- 3 Regularization
- 4 Conclusion

This part of the course is mainly based on the following paper and presentation

- Virieux J. and S. Operto, [2009] An overview of full-waveform inversion in exploration geophysics. *Geophysics*, 74(6), WCC1-WCC26.
- S. Operto [2006] Seismic imaging by frequency-domain full-waveform inversion Part 1 : synthetic examples. SEISCOPE SUMMER SCHOOL

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# Inverse problem ... various terminologies

- What is seismic tomography ?
- What is seismic inversion ?
- Seismic tomography ... reflection tomography and, therefore, time
- Seismic inversion ... MVA/FWI and, therefore, amplitude
- **tomography**; a generic term : model characterization from various observations
- **inversion**; a technical term : given a transformation between model and observations, provide the inverse transformation from observations to models
- linear formulation
- non-linear formulation
- linearized formulation

# Linear inversion problem

- **Linear forward problem**  $d = Gm$  : operator  $G$  does not depend on  $m$
- **Example** : Reflection travel time

$$t_i^2 = t_0^2 + x_i^2/v_{nmo}^2$$

with respect to two parameters  $(t_0^2, 1/v_{NMO}^2)$  ( $X^2$ - $T^2$  method)

- **Sensitivity matrix**  $G$ , also known as Fréchet derivative or Jacobian matrix  
 $G$  has two columns  $G_{i1} = 1$  and  $G_{i2} = x_i^2$
- **Linear algebra** machinery  $Ax=b$  ... to be discussed later on ...

# Non-linear inversion problem

- **Non-linear forward problem**  $d = \mathcal{G}(m)$  : operator  $\mathcal{G}$  does depend on  $m$
- **Example** : Acoustic wave equation

$$\frac{\omega^2}{\kappa(x, z)} P(x, z, \omega) + \frac{\partial}{\partial x} \left( \frac{1}{\rho(x, z)} \frac{\partial P(x, z, \omega)}{\partial x} \right) + \frac{\partial}{\partial z} \left( \frac{1}{\rho(x, z)} \frac{\partial P(x, z, \omega)}{\partial z} \right) = S(x, z, \omega)$$

- **Operator**  $\mathcal{G}(\kappa(x, z), \rho(x, z))$  is a non-linear operator
- Only the forward problem is required in this truly non-linear approach
- Need of an efficient forward problem ...
- **Finding model parameters?**
  - Global search : *exhaustive* sampling (grid search, Monte-Carlo)

(Backus and Gilbert, 1967)

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  - Semi-global search : Simulated annealing, Genetic algorithm, Ant search, Particle swarm optimization
  - Local search : Simplex method

(Backus and Gilbert, 1967)

# Linearized inverse problem

- Selection of a model  $m_0$
- Differentiability : derivative  $\frac{\partial \mathcal{G}}{\partial m}(m_0)$  exists

Linearized search is based on a local linearized forward problem

$$\begin{aligned}d &= \mathcal{G}(m_0) + \partial \mathcal{G} / \partial m_0 (m - m_0) \\d_0 &= \mathcal{G}(m_0) \\d - d_0 &= \partial \mathcal{G} / \partial m_0 (m - m_0) \\ \delta d &= \partial \mathcal{G} / \partial m_0 \delta m\end{aligned}$$

Forward problem  $\mathcal{G}(m_0)$  and first-derivative (gradient)  $\frac{\partial \mathcal{G}}{\partial m}(m_0)$  estimated at  $m_0$   
as non-linear relations

Model  $m_0$  fixed (linear) or changing (linearized) during iterative inversion

- Back to linear algebra machinery
- Except that the forward problem is non-linear

Objective function or misfit function

$$\ell^2 \text{ norm} : \mathcal{C}^2(m) = \frac{1}{2} \|d^{obs} - d^{syn}(m)\|^2$$

$$\ell^1 \text{ norm} : \mathcal{C}^1(m) = \frac{1}{2} |d^{obs} - d^{syn}(m)|$$

$$\ell^p \text{ norm} : \mathcal{C}^p(m) = \frac{1}{2} \sqrt[p]{\|d^{obs} - d^{syn}(m)\|^p}$$

