SEMI-AUTOMATIC ADJOINT PE MODELING FOR GEOACOUSTIC INVERSION*

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Recently, an analytic adjoint-based method of optimal nonlocal boundary control has been proposed for inversion of a waveguide acoustic field using the wide-angle parabolic equation [Meyer & Hermand, J. Acoust. Soc. Am. **117**, 2937–2948 (2005)]. In this paper a numerical extension of this approach is presented that allows the direct inversion for the geoacoustic parameters which are embedded in a discrete representation of the nonlocal boundary condition. The adjoint model is generated numerically and the inversion is carried out jointly across multiple frequencies. To demonstrate the effectiveness of the implemented numerical adjoint, an illustrative example is presented for the geoacoustic characterization of a Mediterranean shallow water environment using realistic experimental conditions.

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1. Introduction

Given an oceanic environment, a model G describing the acoustic propagation $\mathbf{y} = G(\mathbf{x})$ for a set of input variables $\mathbf{x}$ and a differentiable scalar measure $J(\mathbf{y})$ which quantifies the fit between the model solution $\mathbf{y}$ and a corresponding set of observations, a first order Taylor series approximation to the perturbation of the cost function

$$J' = \sum_j \frac{\partial J}{\partial y_j} y'_j \tag{1}$$

can be obtained via

$$y'_j = \sum_k \frac{\partial y_j}{\partial x_k} x'_k \,. \tag{2}$$

Here $\mathbf{x}'$ and $\mathbf{y}'$ denote perturbations of the model input and output, respectively, and the indices k and j refer to the corresponding components. Following the description of the adjoint derivation in Ref.[1] primes are used to denote linear estimates of perturbation quantities. Considering the propagation model G as a sequence of operations, such as e.g., individual range step integrations, physical or algorithmic components of the model,

$$G(\mathbf{x}) = C_N \left((\ldots \langle C_2 \left\{ C_1 \left[C_0(\mathbf{x}) \right] \right\} \rangle \ldots) \right) \,, \tag{3}$$

the chain rule of elementary calculus yields a sequential formulation for $y'_j = y'^{(N)}_j$ in Eq. (2)

$$\begin{cases} y'^{(n)}_j = \sum_k \frac{\partial y^{(n)}_j}{\partial y^{(n-1)}_k} y'^{(n-1)}_k & \text{, for } N \geq n \geq 1 \\ y'^{(n)}_j = \sum_k \frac{\partial y^{(n)}_j}{\partial x_k} x'_k & \text{, for } n = 0 \end{cases} \tag{4}$$

where $y^{(n)}_j$ refers to the jth component of the output after step n. The matrix that describes the set of derivatives appearing in Eq. (2) is called the Jacobian of the model, determined with respect to model input perturbations. Since Eq. (2) is linear in the perturbation quantities it is generally referred to as *tangent linear model.*

In analogy to Eq. (1), an approximation to the perturbation of the cost function with respect to model input perturbations is given by

$$J' = \sum_j \frac{\partial J}{\partial x_j} x'_j \,. \tag{5}$$

Application of the chain rule of elementary calculus for $J = J(\mathbf{y}) = J[G(\mathbf{x})]$ yields a linear relationship comparable to Eq. (2):

$$\frac{\partial J}{\partial x_j} = \sum_k \frac{\partial y_k}{\partial x_j} \frac{\partial J}{\partial y_k} \,. \tag{6}$$

The reversal of the subscripts j, k in Eq. (6) indicates that the Jacobian matrix in Eq. (2) has been replaced by its transpose, or in more general mathematical terms by its adjoint. Equation (6) is therefore called the *adjoint model* corresponding to Eq. (2). Returning to the sequential formulation of the tangent linear model, the adjoint of the sequence of operators in Eq. (4) is by definition the sequence of the adjoint operators, taken in reverse order. In particular, if G represents the range marching solution algorithm of the propagation model and the operators C_n describe a succession of elementary range step integrations, the corresponding adjoint integration is always performed backwards in range.

