Inverse problems and applications for marine environment monitoring

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Outline

- Introduction: direct and inverse problems
  - Definitions.
  - Deterministic vs. stochastic/statistical approaches.
  - Equivalence?
- Acoustic wave propagation for ocean analysis and monitoring
  - Why use acoustics?
  - Direct and inverse models.
- Applications and Results:
  - Geoacoustic inversion.
  - Applications in sedimentation, archeology, marine environment monitoring.
- Conclusions and *perspectives*.

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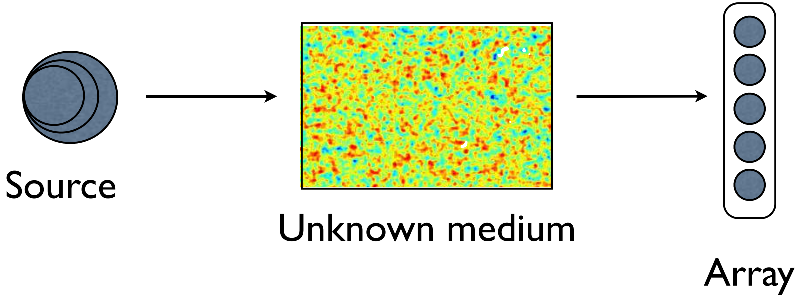
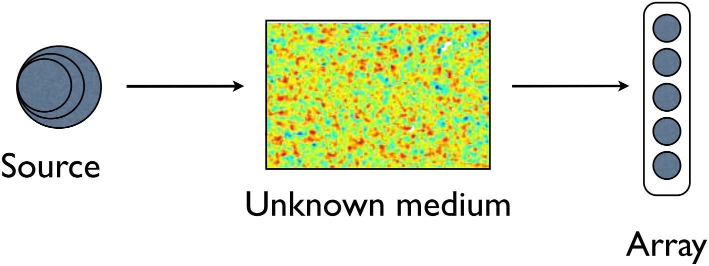
Direct and inverse models



Direct and inverse models



$s(x,t) \longrightarrow$ $\mathcal{L}(u;m) = s$ $\longrightarrow u(x_r, t),$

$r = 1, \dots, N_r$

Model

The inverse problem

Inverse problem:

By comparing the simulations and the observations, find the unknown model parameters - this produces a highly nonlinear inverse problem... (no direct solution possible).

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Two approaches:

1. Classical variational formulation.
2. Statistical formulations.

In fact there is a 3rd: BFN...

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Introduction

- Variational inversion/assimilation is based on optimal control theory.
- The analyzed state is not defined as the one that maximizes a certain pdf (see below...), but as the one that *minimizes a cost function*.
- The minimization requires numerical optimization techniques.
- These techniques all rely on the *gradient* of the cost function.
- This gradient will be obtained here with the aid of *adjoint methods*.

Definition

The adjoint method is a mathematical technique that enables us to compute the gradient of an objective functional with respect to the model parameters in a very efficient manner.

Formulation

Let $\mathbf{u}$ be the state of a dynamical system whose behaviour depends on model parameters $\mathbf{m}$ and is described by a differential operator equation

$$\mathbf{L}(\mathbf{u}, \mathbf{m}) = \mathbf{f},$$

where $\mathbf{f}$ represents external forces.

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where $\mathbf{f}$ represents external forces.
Define a cost function $J(\mathbf{m})$ as an energy functional or, more commonly, as a misfit functional that quantifies the L^2-distance between the observation and the model predicition $\mathbf{u}(\mathbf{x}, t; \mathbf{m})$. For example,

$$J(\mathbf{m}) = \int_0^T \int_\Omega \Big(\mathbf{u}(\mathbf{x}, t; \mathbf{m}) - \mathbf{u}^{\mathrm{obs}}(x, t)\Big)^2 \, \delta(\mathbf{x} - \mathbf{x}_r) \, \mathrm{d}x \, \mathrm{d}t,$$

where $x \in \Omega \subset \mathbb{R}^n, \quad n = 2, 3,$ $0 \leq t \leq T$ and $\mathbf{x}_r$ are the receiver positions.

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where $x \in \Omega \subset \mathbb{R}^n, \quad n = 2, 3,\ 0 \leq t \leq T$ and $\mathbf{x}_r$ are the receiver positions.

Objective:

Choose the model parameters $\mathbf{m}$ as a function of the observed output, such that the cost function $J(\mathbf{m})$ is minimized.

Adjoint derivation

Define the variation of $\mathbf{u}$ with respect to $\mathbf{m}$ in the direction $\delta\mathbf{m}$ (Gâteaux derivative) as

$$\delta\mathbf{u} \doteq \nabla_m \mathbf{u}\, \delta\mathbf{m},$$

then the corresponding directional derivative of J can be written as

$$\nabla_m J\, \delta\mathbf{m} = \nabla_u J\, \delta\mathbf{u} = \langle \nabla_u J_1\, \delta\mathbf{u} \rangle\,, \qquad (1)$$

where $\langle\cdot\rangle$ denotes the space-time integral.

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Difficulty:

The variation $\delta\mathbf{u}$ is impossible/unfeasible to compute numerically (for all directions $\delta\mathbf{m}$).

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The variation $\delta\mathbf{u}$ is impossible/unfeasible to compute numerically (for all directions $\delta\mathbf{m}$).

Solution:

Eliminate $\delta\mathbf{u}$ from (1) by introducing an adjoint state (Lagrange multiplier).