When considering complex numbers, we define

$$\mathcal{C}^2(m) = \frac{1}{2} (d^{obs} - d^{syn}(m))^\dagger (d^{obs} - d^{syn}(m))$$

or

$$\mathcal{C}^2(m) = \frac{1}{2} (d^{obs} - d^{syn}(m))^t (d^{obs} - d^{syn}(m))^*$$

† adjoint = transpose and conjugate

<sup>t</sup> transpose

\* conjugate

Correct normalization by the number of data is required in these formulae

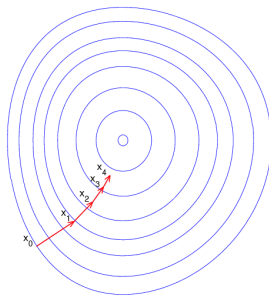
- 1 Introduction
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# Local search (1)

Best fitting model  $x$  in the vicinity  
of a running model  $x_i$

$$x_{i+1} = x_i + \delta x_i$$

$\delta x_i$  is the model perturbation



## Local search (2)

Locally around the model  $m^i$

$$\begin{aligned} \mathcal{C}(m) = \mathcal{C}(m_0 + \Delta m) = \mathcal{C}(m^i) &+ \frac{\partial \mathcal{C}}{\partial m_j}(m^i) \delta m_j \\ &+ \frac{1}{2} \frac{\partial^2 \mathcal{C}}{\partial m_j \partial m_k}(m^i) \delta m_j \delta m_k + \mathcal{O}(m^3) \end{aligned}$$

in explicit form

$$\frac{\partial \mathcal{C}}{\partial m_j}(m) \sim \frac{\partial \mathcal{C}}{\partial m_j}(m^i) + \frac{\partial^2 \mathcal{C}}{\partial m_j \partial m_k}(m^i) \delta m_k$$

in matrix form

$$\frac{\partial \mathcal{C}}{\partial m}(m) \sim \frac{\partial \mathcal{C}}{\partial m}(m^i) + \frac{\partial^2 \mathcal{C}}{\partial m^2}(m^i) \delta m$$

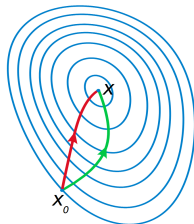
## Local search (3)

$\frac{\partial C}{\partial m}(m) = 0$  around the model  $m^i$  gives

$$\delta m = - \left[ \frac{\partial^2 C}{\partial m^2}(m^i) \right]^{-1} \frac{\partial C}{\partial m}(m^i)$$

$$\nabla C^i = \frac{\partial C}{\partial m}(m^i)$$

$$\mathcal{H}^i = \frac{\partial^2 C}{\partial m^2}(m^i)$$



Line **green** is gradient descent while line **red** is the Newton method which uses the curvature for a more direct road

Gradient  $\nabla C^i$  defines the local direction of the steepest ascent of the point  $m^i$

Hessian  $\mathcal{H}^i$  defines the local curvature of the misfit function

linear problem : the relation is exact

Dimension analysis OK when the Hessian is included ...

# Gradient estimation for the $\ell^2$ norm

$$\nabla C = \sum_{s=1}^{N_s} \nabla C^s \quad \text{sum over sources}$$

$$\nabla C_j^s = \frac{1}{2} \sum_{n=1}^{N_d} \frac{\partial (d_n^{\text{obs}} - u_n(m^i))^* (d_n^{\text{obs}} - u_n(m))}{\partial m_j}$$

$$\nabla C_j^s = -\frac{1}{2} \sum_{n=1}^{N_d} (d_n^{\text{obs}} - u_n(m^i))^* \frac{\partial u_n(m^i)}{\partial m_j} + \frac{\partial u_n(m^i)^*}{\partial m_j} (d_n^{\text{obs}} - u_n(m^i))$$