2. Modular graph approach

2.1. *General concept*

The so-called modular graph is a process and data flow diagram which describes the underlying acoustic model. It consists of a complete set of inter-connected modules M, where the input of each module M_n is provided by the output of its predecessors $M_{p,p<n}$ (Fig. 1). In general, the first module M_1 provides the propagation model with the initial data and as such has no formal input variables x_k whereas the last module simply calculates the cost function J and has no other output variables y_j. There are no restrictions as to the size of each module; from a practical point of view

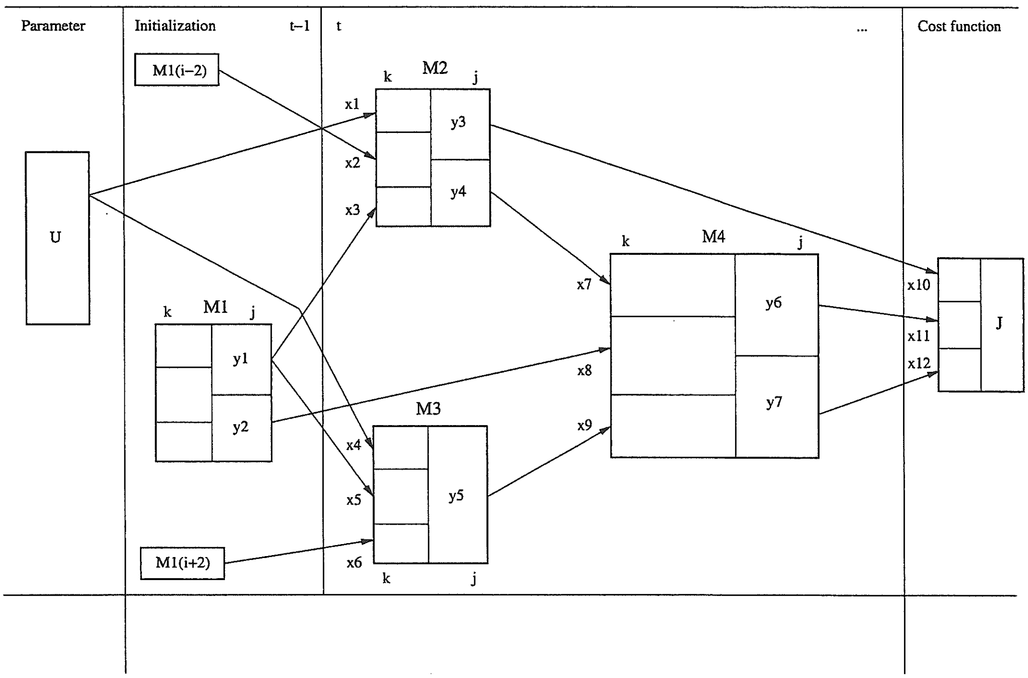

Figure 1. Modular graph: Direct model. For each module M_n the input and output variables are denoted by x_k and y_j, respectively.

the decomposition may depend on the module semantic. Each module represents one or more differentiable functions f_j, which may be simple functions or complex ones represented in turn by a sub-graph. Especially, modifying the model or the cost function at any time is straightforward due to the modular graph structure. If the underlying model is properly decomposed by the user into a number of differentiable modules M, the modular graph methodology presents a convenient way to generate the adjoint by encoding the local Jacobian and backpropagating the result to the preceding modules.

2.2. *Lagrangian formalism*

For the derivation of the reverse adjoint calculation scheme using Lagrangian formalism $\mathcal{M}, \mathcal{I}, \mathcal{O}$, and $\mathcal{P}$ shall denote in the following the complete sets of indices of all modules, module input variables, module output variables and module parameters of the system, respectively. One can then define three mappings

$$\begin{aligned} X : \mathcal{I} \to \ & \mathcal{M} \\ k \mapsto \ & X(k)\,, \end{aligned} \tag{7}$$

$$\begin{aligned} Y : \mathcal{O} \to \ & \mathcal{M} \\ j \mapsto \ & Y(j)\,, \end{aligned} \tag{8}$$

$$\begin{aligned} W : \mathcal{P} \to \ & \mathcal{M} \\ i \mapsto \ & W(i)\,, \end{aligned} \tag{9}$$

where $X(k)$ represents the index of the module for which k is the index of one of its input variables, $Y(j)$ the index of the module for which j is the index of one of its output variables, and $W(i)$ returns the corresponding index of the module for which i is the index of one of the module parameters. With these definitions the module M_n can be formally defined as

$$\forall j \in Y^{-1}(n)\,,\ y_j = f_j\left((x_k)_{k \in X^{-1}(n)}, (w_i)_{i \in W^{-1}(n)}\right)\,. \tag{10}$$