Adjoint derivation II

Differentiate the state equation with respect to the model $\mathbf{m}$ and apply the necessary condition for optimality,

$$\nabla_m \mathbf{L}\,\delta\mathbf{m} + \nabla_u \mathbf{L}\,\delta\mathbf{u} = 0.$$

Multiply by an arbitrary test function $\mathbf{u}^\dagger$ (Lagrange multiplier) and integrate,

$$\left\langle \mathbf{u}^\dagger \cdot \nabla_m \mathbf{L}\,\delta\mathbf{m} \right\rangle + \left\langle \mathbf{u}^\dagger \cdot \nabla_u \mathbf{L}\,\delta\mathbf{u} \right\rangle = 0.$$

Add to (1) and integrate by parts, regrouping terms in $\delta\mathbf{u}$,

$$\begin{aligned} \nabla_m J\,\delta\mathbf{m} &= \langle \nabla_u J_1\,\delta\mathbf{u} \rangle + \left\langle \mathbf{u}^\dagger \cdot \nabla_m \mathbf{L}\,\delta\mathbf{m} \right\rangle + \left\langle \mathbf{u}^\dagger \cdot \nabla_u \mathbf{L}\,\delta\mathbf{u} \right\rangle \\ &= \left\langle \delta\mathbf{u} \cdot \left(\nabla_u J_1^\dagger + \nabla_u \mathbf{L}^\dagger \mathbf{u}^\dagger \right) \right\rangle + \left\langle \mathbf{u}^\dagger \cdot \nabla_m \mathbf{L}\,\delta\mathbf{m} \right\rangle, \end{aligned}$$

where we have defined the adjoint operators $\nabla_u J_1^\dagger$ and $\nabla_u \mathbf{L}^\dagger$.

Adjoint derivation III

Finally, to eliminate $\delta\mathbf{u}$, the adjoint state $\mathbf{u}^\dagger$ should satisfy

$$\nabla_u \mathbf{L}^\dagger \mathbf{u}^\dagger = -\nabla_u J_1^\dagger$$

which is known as the adjoint equation.
Once the adjoint solution $\mathbf{u}^\dagger$ is found, the derivative of the objective functional reduces to

$$\boxed{\nabla_m J\,\delta\mathbf{m} = \left\langle \mathbf{u}^\dagger \cdot \nabla_m \mathbf{L}\,\delta\mathbf{m} \right\rangle}$$

which enables us to compute the desired gradient, $\nabla_m J$ without the explicit knowledge of $\delta\mathbf{u}$.

Adjoint remarks

1. We obtain explicit formulas for the gradient with respect to each model parameter.
2. The computational cost is one solution of the adjoint equation which is usually identical to the direct equation, but with a reversal of time.
3. The optimization of the misfit functional leads to multiple local minima and to very "flat" cost functions which are hard problems to overcome with gradient-based methods.
4. Regularization terms can alleviate the non-uniqueness problem. Rescaling can help with the "flatness". SA algorithms can be mobilized.
5. When measurement and modelling errors can be modelled by Gaussian distributions and a background (prior) solution exists, the objective function may be generalized by including suitable covariance matrices.

Adjoint methods for inverse problems: summary

- Solid theoretical basis: calculus of variations.
- Can treat general partial differential equations and associated boundary and initial conditions.
- Widely-used in meteorology (3D-Var and 4D-Var).
- Applications to geoacoustic inversion...

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Why should we use acoustics?

- Facts:
  1. Electromagnetic waves do not penetrate into the sea water.
  2. Satellites only see and measure surface phenomena.
  3. Hydrographic measurements are too expensive and too sparse.

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Acoustic waves

are the only means of remotely sensing the depths of the ocean, and can provide oceanographers, meteorologists and other ocean researchers with large quantities of significant field data, cheaply and easily.

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Acoustics

- Linear (acoustic) wave Equation: $p_{tt} - \nabla \cdot (c^2 \nabla p) = 0$
- Elastodynamic wave equation:
  $\rho \boldsymbol{u}_{tt} - (\lambda + 2\mu)\nabla\nabla \cdot \boldsymbol{u} + \mu \nabla \times \nabla \times \boldsymbol{u} = 0$
- Helmholtz equation: $k^2\psi + \nabla \cdot (c^2 \nabla \psi) = 0$
- Paraxial equation in waveguides:$\phi_r = \frac{\mathrm{i}}{2k_0}\phi_{zz} + \mathrm{i}\frac{k_0}{2}(n^2 - 1)\phi$ (equation of Schrödinger type)
- Others : normal modes (Fourier series) , rays (Eikonal equation).

Note:

Must add physically relevant, initial and boundary conditions...

Numerical approaches

- finite difference methods
- finite element and spectral element methods
- ray-tracing methods
- Fourier-mode methods

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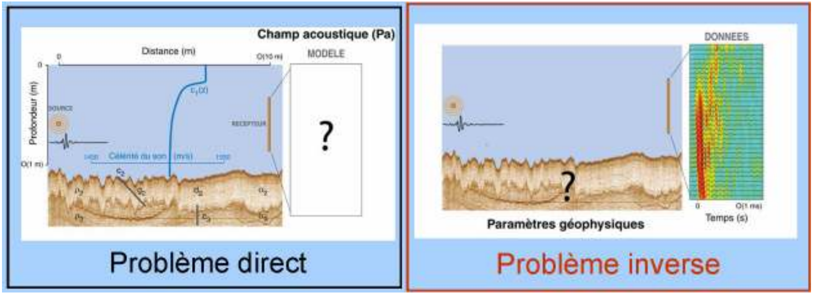
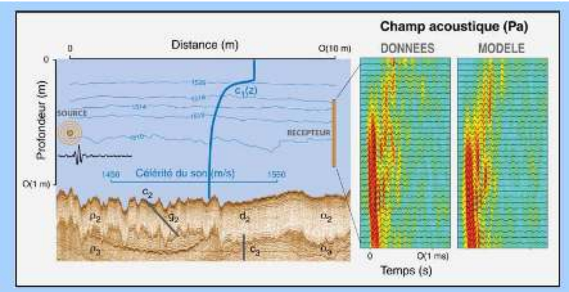
What is geoacoustic inversion?