Because  $x + \bar{x} = 2\mathcal{R}(x)$

$$\nabla C_j^s = -\sum_{n=1}^{N_d} \mathcal{R} \left[ \frac{\partial u_n(m^i)}{\partial m_j} (d_n^{\text{obs}} - u_n(m^i))^* \right]$$

in vector form  $\nabla C^s = -\mathcal{R} \left[ \frac{\partial u(m^i)^t}{\partial m} \cdot (d^{\text{obs}} - u(m^i))^* \right]$

# Gradient estimation for the $\ell^1$ norm

Because  $C_{\ell^1} \sim \sqrt{C_{\ell^2}}$ , we have

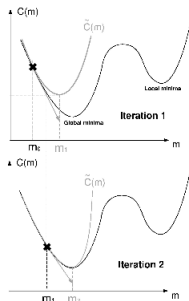
$$\frac{\partial C_{\ell^1}}{\partial m_l} = -\frac{1}{2} \frac{1}{C_{\ell^1}} \frac{\partial C_{\ell^2}}{\partial m_l}$$

$$\nabla C_{\ell^1}^s = \frac{\sqrt{2}}{4} \mathcal{R} \left[ \frac{\partial u(m^i)^t}{\partial m} \cdot \frac{(d^{obs} - u(m^i))^*}{|d^{obs} - u(m^i)|} \right]$$

One can see the effect of residues  $d^{obs} - u(m^i)$  through a normalized amplitude.

# Sensitivity or Jacobian matrix - Fréchet derivative

$$\nabla C(m^i) = - \sum_{s=1}^{N_s} \mathcal{R} [J_s^t \Delta d_s^*] \quad (1)$$



where  $\Delta d_s = d^{obs} - u(m^i) = d^{obs} - Rv(m^i)$  with  $R$  is the restriction projector to receivers of the field  $v$  computed through the wave equation  $Av = b$

where the dimension of the jacobian matrix is  $\dim(J) = [N_s N_d \times M]$ .

## □ Newton approach

$$\frac{\partial^2 \mathcal{C}}{\partial m_k \partial m_l}(m^i) = - \sum_{n=1}^{N_d} \frac{\partial u_n}{\partial m_k}(m^i)^* \frac{\partial u_n}{\partial m_l}(m^i) + \frac{\partial^2 u_n}{\partial m_k \partial m_l}(m^i)(d_n^{obs} - u_n(m^i))^*$$

$$\frac{\partial^2 \mathcal{C}}{\partial m^2}(m^i) = -\mathcal{R}(J^t(m^i)J(m^i)^*) - \mathcal{R} \left[ \sum_{k=1}^M \frac{\partial J^t}{\partial m_k} \Delta d^* \right]$$

$$\frac{\partial^2 \mathcal{C}}{\partial m^2}(m^i) = -\mathcal{R}(J^t(m^i)J(m^i)^*) - \mathcal{R} \left[ \frac{\partial J^t}{\partial m} \cdot (\Delta d_1 \dots \Delta d_{N_s})^* \right]$$

Multi-scattering is considered through the influence of  $m_k$  over  $m_l$

Check the dimensions of the matrix  $\dim(J^t) = [M \times N_s N_d]$

## □ Gauss-Newton approach

$$\frac{\partial^2 \mathcal{C}}{\partial m^2}(m^i) \sim -\mathcal{R}(J^t(m^i)J(m^i)^*)$$

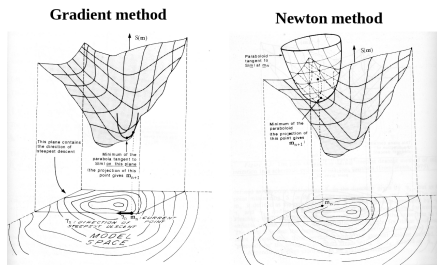
## □ Newton approach

$$\delta m^{i+1} = - \left( \mathcal{R} \left[ J^t(m^i) J^*(m^i) + \frac{\partial J^t}{\partial m}(m^i) \cdot (\Delta d_1 \dots \Delta d_{N_s})^* \right] \right)^{-1} \mathcal{R} [J^t(m^i) \Delta d^*(m^i)]$$

