Numerical optimization and adjoint state methods for large-scale nonlinear least-squares problems

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Outline

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Numerical optimization for inverse problems in geosciences

Nonlinear least-squares problem

In this presentation, we will consider the inverse problem

$$\min_m f(m) = \frac{1}{2}\|d_{cal}(m) - d_{obs}\|^2$$

where

- d_{obs} are data associated with a physical phenomenon and a measurement protocol: seismic waves, electromagnetic waves, gravimeter, ultrasounds, x-ray,...
- m is the parameter of interest we want to reconstruct: P and S-wave velocities, density, anisotropy parameters, attenuation, or a collection of these parameters
- $d_{cal}(m)$ are synthetic data, computed numerically, often through the solution of partial differential equations
- $f(m)$ is a misfit function which measures the discrepancy between observed and synthetic data

Numerical optimization for inverse problems in geosciences

Nonlinear least-squares problem

In this presentation, we will consider the inverse problem

$$\min_{m} f(m) = \frac{1}{2}\|d_{cal}(m) - d_{obs}\|^2$$

Of course, in joint inversion, we may consider a misfit function as a sum of these functions associated with different measurements: the theory remains the same

Numerical optimization for inverse problems in geosciences

Nonlinear least-squares problem

In this presentation, we will consider the inverse problem

$$\min_m f(m) = \frac{1}{2}\|d_{cal}(m) - d_{obs}\|^2$$

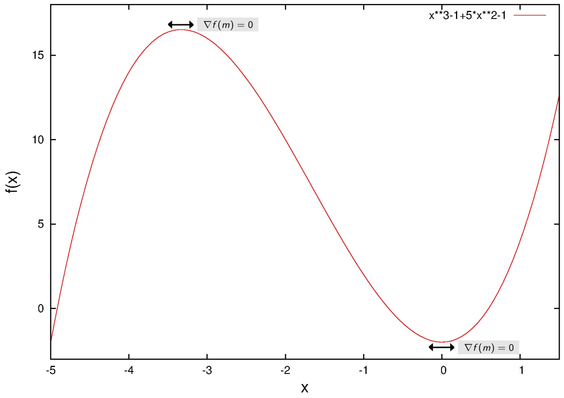
- We will also assume that $f(m)$ is a continuous and twice differentiable function: the gradient is continuous, and the second-order derivatives matrix $H(m)$ (Hessian matrix) is also continuous
- The methods we are going to review are local optimization method: we put aside the global optimization methods and stochastic/genetic algorithms which are unaffordable for large-scale optimization problems
- All the methods we review are presented in (Nocedal and Wright, 2006)

Local methods to find the minimum of a function

Necessary condition

To detect the extremum of a differentiable function $f(m)$, we have the necessary condition

$$\nabla f(m) = 0$$



Local methods to find the minimum of a function

Necessary condition

To detect the extremum of a differentiable function $f(m)$, we have the necessary condition

$$\nabla f(m) = 0$$

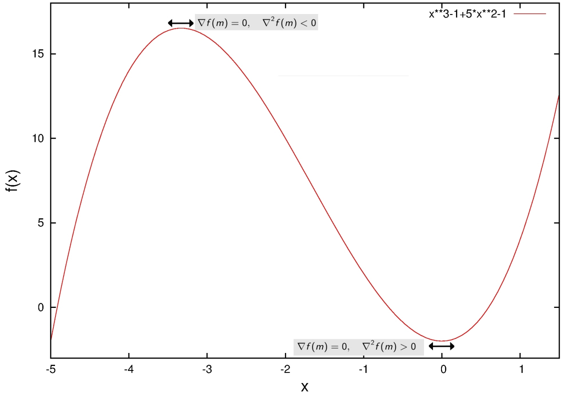
This is not enough: is it a minimum or maximum?