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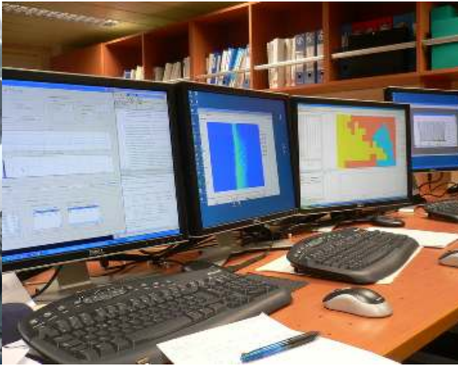
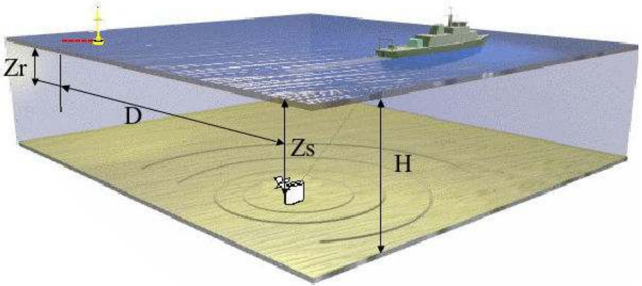
Physical problem I

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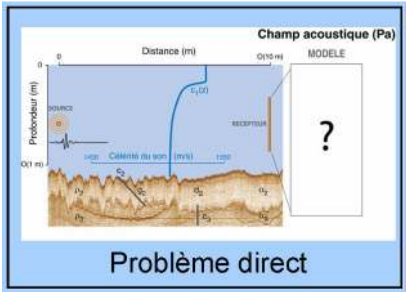
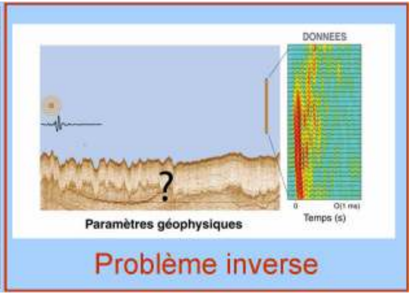
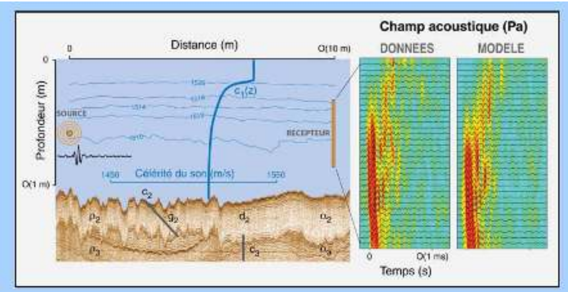
Physical problem II: waveguide model







Program

We now prepare all the ingredients for the solution of the inverse problem:

- direct propagation model;
- cost function for mismatch;
- adjoint model obtained by integration by parts (same as direct equation, but with reversal of time);
- gradient of cost function (in terms of adjoint field) with respect to the model (geoacoustic) parameters;
- gradient-based (quasi-Newton) algorithm for the minimization.

Direct (forward) model

- SPE: Small angle parabolic approximation ($\psi-$diff. 1st order approx. of Helmholtz eq.) : $p(r,z) = \psi(r,z)H_0^{(1)}(k_0 r)$

$$2ik_0 \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} + k_0^2(n^2-1)\psi = 0 \qquad , 0 < r < R,\ 0 < z < H.$$
$$\psi(0,z) = S(z), \quad \psi(0,r) = 0,\ G_1(\psi(r,H),\gamma) = 0.$$

- WAPE: Large angle parabolic approximation ($\psi-$diff. Padé 1st order) :

$$2ik_0 \left[1 + \frac{1}{4}(n^2-1)\right] \frac{\partial \psi}{\partial r} + \frac{\partial^2 \psi}{\partial z^2} + k_0^2(n^2-1)\psi + \frac{i}{2k_0}\frac{\partial^3 \psi}{\partial r \partial z^2} = 0 \quad , 0 < r < R,\ 0 <$$
$$\psi(0,z) = S(z),\ \psi(0,r) = 0,\ G_2(\psi(r,H),\gamma) = 0.$$

- Impedance condition on sea bottom $z = H$ that contains the unknown geoacoustic parameters: densité ρ, célérité c et attenuation α.

Modeling: impedance conditions

- LBC: Local Condition (non-physical) : $\frac{\partial \psi}{\partial z} + im(r)\psi = 0$ where $m(r)$ is the control variable.
- NLBC: Non-Local Condition: that includes all physical parameters explicitly,

$$\left\{ \frac{\partial}{\partial z} - i\mathcal{B} \right\} \psi \left[(J+1)\Delta r, z_b \right] = i\mathcal{B} \sum_{j=1}^{J+1} g_{0,j} \psi \left[(J+1-j)\Delta r, z_b \right]$$

  - $\mathcal{B} = \frac{\rho_b}{\rho_w} k_0 \sqrt{N_b^2 - 1 + \nu^2}$, $k_0 = \frac{\omega}{c_0}$,
  - $N_b = n_b[1 + i\alpha]$, $n_b = \frac{c_0}{c_b}$, $\nu^2 = \frac{4i}{k_0 \Delta r}$.
- Control Vector $\mathbf{m}(r) = [N_b(r),\ \rho_b(r)]^T$.

Application of adjoint method

- Cost Functional: $J[\mathbf{m}] = \frac{1}{2}\int_0^H |\psi - \psi^*|^2_{r=R}\, dz +$ regularization terms
- Adjoint System derived by necessary condition for optimality.
- Compute exact gradients for different models:
  - SPE+LBC: $\nabla_{\mathbf{m}} J = \frac{1}{2k_0}\ \bar{\psi} p \big|_{z=H}$,
  - SPE+NLBC: $\nabla_{\mathbf{m}} J = \frac{1}{2k_0}\begin{bmatrix} \bar{\psi} p \\ ip \end{bmatrix}_{z=H}$,
  - WAPE+NLBC: $\nabla_{\mathbf{m}} J = \begin{bmatrix} (i\bar{\psi} - \bar{F})(p + \frac{i}{2k_0} p_r) \\ -\bar{\beta}(p + \frac{i}{2k_0} p_r) \end{bmatrix}_{z=H}$.