## □ Gauss-Newton approach

$$\delta m^{i+1} \sim - \mathcal{R} [J^t(m^i) J^*(m^i)]^{-1} \mathcal{R} [J^t(m^i) \Delta d^*(m^i)]$$

# Gradient method versus Newton method



From Tarantola (1987)

$$\begin{aligned}\delta m_i^{\text{Gradient}} &= -\alpha \mathcal{R}(J_i^t \Delta d_i^*) \\ \delta m_i^{\text{Gauss}} &= -\mathcal{R}[J_i^t J_i]^{-1} \mathcal{R}(J_i^t \Delta d_i^*) \\ \delta m_i^{\text{Newton}} &= -[\mathcal{H}_i]^{-1} \mathcal{R}(J_i^t \Delta d_i^*)\end{aligned}$$

where the iteration is taken as an index

Gradient method :  $\alpha$  scaling factor distance and proper units

Approximate Gauss-Newton method : diagonal Hessian matrix

Quasi-Newton method : better estimation of the Hessian or its inverse

or its effect onto the gradient (DFP ; BFGS ; L-BFGS ; L-BFGS-B ; KKT ...)

(Pratt et al., 1998; Nocedal and Wright, 1999)

# Adjoint approach for the gradient estimation

No need to estimate the Jacobian matrix  $J$  for the gradient estimation. At a given iteration  $i$ , we have

$$\nabla C = \mathcal{R} [J^t \Delta d^*].$$

The adjoint formulation allows the writing for each source

$$\nabla C_i^s = \mathcal{R} \left[ u^t \left( \frac{\partial B}{\partial m_i} \right)^t r_b^* \right] \quad \text{with} \quad Bu = s$$

- $[M \times 1]$   $u^s$  incident wave for the source  $s$  :  $B^{-1}s$
- $[M \times 1]$   $r_b^s$  backpropagated residues :  $B^{-1}\Delta d$
- $[M \times M]$   $\frac{\partial B}{\partial m_i}$  sparse diffraction kernel

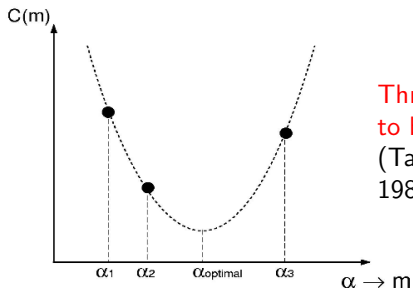
$$\nabla C = \sum_{s=1}^{N_s} \mathcal{R} \left[ u^{s^t} \left( \frac{\partial B}{\partial m} \right)^t r_b^{s^*} \right],$$

Two forward problems to be solved at least (Plessix, 2006)

# Gradient method

$$\delta m_i^{gradient} = -\alpha \mathcal{R} [J_i^t \Delta d_i^*]$$

step length  $\alpha$  parabolic fitting

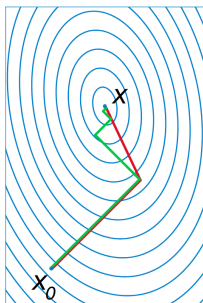


Three forward problems  
to be solved at least  
(Tarantola, 1984; Gauthier et al.,  
1986)

Improved method : approximate Gauss-Newton method but need estimation of diagonal terms of Jacobian matrix

$$\delta m_i^{gradient} = -Diag(\mathcal{R} [J_i^t J_i^*])^{-1} \mathcal{R} [J_i^t \Delta d_i^*]$$

$N_d$  forward problems for each source to be solved at most



$$p^i = \nabla C^i + \beta^i p^{i-1} \quad (2)$$

$p^i$  is the new search direction from

- previous direction  $p^{i-1}$
- new gradient  $\nabla C^i$
- factor  
 $\beta^i = \langle \nabla C^i - \nabla C^{i-1} | \nabla C^i \rangle / (\nabla C^i)^2$

(Polak and Ribière, 1969; Mora, 1987)

green line is the gradient descent while red is the conjugate gradient

$$\delta m_i \sim \mathcal{H}_i^{-1} \mathcal{R}(J^t \Delta d^*)_i$$

with notation  $\nabla C(m_i + \delta m_i) \sim \nabla C(m_i) + \mathcal{H}_i \delta m_i$ , we have