Local methods to find the minimum of a function

Necessary and sufficient conditions

In a local minimum, the function is locally convex: the Hessian is definite positive

$$\nabla f(m) = 0, \quad \nabla^2 f(m) > 0$$



Local methods to find the minimum of a function

Practical implementation

However, this not what we implement in practice. From an initial guess m_0, a sequence m_k is built such that

- the limit m_* should satisfy the necessary condition

$$\nabla f(m_*) = 0$$

- at each iteration

$$f(m_{k+1}) < f(m_k)$$

We have to guarantee the decrease of the misfit function at each iteration

Outline

How to find the zero of the gradient: first-order method

The fixed-point method

We want to find m_* such that

$$\nabla f(m_*) = 0 \qquad (1)$$

The simplest method is to apply the fixed point iteration on $I - \alpha \nabla f$

$$m_{k+1} = (I - \alpha \nabla f) m_k = m_k - \alpha \nabla f(m_k), \quad \alpha \in \mathbb{R}_*^+$$

At convergence we should have

$$m_* = (I - \alpha \nabla f) m_* = m_* - \alpha \nabla f(m_*) \implies \nabla f(m_*) = 0$$

How to find the zero of the gradient: first-order method

Ensuring the decrease of the misfit function

We need to ensure

$$f(m_{k+1}) < f(m_k)$$

We have

$$f(m+dm) = f(m) + \nabla f(m)^T dm + o(||dm||^2)$$

Therefore, if

$$m_{k+1} = m_k - \alpha \nabla f(m_k),$$

we have

$$f(m_{k+1}) = f(m_k - \alpha \nabla f(m_k)) = f(m_k) - \alpha \nabla f(m_k)^T \nabla f(m_k) + \alpha^2 o(||\nabla f(m_k)\|^2$$

that is

$$f(m_{k+1}) = f(m_k) - \alpha ||\nabla f(m_k)^T||^2 + \alpha^2 o(||\nabla f(m_k)\|^2$$

Therefore for α small enough, we can ensure the decrease condition

How to find the zero of the gradient: first-order method

Fixed point on $I - \alpha F$ = steepest-descent method

To summarize, using the fixed-point iteration on $I - \alpha \nabla f(m)$ yields the sequence

$$m_{k+1} = m_k - \alpha \nabla f(m_k),$$

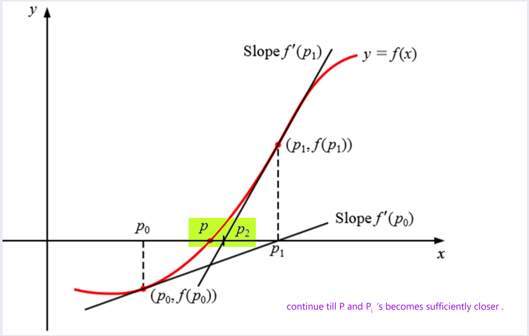
We have just rediscovered the steepest-decent iteration

Outline

How to find the zero of the gradient: second-order method

Newton method: graphical interpretation

A faster (quadratic) convergence can be achieved for finding the zero $\nabla f(m)$ if we use the Newton method.



How to find the zero of the gradient: second-order method

Newton method

We approximate $\nabla f(m_{k+1})$ as its first-order Taylor development m_k

$$\nabla f(m_{k+1}) \simeq \nabla f(m_k) + \left(\frac{\partial \nabla f(m_k)}{\partial m_k}\right)(m_{k+1} - m_k) \tag{1}$$

We look for the zero of this approximation

$$\nabla f(m_k) + \left(\frac{\partial \nabla f(m_k)}{\partial m_k}\right)(m_{k+1} - m_k) = 0 \tag{2}$$

which yields

$$m_{k+1} = m_k - \left(\frac{\partial \nabla f(m_k)}{\partial m_k}\right)^{-1} \nabla f(m_k)$$

How to find the zero of the gradient: second-order method

Notations

In the following, we use the notation

$$\frac{\partial \nabla f(m_k)}{\partial m_k} = H(m_k) \quad (1)$$

for the Hessian operator (second-order derivatives of the misfit function).