This is the formal statement of the constraint that each output variable y_j of a given module M_n be defined as a function f_j of the input variables $(x_k)_{k \in X^{-1}(n)}$ and the parameters $(w_i)_{i \in W^{-1}(n)}$ of that module. At the same time each input variable x_k of the module M_n is required to emanate from one and only one output variable of a preceding module $M_{l,\, l<n}$. This can be formally expressed as

$$\forall k \in X^{-1}(n)\,,\ x_k = y_{\phi(k)} \tag{11}$$

$$\text{with} \qquad \phi(k) \in \bigcup_{p=0}^{n-1} Y^{-1}(p)\,. \tag{12}$$

The Lagrangian $\mathcal{L}$ of the system can then be defined as the cost function J measuring the fit between the model result and the observations subject to the two constraints formulated in Eqs. (10) and (11)–(12)

$$\mathcal{L} = J - \sum_{j\in\mathcal{O}} \alpha_j \left(y_j - f_j\left((x_k)_{k\in X^{-1}(Y(j))}, (w_i)_{i\in W^{-1}(Y(j))}\right)\right) - \sum_{k\in\mathcal{I}} \beta_k \left(x_k - y_{\phi(k)}\right) . \quad (13)$$

The Lagrange multipliers α_j and β_k can thus be obtained via

$$\frac{\partial\mathcal{L}}{\partial y_j} = -\alpha_j + \sum_{k\in\phi^{-1}(j)} \beta_k = 0 \quad (14)$$

and[a]

$$\frac{\partial\mathcal{L}}{\partial x_k} = -\beta_k + \sum_{j\in Y^{-1}(X(k))} \alpha_j \frac{\partial f_j}{\partial x_k} = 0 \quad (15)$$

as

$$\alpha_j = \sum_{k\in\phi^{-1}(j)} \beta_k \quad (16)$$

and[a]

$$\beta_k = \sum_{j\in Y^{-1}(X(k))} \alpha_j \frac{\partial f_j}{\partial x_k} . \quad (17)$$

The reverse calculation (backpropagation) of the Lagrange multipliers via Eqs. (16) and (17) (Fig. 2) is initiated at the last module for which β_k simply reduces to[a]

$$\beta_k = \frac{\partial J}{\partial x_k} . \quad (18)$$

For comparison, the corresponding forward calculation scheme via the tangent linear model is further illustrated in Appendix A. Once all Lagrange multipliers $\{\alpha_j, \beta_k\}$ of the system are computed, the Lagrangian formalism allows the calculation of the local gradient of the cost function J with respect to any given model parameter w_i as

$$\frac{\partial J}{\partial w_i} = \sum_{j\in Y^{-1}(W(i))} \alpha_j \frac{\partial f_j}{\partial w_i} . \quad (19)$$

Based on this reverse modular graph formalism an algorithmic tool can thus facilitate the generation and coding of the adjoint of the complex acoustic propagation model. YAO[2], the tool that is used in this paper further provides several routines to test the validity of the local derivatives of the different modules, the cost function and an automatic validation can also be performed for the tangent linear and the adjoint model. In the past this semi-automatic adjoint approach has

[a] If the index $k \in \mathcal{I}$ belongs to an input variable of the last module (cost function) the derivative reduces to $\frac{\partial\mathcal{L}}{\partial x_k} = \frac{\partial J}{\partial x_k} - \beta_k = 0 \Leftrightarrow \beta_k = \frac{\partial J}{\partial x_k}$.