Recap

We now have all the ingredients for the solution of the inverse problem:

- direct propagation model;
- cost function for mismatch;
- adjoint model; here we have used the approach "adjoint-then-discretize" - the other possibility is "discretize-then-adjoint" which is commonly used in meteorology...
- gradient of cost function with respect to the model (geoacoustic) parameters;
- gradient-based (quasi-Newton) algorithm for the minimization.

Results

It works!
Key references:

Meyer, Hermand, Optimal nonlocal boundary control of the wide-angle parabolic equation for inversion of a waveguide acoustic field, *J. Acoust. Soc. Am.* ***117***, *5 (2005).*

Meyer, Hermand, Asch, Legac, An analytic multiple frequency adjoint-based inversion algorithm for parabolic-type approximations in ocean acoustics. *Inverse Problems in Science and Engineering,* ***13***, *3, (2006).*

But we're interested in more realistic problems...

More realistic problems

The complexity of real pde models (especially the boundary conditions), imposes the choice between 2 adjoint strategies:

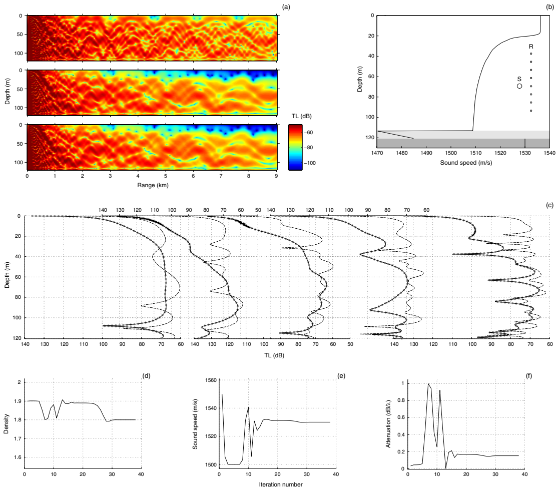
1. Automatic differentiation.
2. Semi-automatic, graph theoretical approach.

Our choice

We choose the 2nd and use the YAO package which requires the construction of a *modular graph* of the direct model. The linear tangent and the *adjoint* are then automatically generated by YAO, which also solves the functional *minimization* problem by using quasi-Newton methods.

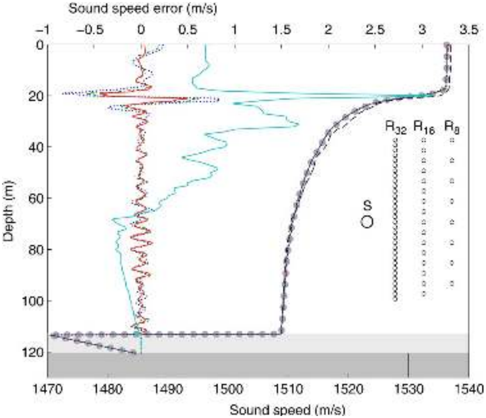
[J.-P. Hermand, M. Meyer, M. Asch, and M. Berrada. Adjoint-based acoustic inversion for the physical characterization of a shallow water environment. *J. Acoust. Soc. Am.*, 119 (6): 3860–3871, June 2006.]

Numerical results: geoacoustic inversion



Adjoint-based geoacoustic characterization of a shallow water environment: joint optimization across 5 source frequencies using an 8-element VRA. (a) Initial (top), true (middle) and calculated (bottom) acoustic field for source frequency (400Hz); (b) environmental input data and experimental configuration; (c) initial (dashed), true (gray dots) and calculated (solid) acoustic fields at 9 km range for 200, 315, 400, 500, 630 Hz from left to right; (d)–(f) evolution of the estimated density, sound speed and attenuation vs. iteration number. (*JASA*, **119**(6), 2006)

Numerical results: ocean acoustic tomography



Correction for an uncertain SSP during GI using three partial water column spanning VRAs with 32, 16 and 8 hydrophones at 1.5 km range. For the inversion seven frequencies were used; the initial SSP profile (dashed, black) is calculated from the CTD cast that deviates the most from the true ensemble average (large dots, gray). The inverted profiles are obtained with a 32 (solid,) a 16 (dash-dot), and an 8-element (dotted), VRA. Left: Inversion errors for the three estimated and the initial profile (solid, turkey) (top scale.)

Extensions

- Broadband, multiple frequency formulation.
- Regularization of the cost function and treatment of measurement uncertainty.
- Multiple sediment layers.
- Sparse arrays and missing measurements.
- PCA/EOF representation of sound speed profile (SSP).
- Particle velocities (gradient of pressure).

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Introduction

- Recall the inverse problem: assume a vector of model parameters $\mathbf{m} = \{m_i,\ i = 1, \ldots, M\}$ representing the unknown geoacoustic properties and estimate the parameter values that minimize the misfit between measured and modeled acoustic fields.
- Optimization alone provides no information on the parameter uncertainties and data information content.
- Bayesian theory can provide a more complete approach to the inverse problem:
  - model parameters are considered as random variables constrained by noisy data and prior information;
  - Bayesian inversion is then formulated in terms of the posterior probability density (ppd), parameter uncertainties (variances, marginals), and parameter correlations.
- Kalman filters can be developed from Bayesian theory (when errors are Gaussian...)

Bayesian formulation I

- Data information formulated in terms of the likelihood function.
- This function represents the conditional data uncertainty distribution interpreted as a function of the model parameters.
- Data uncertainties (measurement error, theory error) are not well-known and physically reasonable estimates are needed.
- Simple distributions (e.g. multi-variate Gaussian) are assumed with μ and σ estimated from the data.
- Model selection can be applied across a range of parametrizations by using an information criterion.