How to find the zero of the gradient: second-order method

Decrease of the misfit function

Do we ensure the decrease of the misfit function?

$$\begin{array}{rcl} f(m_{k+1}) & = & f(m_k - \alpha_k H(m_k)^{-1} \nabla f(m_k)) \\ & = & f(m_k) - \alpha_k \nabla f(m_k)^T H(m_k)^{-1} \nabla f(m_k) + \alpha_k^2 o(||H(m_k)^{-1} \nabla f(m_k)\|^2 \end{array}$$

We have

$$\nabla f(m_k)^T H(m_k)^{-1} \nabla f(m_k) > 0 \tag{1}$$

if and only if $H(m_k)^{-1} > 0$.

How to find the zero of the gradient: second-order method

Difficulties

- The Hessian operator may not be necessary strictly positive: the function $f(m)$ may not be strictly convex as the forward problem is nonlinear ($f(m)$ is not quadratic)
- For large-scale application, how to compute $H(m)$ and its inverse $H(m^{-1})$?

Outline

The l-BFGS method

Principle

l-BFGS method (Nocedal, 1980) relies on the iterative scheme

$$m_{k+1} = m_k - \alpha_k Q_k \nabla f(m_k) \quad (1)$$

where

$$Q_k \simeq H(m_k)^{-1}, \mathrm{sym} > 0 \quad (2)$$

and

$$\alpha_k \in \mathbb{R}_*^+ \quad (3)$$

is a scalar parameter computed through a linesearch process

The l-BFGS method

l-BFGS approximation

The l-BFGS approximation consists in defining Q_k as

$$\begin{array}{rcl} Q_k & = & \left(V_{k-1}^T \dots V_{k-l}^T\right) Q_k^0 \left(V_{k-l} \dots V_{k-1}\right) \\ & & +\rho_{k-l} \left(V_{k-1}^T \dots V_{k-l+1}^T\right) s_{k-l} s_{k-l}^T \left(V_{k-l+1} \dots V_{k-1}\right) \\ & & +\rho_{k-l+1} \left(V_{k-1}^T \dots V_{k-l+2}^T\right) s_{k-l+1} s_{k-l+1}^T \left(V_{k-l+2} \dots V_{k-1}\right) \\ & & + \dots \\ & & +\rho_{k-1} s_{k-1} s_{k-1}^T, \end{array} \tag{1}$$

where the pairs s_k, y_k are

$$s_k = m_{k+1} - m_k, \quad y_k = \nabla f(m_{k+1}) - \nabla f(m_k), \tag{2}$$

the scalar ρ_k are

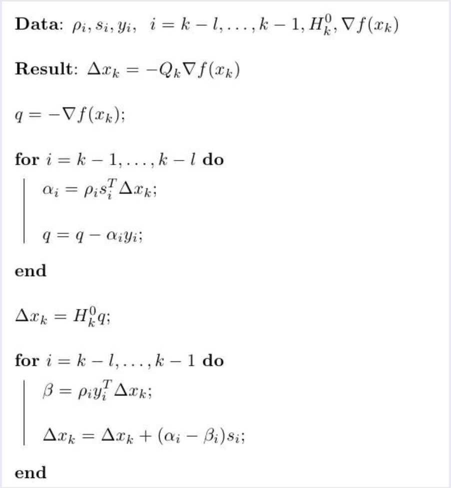
$$\rho_k = \frac{1}{y_k^T s_k}, \tag{3}$$

and the matrices V_k are defined by

$$V_k = I - \rho_k y_k s_k^T. \tag{4}$$

The *l*-BFGS method

Implementation: two-loops recursion



```
**Data**: $\rho_i, s_i, y_i, \;\; i = k-l, \dots, k-1, H_k^0, \nabla f(x_k)$
**Result**: $\Delta x_k = -Q_k \nabla f(x_k)$
$q = -\nabla f(x_k);$
**for** $i = k-1, \dots, k-l$ **do**
    $\alpha_i = \rho_i s_i^T \Delta x_k;$
    $q = q - \alpha_i y_i;$
**end**
$\Delta x_k = H_k^0 q;$
**for** $i = k-l, \dots, k-1$ **do**
    $\beta = \rho_i y_i^T \Delta x_k;$
    $\Delta x_k = \Delta x_k + (\alpha_i - \beta_i) s_i;$
**end**
```