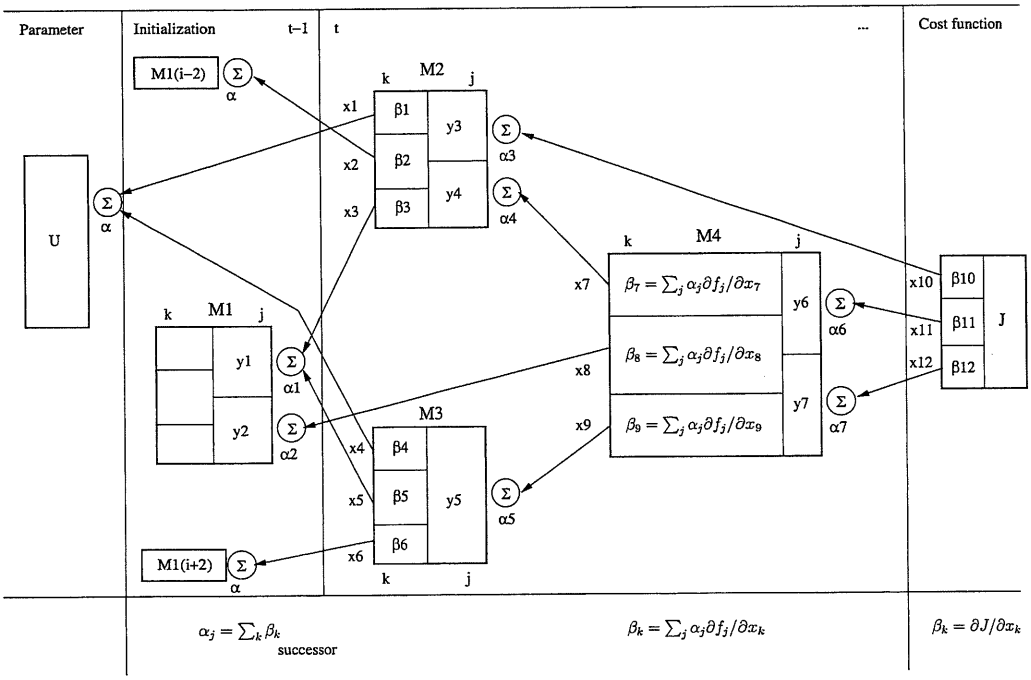

Figure 2. Modular graph: Adjoint model. Illustration of the reverse calculation (backpropagation) of the Lagrange multipliers $\{\alpha_j, \beta_k\}$.

been successfully applied e.g., for multi-dimensional variational data assimilation in meteorological and climate modeling, for variational data assimilation with several models in oceanography (three-dimensional modeling of phytoplankton growth[3,4]) and for land hydrology with the ISBA code of Météo-France[5].

3. Wide-angle PE

In continuation of the analytic optimal control approach introduced in Ref. [6] the propagation model G that is chosen to demonstrate the semi-automatic adjoint approach for ocean acoustic inversion purposes is the wide-angle PE due to Claerbout[7]. For a stratified medium with varying density $\rho(z)$, sound speed $c(z)$ and absorption loss $\alpha(z)$ the wide angle PE model can be summarized as

$$\begin{cases} 2ik_0\left(1+\frac{1}{4}(N^2-1)\right)\frac{\partial\psi}{\partial r}+\rho\frac{\partial}{\partial z}\left(\rho^{-1}\frac{\partial\psi}{\partial z}\right) & \\ +\frac{i}{2k_0}\rho\frac{\partial}{\partial z}\left(\rho^{-1}\frac{\partial^2\psi}{\partial z\partial r}\right)+k_0^2(N^2-1)\psi = 0 & \\ \psi(r,z=0) = 0 & \\ \psi(r=0,z) = S(z) & \\ \text{NLBC} \quad \left[\frac{\partial}{\partial z}-i\beta\right]\psi(z)\Big|_{z=H} = i\beta\sum_j g_{1,j}\psi_j(z)\Big|_{z=H} & \end{cases} \tag{20}$$