Bayes' rule

Let $\mathbf{d} = [d_i]_{i=1,\ldots,N}$ be a vector of data representing physical observations, $\mathcal{I}$ denote the model that specifies the choice of parametrization of the physical system, $\mathbf{m} = [m_i]_{i=1,\ldots,M}$ be the vector of free parameters representing a realization of $\mathcal{I}$. Then, in a Bayesian approach, these obey Bayes' rule

$$P(\mathbf{m}|\mathbf{d},\mathcal{I}) = \frac{P(\mathbf{d}|\mathbf{m},\mathcal{I})P(\mathbf{m}|\mathcal{I})}{P(\mathbf{d}|\mathcal{I})},$$

where (suppressing $\mathcal{I}$)

- $P(\mathbf{m})$ is the prior probability density function representing the available parameter information independent of the data,
- $P(\mathbf{d}|\mathbf{m})$ is the conditional pdf of the data given the parameters - this represents the error distribution (as a function of $\mathbf{d}$) or likelihood function (as a function of $\mathbf{m}$),
- $P(\mathbf{d})$ is a normalization.

Likelihood function

The likelihood function can generally be written as

$$L(\mathbf{m}) \propto \exp\left[-E(\mathbf{m})\right],$$

where $E(\mathbf{m})$ represents an appropriate data misfit function. Now define the generalized misfit function, combining data and prior, as

$$\phi(\mathbf{m}) = E(\mathbf{m}) - \ln P(\mathbf{m}).$$

Then Bayes' rule becomes

$$P(\mathbf{m}|\mathbf{d}) = \frac{\exp\left[-\phi(\mathbf{m})\right]}{\int \exp\left[-\phi(\mathbf{m}')\mathrm{d}\mathbf{m}'\right]}.$$

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PPD

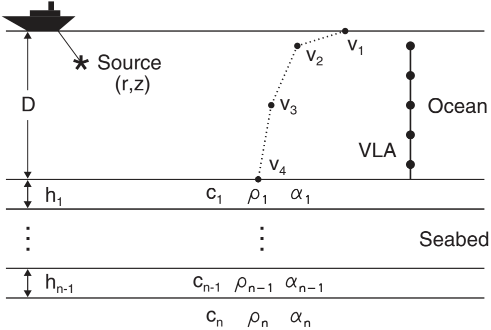
This posterior probability density represents the most general solution to an inverse problem.

PPD

To intrepret the PPD in multi-dimensional problems, we need to estimate the following quantities:

MAP	$\hat{\mathbf{m}} = \arg\max_{\mathbf{m}} P(\mathbf{m}\vert\mathbf{d})$
Mean	$\bar{\mathbf{m}} = \int \mathbf{m} P(\mathbf{m}\vert\mathbf{d}) \mathrm{d}\mathbf{m}$
Covariance	$\mathbf{C}_{\mathbf{m}} = \int (\mathbf{m}-\bar{\mathbf{m}})(\mathbf{m}-\bar{\mathbf{m}})^T P(\mathbf{m}\vert\mathbf{d}) \mathrm{d}\mathbf{m}$
Marginals	$P(m_i\vert\mathbf{d}) = \int \delta(m_i - m_i') P(\mathbf{m}'\vert\mathbf{d}) \mathrm{d}\mathbf{m}'$
Correlations	$R_{ij} = C_{m_{ij}} / \sqrt{C_{m_{ii}} C_{m_{jj}}}.$

Model selection



- Over parametrization can lead to spurious model structure and over-estimation of model uncertainties.
- Under parametrization can leave structure unresolved and underestimate uncertainties.

BIC

Bayesian inversion can determine an appropriate model parametrization based on an objective criterion. For this, we need to compute the conditional probability $P(\mathbf{d}|\mathcal{I})$ that expresses the likelihood of the parametrization given the data, or the Bayesian evidence for $\mathcal{I}$. We have

$$P(\mathbf{d}|\mathcal{I}) = \int P(\mathbf{d}|\mathbf{m}, \mathcal{I}) P(\mathbf{m}|\mathcal{I}) \mathrm{d}\mathbf{m}$$

which is very difficult to compute.
By using an asymptotic point estimate of $\ln P(\mathbf{d}|\mathcal{I})$, the BIC, we can easily compute this Bayesian evidence,

$$\begin{aligned} -2 \ln P(\mathbf{d}|\mathcal{I}) \approx \mathrm{BIC} &= -2 \ln L(\hat{\mathbf{m}}) + M \ln N, \\ &= 2E(\hat{\mathbf{m}}) + M \ln N, \end{aligned}$$

where N is the number of unknown parameters in the model.

BIC

Bayesian inversion can determine an appropriate model parametrization based on an objective criterion. For this, we need to compute the conditional probability $P(\mathbf{d}|\mathcal{I})$ that expresses the likelihood of the parametrization given the data, or the Bayesian evidence for $\mathcal{I}$. We have

$$P(\mathbf{d}|\mathcal{I}) = \int P(\mathbf{d}|\mathbf{m},\mathcal{I})P(\mathbf{m}|\mathcal{I})\mathrm{d}\mathbf{m}$$

which is very difficult to compute.
By using an asymptotic point estimate of $\ln P(\mathbf{d}|\mathcal{I})$, the BIC, we can easily compute this Bayesian evidence,

$$\begin{aligned} -2\ln P(\mathbf{d}|\mathcal{I}) \approx \mathrm{BIC} &= -2\ln L(\hat{\mathbf{m}}) + M\ln N, \\ &= 2E(\hat{\mathbf{m}}) + M\ln N, \end{aligned}$$

where N is the number of unknown parameters in the model.

Minimization

The parametrization with the smallest BIC is selected as the most appropriate model.