Truncated Newton method

Principle

The truncated Newton method (Nash, 2000) relies on the iterative scheme

$$m_{k+1} = m_k + \alpha_k \Delta m_k \tag{1}$$

where Δm_k is computed as an approximate solution of the linear system

$$H(m_k)\Delta m_k = -\nabla f(m_k) \tag{2}$$

Truncated Newton method

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$$m_{k+1} = m_k + \alpha_k \Delta m_k \tag{1}$$

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Implementation

- A matrix-free conjugate gradient is used to solve this linear system (Saad, 2003)
- This only requires the capability to compute matrix-vector products $H(m_k)v$ for given vectors v: the full Hessian matrix needs not to be formed explicitly
- The resulting approximation of the Hessian only accounts for positive eigenvalues of $H(m_k)$: Δm_k is ensured to be a descent direction

Outline

Conjugate gradient

Conjugate gradient for symmetric positive linear systems

The conjugate gradient is an iterative method for the solution of symmetric positive definite linear systems

$$Am = b \tag{3}$$

The method enjoys several interesting properties

- Convergence in at most n iterations for a system of size n (ok)
- Fast convergence rate possible depending on the eigenvalues distribution of A: in practice, an acceptable approximation of the solution can be obtained in k iterations with $k << n$

Conjugate gradient

Only matrix-vector products to perform

Implementation

```
**Data**: $m_0, \varepsilon$
**Result**: $A^{-1}b$
$r_0 = Am_0 - b$;
$\Delta m_0 = -r_0$;
$k = 0$;
**while** $||r_k|| > \varepsilon$ **do**
    Compute $A\Delta m_k$;
    $\alpha_k = \frac{r_k^T r_k}{\Delta m_k^T A \Delta m_k}$;
    $m_{k+1} = m_k + \alpha_k \Delta m_k$;
    $r_{k+1} = r_k + \alpha_k A \Delta m_k$;
    $\beta_{k+1} = \frac{r_{k+1}^T r_{k+1}}{r_k^T r_k}$;
    $\Delta m_{k+1} = -r_{k+1} + \beta_{k+1} \Delta m_k$;
    $k = k + 1$;
**end**
```

Algorithm 1: Conjugate gradient for linear symmetric positive definite systems

Conjugate gradient

Nonlinear conjugate gradient

How to extend the conjugate gradient for the solution of nonlinear minimization problems? There is a link: solving

$$Am = b \tag{3}$$

where A is symmetric positive definite is equivalent to solve

$$\min_m f(m) = m^T Am - m^T b \tag{4}$$

because

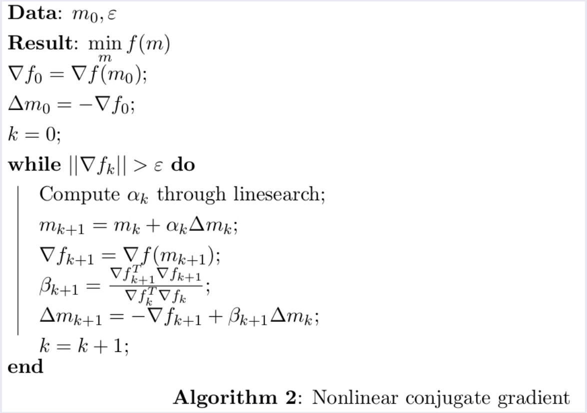
$$\nabla f(m) = Am - b \tag{5}$$

and f is strictly convex (a single extremum which is a minimum)

Conjugate gradient

Implementation

Simply replace r in the preceding algorithm by $\nabla f(m)$



```
**Data**: $m_0, \varepsilon$
**Result**: $\min_m f(m)$
$\nabla f_0 = \nabla f(m_0)$;
$\Delta m_0 = -\nabla f_0$;
$k = 0$;
**while** $||\nabla f_k|| > \varepsilon$ **do**
    Compute $\alpha_k$ through linesearch;
    $m_{k+1} = m_k + \alpha_k \Delta m_k$;
    $\nabla f_{k+1} = \nabla f(m_{k+1})$;
    $\beta_{k+1} = \frac{\nabla f_{k+1}^T \nabla f_{k+1}}{\nabla f_k^T \nabla f_k}$;
    $\Delta m_{k+1} = -\nabla f_{k+1} + \beta_{k+1} \Delta m_k$;
    $k = k + 1$;
**end**
```