where $k_0 = \omega/c_0$ is a reference wavenumber, $N(z) = n(z)[1+i\alpha(z)]$ and $n(z) = c_0/c(z)$ the refractive index, $S(z)$ is an analytical source term and NLBC denotes the nonlocal boundary condition at the bottom. For convenience Yevick and Thomson's original notation for the NLBC [8]

$$\left[\frac{\partial}{\partial z} - i\beta\right] \psi[(L+1)\Delta r, z_b] = i\beta \sum_{j=1}^{L+1} g_{1,j} \psi[(L+1-j)\Delta r, z_b] \tag{21}$$

with the convolution coefficients $g_{1,j}$ and[6]

$$\beta = \frac{\rho_w}{\rho_b} k_0 \sqrt{\frac{(N_b^2 - 1)\left(1 + \frac{1}{4}\nu^2\right) + \nu^2}{\left(1 + \frac{1}{4}\nu^2\right)}}\,, \tag{22}$$

is simplified here by dropping the range coordinate and using $\psi_j(z_b) = \psi[(L + 1 - j)\Delta r, z_b]$. Furthermore $\nu^2 = 4i/k_0 \Delta r$, and the subscripts w and b indicate the water column and bottom, respectively.

The finite difference implementation of the direct problem given in Eq. (20) is an implicit Crank-Nicolson scheme and the NLBC in Eq. (21) is treated as a first order ODE in depth. Integration with respect to the depth z yields the calculation[b] of the field on the boundary ($H = z_b$)

$$\begin{aligned} \psi(H) = &\underbrace{e^{i\beta(1/2\Delta z)}}_{\doteq e_1} \psi(H - 1/2\Delta z) \\ &+ \underbrace{i\, e^{i\beta(1/4\Delta z)} \sin(1/4\,\beta\Delta z)}_{\doteq e_2} \sum_j g_{1,j} \left[\psi_j(H) + \psi_j(H - 1/2\Delta z)\right]. \end{aligned} \tag{23}$$

Following the discretization of the direct WAPE system, the forward model can then be decomposed according to the modular graph concept described in Sec. 2.

3.1. *Modular decomposition*

The resulting modular graph (Fig. 3) is divided into four blocks (a)–(d), each of which can be further subdivided vertically and/or horizontally. Given a finite difference discretization with NZ and NR gridpoints in depth and range respectively

- Space (a) is of the dimension NZx1 and is used to initialize the tridiagonal finite difference matrices (Crank-Nicolson scheme), which are represented by the modules *diaGt* and *diaG* respectively. The sound speed profile, the depth-dependent density and sound attenuation in the water column are represented accordingly by the by modules ρ_w, $c(z)$ and α_w. Furthermore, also the LU decomposition[10] of the finite difference system which is represented by modules *bet* and *gag* is initialized in this space.

[b] A similar treatment of Papadakis' original spectral integral formulation of the NLBC (Neumann to Dirichlet map) is proposed in Eqs. (2.20)–(2.23) in Ref[9].