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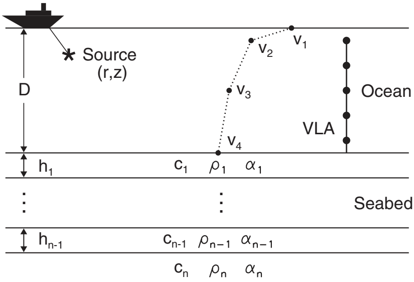
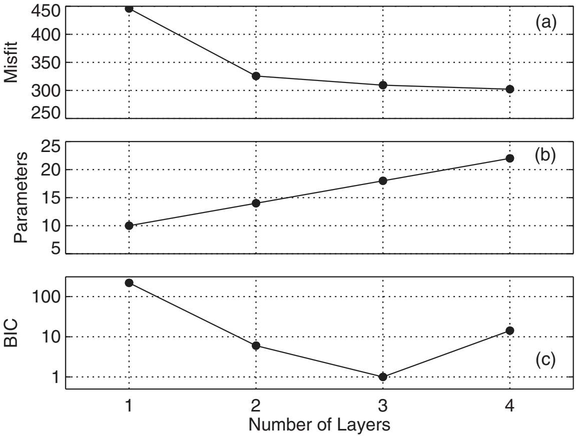
Problem setup



- Mediterranean sea, depth 132 m, chirp signal 300-800 Hz, VLA of 48 hydrophones, range 3.85 km.
- SSP parametrized by 4 unknowns, $v_1, \ldots, v_4$.
- Seabed parametrized by n layers, each represented by sound speed c, density ρ, attenuation α and thickness h.
- Uniform priors assigned to all parameters within physical bounds.

[S. Dosso, J. Dettmer. Bayesian matched-field geoacoustic inversion. Inverse Problems 27, 2011.]

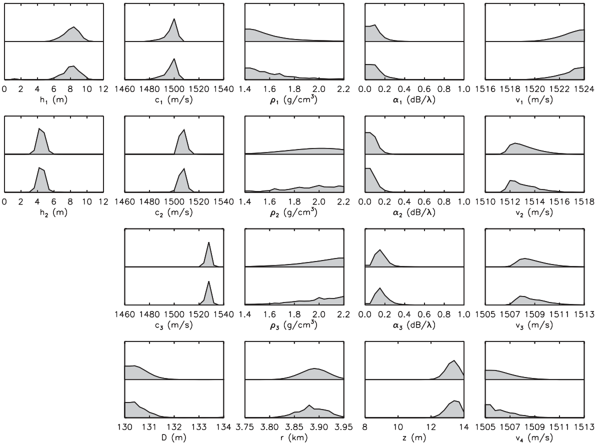
Results: model selection



Conclusion

Use a three-layer model.

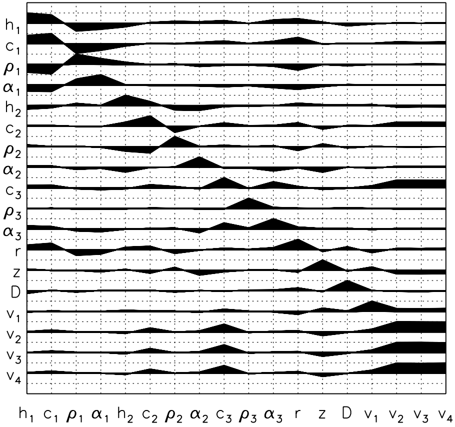
Results: marginals for 3-layer model

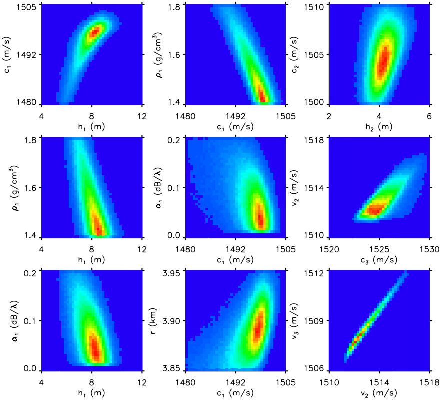


Problem

Requires a very large number of forward simulations $\sim 10^6$...

Results: correlation matrix & joint marginals





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New Inverse problem #1: the ocean observatory

- **Aim:** monitor environmental parameters using active and passive acoustic signals

- **Equation:** elastic wave/Helmholtz equation, with variable layers (water, vegetation, sediments), continuity conditions on layer interfaces, absorbing conditions on lateral boundaries and sea bottom below sediment layers , Dirichlet condition (zero pressure) on water surface, known (active) source or unknown (passive) source.
- **Inverse problem:** from observations of acoustic pressures, track environmental parameters (density, salinity, temperature, etc.)
- **Question:** how?

New Inverse problem #2: acoustical archeology

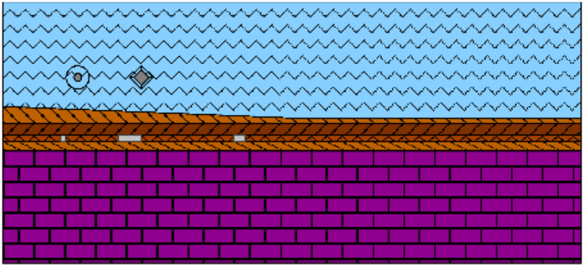
- **Aim:** map archeological sites, in coastal waters, for heritage preservation

- **Equation:** elastic wave equation, bc's, known (active) source
- **Inverse problem:** from observations of (time dependent) acoustic pressures, detect the presence (or absence) of archeological artefacts
- **Question:** how?

Preliminary results for the direct problem

- Realistic layer and flint geometry
- Time-domain seismo-acoustic simulations using **SPECFEM2D**
- Computation of spectra and comparison with lab measurements.