□ **Davidon-Fletcher-Powell (DFP)** formulae (secant formulae)

$$\begin{aligned}\mathcal{H}_{i+1} &= (I - \gamma_i y_i \delta m_i^t) \mathcal{H}_i (I - \gamma_i \delta m_i^t y_i) + \gamma_i y_i y_i^t \\ \mathcal{H}_{i+1}^{-1} &= \mathcal{H}_i^{-1} + \gamma_i \delta m_i \delta m_i^t - \frac{\mathcal{H}_i y_i (\mathcal{H}_i y_i)^t}{y_i^t \mathcal{H}_i y_i}\end{aligned}$$

with  $y_i = \nabla C(m_i + \delta m_i) - \nabla C(m_i)$  and  $\gamma_i = 1/y_i^t \delta m_i$

while the more efficient BFGS formula has a very analog expression

□ **Broyden-Fletcher-Goldfarb-Shanno (BFGS)** formula

$$\begin{aligned}\mathcal{H}_{i+1} &= \mathcal{H}_i + \gamma_i y_i y_i^t - \frac{\mathcal{H}_i \delta m_i (\mathcal{H}_i \delta m_i)^t}{\delta m_i^t \mathcal{H}_i \delta m_i} \\ \mathcal{H}_{i+1}^{-1} &= (I - \gamma_i y_i \delta m_i^t) \mathcal{H}_i^{-1} (I - \gamma_i \delta m_i^t y_i) + \gamma_i \delta m_i \delta m_i^t\end{aligned}$$

- **Limited-memory Broyden–Fletcher–Goldfarb–Shanno (L-BFGS)** formula  
This approach is different on how matrix-vector multiplication is performed for finding the search direction
- **Limited-memory Broyden–Fletcher–Goldfarb–Shanno for bound constrained optimization (L-BFGS-B)** formula  
when bound limites for model parameters are required (Nocedal, 1980).
- **Karush-Kuhn-Tucker conditions (KKT)** formula  
with inegality and equality constraints ...  
Other conditions for allowing various constraints (the use of Lagrange multipliers)

- 1 Introduction
- 2 Local search
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# Ill-posed inversion problem

- Seismic data : incomplete illumination of the medium
  - under-determined problem
  - over-determined problem
  - mixed-determined problem
  
- Remedy : regularization (Tikhonov and Arsenin, 1977)
  - data space  $W_d$  weighting operator (quality and/or compression)
  - model space  $W_m$  weighting operator (could be a combination)

# Weighted least-square problem $\ell^2 \ell^2$

$$\mathcal{C} = \mathcal{C}_{data} + \mathcal{C}_{model} = \frac{1}{2}(\Delta d^\dagger W_d \Delta d) + \frac{1}{2}\epsilon(\Delta m^\dagger W_m \Delta m)$$

$W_d$  : data are often not correlated - diagonal matrix

$W_m$  : model parameter weighting smoothing or roughing or both ...

$\epsilon$  : added this extra parameter for easiness (although could be included in  $W_m$ )

sometimes called Ridge regression or Tikhonov regularisation ( $W_m \sim I$ )

related to the Levenberg-Marquardt algorithm

$[dim(W_d)] =$  inverse of the square of the data units

$[dim(W_m)] =$  inverse of the square of the model units

$\Delta m = m^i - m_{prior}$  where  $m_{prior}$  might take various values

as  $m^i$  or  $m^{i-1}$  or  $m_{ref}$ .

Higher-order Tikhonov ( $W_m$  is a first-order or second-order differential operator)

# Least Absolute Shrinkage and Selection Operator

“LASSO”  $\ell^2 \ell^1$  regression

$$\mathcal{C} = \mathcal{C}_{data} + \mathcal{C}_{model} = \frac{1}{2}(\Delta d^\dagger W_d \Delta d) + \frac{1}{2} \epsilon |\sqrt{W_m} \Delta m|$$

$W_d$  : Data are often not correlated - diagonal matrix

$W_m = L$  : In the Total Variation regression, the operator  $L$  is the first-order differential operator

For TV regression  $\nabla \mathcal{C}_{model} \sim -\nabla \left( \frac{\nabla m}{|\nabla m| + \beta^2} \right)$

$\beta$  a smoothing factor in order to avoid singularities in the model gradient estimation

Still the numerical estimation is a challenge (work in progress)

although many investigations are performed but not yet extensively for the FWI.