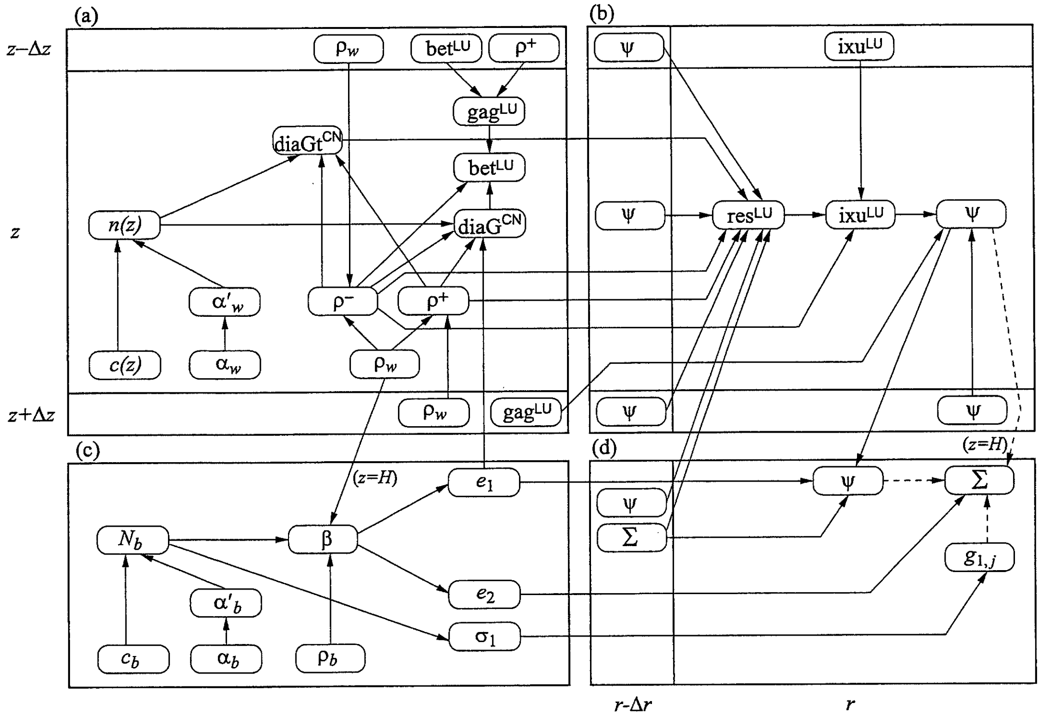

Figure 3. Modular graph representation of the WAPE NLBC model. The nomenclature is consistent with the notation in Sec. 3. Modules with the superscript "LU" or "CN" implement the LU-decomposition[10] and the Crank-Nicolson scheme, respectively. Module "$\sum$" refers to the summation of the boundary-field values in Eq. (23).

- Space (b) is of the dimension NZxNR, and in this space the acoustic field represented by module ψ is calculated by solving the numerical system for each range step r via LU-decomposition (modules res and ixu).
- Space (c) is of the dimension 1x1 and it mainly serves for the initialization of the sediment geoacoustic parameters $\{\rho_b, c_b, \alpha_b\}$ and the calculation of related variables, such as e.g., refractive index N_b and parameters β, e_1, e_2 of the NLBC (Eqs. 21–23).
- Space (d) is of the dimension 1xNR, and is used to calculate the NLBC at the water-sediment interface in order to determine the acoustic field at the bottom (Eq. 23).

Horizontal layering within a block indicates adjacent finite difference depth cells $(z, z{\pm}\Delta z)$ and vertical subdivision represents successive range steps $(r{-}\Delta r, r)$. The dashed arrow further indicates that the module $\sum$ which represents the summation of the boundary-field values in Eq. (23) depends on all the known values (history) of the source modules at previous range steps, not just on the actual value of the current instance.

4. Optimization

With YAO the cost function is calculated automatically from the module that is declared as cost module and from observations that are loaded from an external file. An example of a multiple frequency cost function[c] with two regularization terms is given by

$$
\begin{aligned}
J(\mathbf{x}) &= \sum_{i=1}^{m} \frac{1}{2} \left[(G_i(\mathbf{x}) - \psi_{\mathrm{obs},i})^T R^{-1} (G_i(\mathbf{x}) - \psi_{\mathrm{obs},i}) \right] \\
&\quad + \frac{1}{2} a \, (\mathbf{x} - \mathbf{x}_{\mathrm{apr}})^T B^{-1} (\mathbf{x} - \mathbf{x}_{\mathrm{apr}}) \\
&\quad + \frac{1}{2} b \, || \nabla \mathbf{x} ||^2 , \qquad (24)
\end{aligned}
$$

where the index i denotes different source frequencies and $\psi_{\mathrm{obs},i}$, $i = 1, \ldots, m$ are the corresponding observations at each frequency. The parameter $\mathbf{x}_{\mathrm{apr}}$ is included in the cost function as an *a priori* estimate of the desired solution $\mathbf{x}$, R and B represent the covariance matrices for the field and the control parameter, respectively and (a, b) are the two regularization parameters.