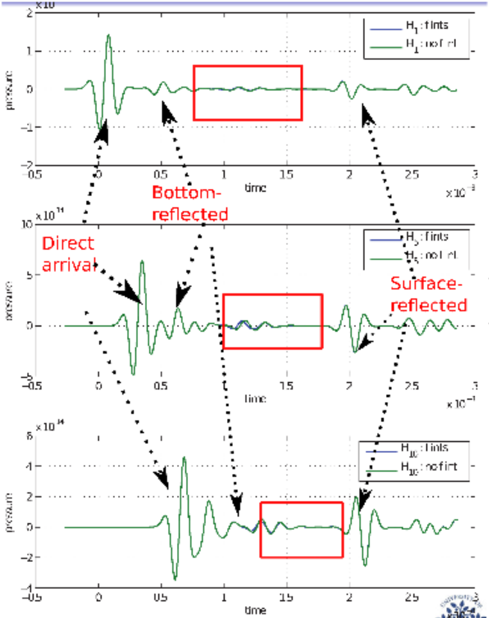
Results: shallow water zone

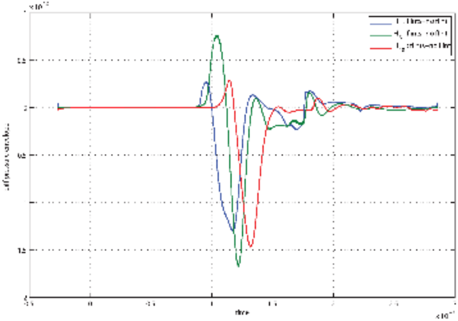


Density	2300 kg/m^3
Compression speed	8433 m/s
Shear speed	5843 kg/m^3
Young's module	185 GPa
Poisson's Ratio	0.27

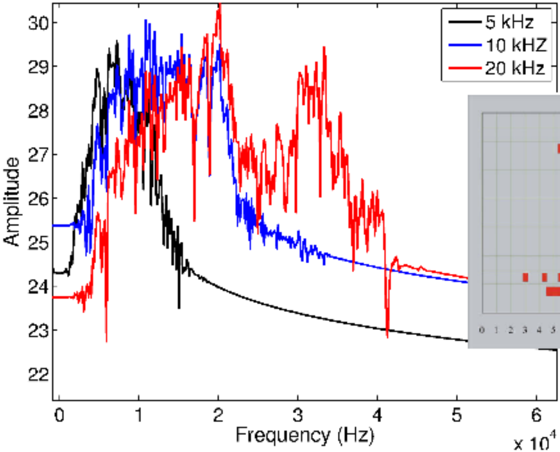
Layer	Thickness (cm)	ρ (kg/m^3)	c_p(m/s)	c_s(m/s)	α_p(dB/λ)	α_s(dB/λ)
seawater	0 – 500 (200)	1000	1500	–	–	–
sand	10 – 25 (10)	1900	1650	110	0.8	–
mud	20 – 30 (20)	1500	1500	50	0.2	–
cultural	5 – 10 (5)	1500	1500	50	0.2	–
sand	15 – 50 (15)	1900	1650	110	0.8	–
substrate (moraine)	semi–∞	2100	1950	600	0.4	1.0

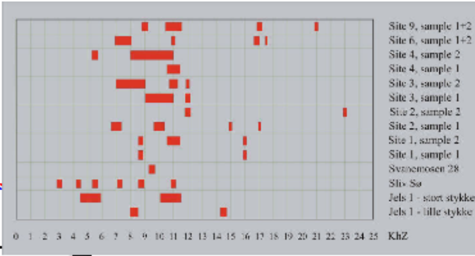
Results: recorded signals



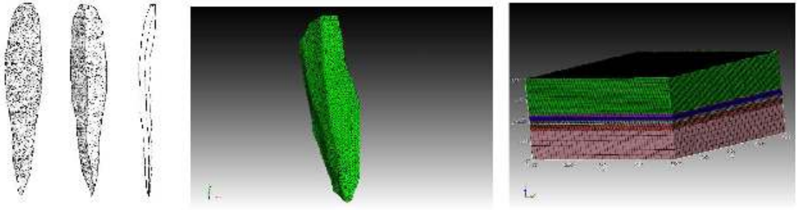


Spectral differences





3D setting and model



(a) (b) (c)

(a) Flint flake geometry, (b) Mesh of flint and flake and (c) Mesh for the coastal environment.

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Conclusions

1. Need for fast, accurate forward and inverse numerical models.
2. Adjoint approach can be efficient, but code maintenance is complex.
3. Bayesian approach gives much more complete information.
4. Hybrid methods are the future: EnsKF, Ens/Var, ...
5. Passive acoustic monitoring for environmental protection is the new grand challenge.

Perspectives

- Participate in "environmental monitoring" projects: Amazon, archeology, aquatic life, ...
- Develop and implement hybrid, deterministic-statistical approaches.
- Full stochastic modeling (*cf.* Garnier-Papanicolaou) with random medium properties and suitable scale separation.

Questions?

Ex. 1: Convection-diffusion (ODE)

$$\begin{cases} -\left(a(x)u'(x)\right)' - u'(x) = q(x) \quad 0 < x < 1 \\ u(0) = 0,\ u(1) = 0. \end{cases} \tag{2}$$

- $J[a] = \frac{1}{2}\int_0^1 |u(x) - u^*(x)|^2\, dx$
- Lagrangian (variational formulation) :
  $J^*[a,p] = \frac{1}{2}\int_0^1 |u(x) - u^*(x)|^2\, dx + \int_0^1 p\left(-(au')' - u' - q\right) dx$
- Variation of J^* :

$$\delta J^* = \int_0^1 (u - u^*)\,\delta u\, dx + \int_0^1 \delta p \overbrace{\left(-(au')' - u' - q\right)}^{=0} dx \\ + \int_0^1 p\left[(-\delta a\, u' - a\,\delta u)' - q\right]$$

Ex. 1: (contd.)

- **KILL terms** by conditions on p: *adjoint equation*, *boundary conditions*.
- $\delta J^* = \int_0^1 [(u-u^*) + p' - (ap')'] \, \delta u \, dx + \int_0^1 \delta a \, u'p' dx$
  $\quad + [-p(\delta u + u'\delta a + a\delta u') + p' a \delta u]_0^1$
  $\quad = \int_0^1 \delta a \, u'p' dx$

  where,
  $$\begin{cases} -(ap')' + p' = -(u-u^*) & 0 < x < 1 \\ p(0) = 0, \; p(1) = 0. \end{cases} \tag{3}$$
- $\Rightarrow$ gradient:
  $$\nabla_{a(x)} J^* = u'p'$$

Example 2: Diffusion equation (PDE)

- IBVP :

$$\begin{cases} \frac{\partial u}{\partial t} - \nabla \cdot (\nu \nabla u) = 0 & x \in (0, L), \qquad t > 0, \\ u(x, 0) = u_0(x), & u(0, t) = 0, \quad u(L, t) = \eta(t). \end{cases}$$

- Controls:
  - internal – $\nu(x)$ (parameter identification / tomography)
  - initial – $\xi(x) = u_0(x)$ (source detection)
  - boundary – $\eta(t) = u(L, t)$ («classical» control / parameter identification)
- Cost Function:

$$J[\nu, \xi, \eta] = \frac{1}{LT} \int_0^T \int_0^L |u - u_{\text{ref}}|^2 \, dx \, dt$$

Ex. 2 (contd.)