# L2L0 regression $\ell^2 \ell^0$ or L1L1 regression $\ell^1 \ell^1$

$$\mathcal{C} = \mathcal{C}_{data} + \mathcal{C}_{model} = \frac{1}{2} \|\Delta d\|_{W_d}^2 + \frac{1}{2} \epsilon \|\delta m\|_{W_m}^0$$

$$\mathcal{C} = \mathcal{C}_{data} + \mathcal{C}_{model} = \frac{1}{2} |\sqrt{W_d} \Delta d| + \frac{1}{2} \epsilon |\sqrt{W_m} \delta m|$$

Not yet investigated as far as we know because problem of convexity ...  
Should be strongly connected with the problem to be solved ...

# Model perturbation $\ell^2$ $\ell^2$

Two identical formulations depending on the availability of  $W_m^{-1}$  or  $W_m$

$$C_{i+1} = \frac{1}{2}((d^{obs} - u(m_i))^t W_d (d^{obs} - u(m_i))^*) + \frac{1}{2}\epsilon((m_i - m_{prior})^t W_m (m_i - m_{prior})^*)$$

$$\delta m_{i+1} = \mathcal{R} [J_i^t W_d J_i^* + \epsilon W_m]^{-1} \mathcal{R} [J_i W_d (d^{obs} - u(m_i))^* + \epsilon W_m (m_i - m_{prior})]$$

$$C_{i+1} = \frac{1}{2}((d^{obs} - u(m_i))^t W_d (d^{obs} - u(m_i))^*) + \frac{1}{2}\epsilon((m_i - m_{prior})^t W_m (m_i - m_{prior})^*)$$

$$\delta m_{i+1} = \mathcal{R} [W_m^{-1} J_i^t W_d J_i^* + \epsilon I]^{-1} \mathcal{R} [W_m^{-1} J_i W_d (d^{obs} - u(m_i))^* + \epsilon (m_i - m_{prior})]$$

In current FWI, the second formulation is used  
with a damping and smoothing in both gradient term and Hessian term using  
 $m_{prior} = m_i$

$$C_{i+1} = \frac{1}{2}((d^{obs} - u(m_i))^t W_d (d^{obs} - u(m_i))^*)$$

$$\delta m_{i+1} = \mathcal{R} [W_m^{-1} J_i^t W_d J_i^* + \epsilon I]^{-1} \mathcal{R} [W_m^{-1} J_i W_d (d^{obs} - u(m_i))^*]$$

Work in progress in this direction of better tuning the a priori information and the smoothing of your medium

# Outline

- 1 Introduction
- 2 Local search
- 3 Regularization
- 4 Conclusion

- Currently, simple formulation of the inversion as the forward problem is quite intensive
- On the side of data space
  - ▶ Different levels of hierarchy in the data processing
  - ▶ Frequency hierarchy from low to high frequencies
  - ▶ Time windowing from EWT to FWT
  - ▶ Slant-stack hierarchy
- On the side of model space
  - ▶ Initial model definition
  - ▶ A priori model influence
  - ▶ A priori uncertainties and correlation lengths estimation
- On the side of objective function
  - ▶ Various formulations of objective functions
  - ▶ cross-correlation (Tape et al., 2009; Baumstein et al., 2011)
  - ▶ time-frequency criteria (Fichtner et al., 2009)
  - ▶ Improved Hessian formulation
  - ▶ Hyper-parameters tuning : weighting operators

# Conclusion

FWI is now going into a mature level with many applications for a better tuning of various parameters.

FWI may provide a macromodel inside which migration will focus on well identified phases.

Thanks you for your attention

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