With a cost function specified in Eq. (24) the numerical implementation of the direct model (Sec. 3) can be differentiated using YAO in reverse mode to generate the adjoint code. Equation (19) then allows the computation of the gradient of the cost function with respect to the control variable. A Taylor test ensures that the derivatives generated with the adjoint code agree with the corresponding finite difference approximations for different directions of perturbation of the control variable. Minimization is generally accomplished through the use of standard iterative gradient methods like e.g. conjugate gradient or Newton-type methods[12]. The routine M2QN1, which is used for the optimization process in the following example, is a solver of bound constrained minimization problems and implements a quasi-Newton (BFGS) technique with line-search. As an illustrative test case the numerical adjoint approach is briefly demonstrated for the geoacoustic characterization of a shallow water environment (Fig. 4). The control variable $\mathbf{x}$ is determined in this case by the geoacoustic parameters $\{\rho_b, c_b, \alpha_b\}$ of the sediment.

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[c]An extensive analytic treatment of multiple-frequency adjoint-based inversion of a locally reacting impedance boundary condition for the standard PE can be found in Ref.[11]

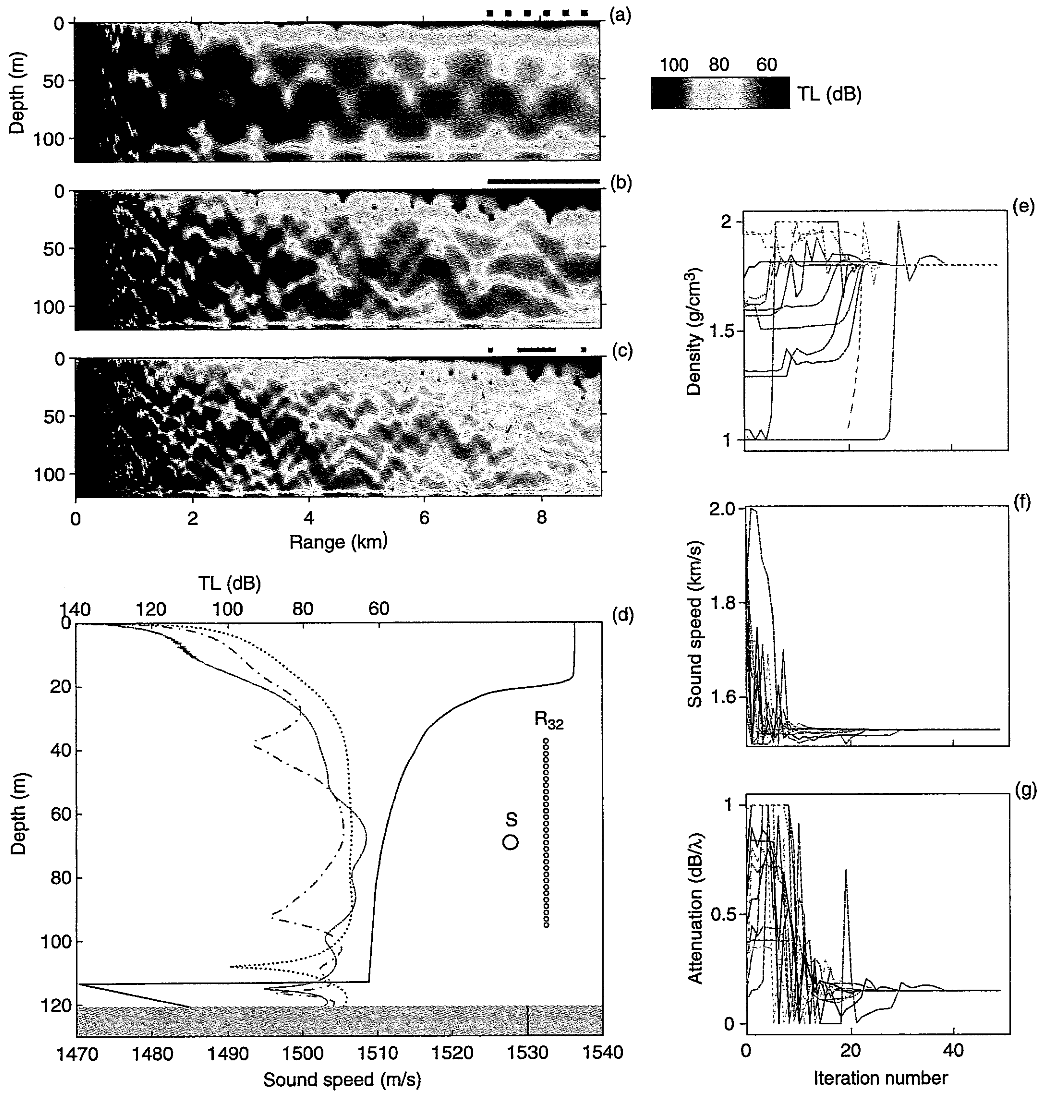

Figure 4. Adjoint-based geoacoustic characterization of a shallow water environment: Acoustic fields for the three source frequencies 200, 400 and 500 Hz (a)–(c); acoustic fields at 9 km range, environmental input data and experimental configuration (d); evolution of the estimated parameters *vs.* iteration number (e)–(g).

Appendix A. Tangent linear model

As a counterpart to the reverse calculation of the Lagrange multipliers in the adjoint model (Fig. 2), the following illustration explains the tangent linear model, which operates forward in the sense that it determines a gradient with respect to output from a gradient with respect to input.

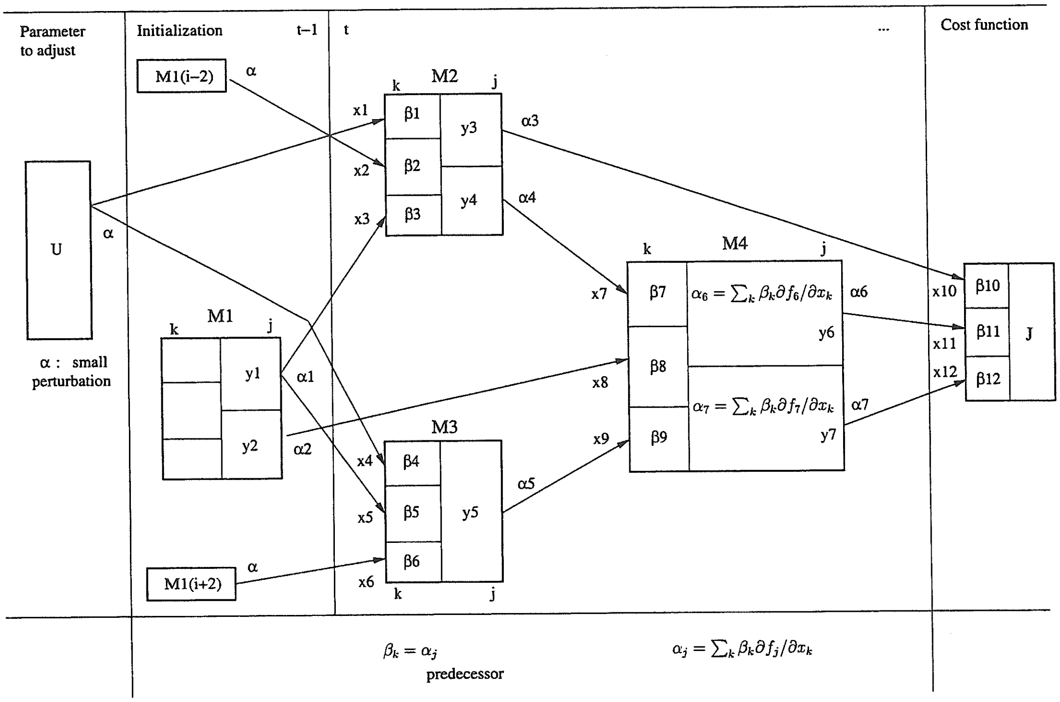

Figure 5. Modular graph: Tangent linear model. Forward calculation of the Lagrange multipliers $\{\alpha_j, \beta_k\}$.

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