- Lagrangian:
$J^* = \frac{1}{LT} \int_0^T \int_0^L |u - u_*|^2 \, dx \, dt + \frac{1}{LT} \int_0^T \int_0^L p \, [u_t - (\nu u_x)_x] \, dx \, dt$

- Variation: $\delta J^* = \frac{1}{LT} \int_0^T \int_0^L 2(u - u_*)\delta u \, dx \, dt + \frac{1}{LT} \int_0^T \int_0^L \delta p \, \overbrace{[u_t - (\nu u_x)_x]}^{=0} \, dx \, dt$
$+ \frac{1}{LT} \int_0^T \int_0^L p \, [\delta u_t - (\delta\nu \, u_x + \nu \delta u_x)_x] \, dx \, dt$

- Integration by parts:
$\delta J^* = \frac{1}{LT} \int_0^T \int_0^L \delta\nu u_x p_x dx \, dt - \frac{1}{LT} \int_0^L p \;\; \delta u|_{t=0} \, dx + \frac{1}{LT} \int_0^T p \;\; \delta\eta|_{x=L} \, dt$

Ex. 2 (contd.)

- Adjoint Equation:

$$\left\{ \begin{array}{lll} \frac{\partial p}{\partial t} + \nabla \cdot (\nu \nabla u) = 2(u - u_*) & x \in (0, L), & t > 0, \\ p(x, T) = 0, & p(0, t) = 0, & p(L, t) = 0. \end{array} \right.$$

- $\Rightarrow$ gradient :

$$\begin{aligned} \nabla_{u|_{t=0}} J^* &= -\, p|_{t=0} \\ \nabla_{\nu(x)} J^* &= \frac{1}{T} \int_0^T u_x p_x dt \\ \nabla_{\eta|_{x=L}} J^* &= p|_{x=L} \,. \end{aligned}$$

Adjoint zoo...

Adjoint equations for other partial differential operators:

Operator	Adjoint
$\frac{du}{dx} - \gamma \frac{d^2u}{dx^2}$	$-\frac{dv}{dx} - \gamma \frac{d^2v}{dx^2}$
$\nabla \cdot (k \nabla u)$	$\nabla \cdot (k \nabla v)$
$\frac{\partial u}{\partial t} - c \frac{\partial^2 u}{\partial x^2}$	$-\frac{\partial v}{\partial t} - c \frac{\partial^2 v}{\partial x^2}$
$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x}$	$-\frac{\partial v}{\partial t} - c \frac{\partial v}{\partial x}$

YAO - modular graph, semi-automatic adjoints

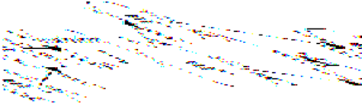

FIG. 1. Example of a modular graph. For each module m_n the input and output variables are denoted by x_k and y_j respectively. α_k and β_j represent the corresponding Lagrange multipliers that are used for the adjoint generation scheme in Sec. II B2.

Lagrange multipliers computed from $\frac{\partial \mathcal{L}}{\partial y_j} = -\alpha_j + \sum \beta_k = 0$ and $\frac{\partial \mathcal{L}}{\partial x_k} = -\beta_k + \sum \alpha_j \frac{\partial f_j}{\partial x_k} = 0$ by back-propagation, initiated at last module where $\beta_k = \frac{\partial f_j}{\partial x_k}$. Then local gradient of the cost function with respect to any model parameter, w_i, is $\frac{\partial J}{\partial w_i} = \sum \alpha_j \frac{\partial f_j}{\partial w_i}$.

YAO - WAPE+NLBC

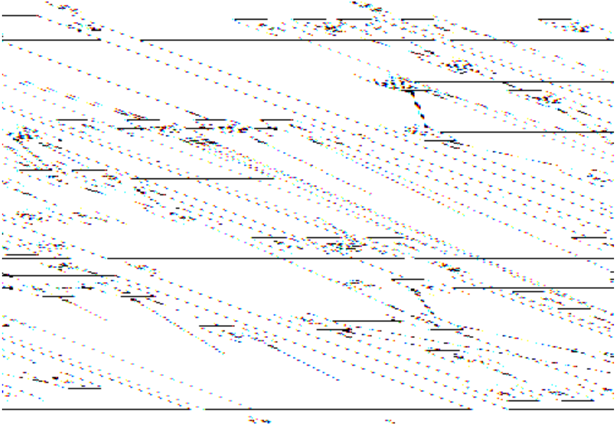

FIG. 2. Modular graph representation of the WAPE NLBC model. The nomenclature is consistent with the notation in Sec. III, particularly Eqs. (18), (20), (21), and (27). Modules with the superscript "LU" or "CN" implement the LU decomposition (Ref. 39) and the Crank-Nicolson scheme, respectively. Module "Σ" refers to the summation of the boundary-field values in Eq. (27).

Blocks (a)–(d) represent 4 different dimensional spaces; block (a) mainly serves for the initialization of the environmental parameters $[\alpha_w, \rho_w, c(z), n(z)]$ in the water column and the setup of the tridiagonal finite difference matrices (diaGt, DiaG), block (b) represents the actual range marching solution for the field in the water column via LU decomposition (res, ixu). Blocks (c) and (d) represent the corresponding counterparts for the initialization (c) and calculation (d) of the field in the bottom in accordance with the NLBC

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