Algorithm 2: Nonlinear conjugate gradient

Outline

Summary

An iterative scheme for local optimization

We have seen 4 different methods all based on the same iterative scheme

$$m_{k+1} = m_k + \alpha_k \Delta m_k \tag{3}$$

Summary

An iterative scheme for local optimization

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$$m_{k+1} = m_k + \alpha_k \Delta m_k \tag{3}$$

Nonlinear optimization methods

The four method only differ in the way to compute Δm_k

Steepest descent	$\Delta m_k = -\nabla f(m_k)$
Nonlinear CG	$\Delta m_k = -\nabla f(m_k) + \beta_k \Delta m_{k-1}$
l-**BFGS**	$\Delta m_k = -Q_k \nabla f(m_k), \quad Q_k \simeq H_k^{-1}$
Truncated Newton	$H(m_k)\Delta m_k = -\nabla f(m_k)$ (solved with CG)

Summary

Large-scale applications

From this quick overview we see that the two key quantities to be estimated for the solution of

$$\min_m f(m) = \frac{1}{2}\|d_{cal}(m) - d_{obs}\|^2 \qquad (3)$$

are

- The gradient of the misfit function $\nabla f(m)$
- Hessian vector products $H(m)v$ for a given v (only for the truncated Newton method)

We shall see in the next part how to compute it at a reasonable computational cost (memory imprint and flops) for large-scale applications using adjoint state methods

Outline

Outline

Gradient computation of a nonlinear least-squares function

Framework

We consider the problem

$$\min_m f(m) = \frac{1}{2}\|d_{cal}(m) - d_{obs}\|^2$$

Gradient computation of a nonlinear least-squares function

For a perturbation *dm* we have

$$\begin{aligned} f(m+dm) &= \frac{1}{2}\|d_{cal}(m+dm) - d_{obs}\|^2 \\ & \frac{1}{2}\|d_{cal}(m) - d_{obs} + J(m)dm + o(\|dm\|^2)\|^2 \end{aligned}$$

where

$$J(m) = \frac{\partial d_{cal}}{\partial m}$$

is the Jacobian matrix

Gradient computation of a nonlinear least-squares function

For a perturbation dm we have

$$\begin{array}{rcl} f(m+dm) & = & \frac{1}{2}\|d_{cal}(m+dm)-d_{obs}\|^2 \\ & & \frac{1}{2}\|d_{cal}(m)-d_{obs}+J(m)dm+o(\|dm\|^2)\|^2 \end{array}$$

where

$$J(m)=\frac{\partial d_{cal}}{\partial m}$$

is the Jacobian matrix

$$\begin{array}{rcl} f(m+dm) & = & \frac{1}{2}\|d_{cal}(m)-d_{obs}\|^2+(d_{cal}-d_{obs},J(m)dm)+o(\|dm\|^2) \\ & & \frac{1}{2}\|d_{cal}(m)-d_{obs}\|^2+\left(J(m)^T\left(d_{cal}-d_{obs}\right),dm\right)+o(\|dm\|^2) \end{array}$$

Gradient computation of a nonlinear least-squares function

For a perturbation *dm* we have

$$\begin{array}{rcl} f(m+dm) & = & \frac{1}{2}\|d_{cal}(m+dm)-d_{obs}\|^2 \\ & & \frac{1}{2}\|d_{cal}(m)-d_{obs}+J(m)dm+o(\|dm\|^2)\|^2 \end{array}$$

where

$$J(m)=\frac{\partial d_{cal}}{\partial m}$$

is the Jacobian matrix

$$\begin{array}{rcl} f(m+dm) & = & \frac{1}{2}\|d_{cal}(m)-d_{obs}\|^2+(d_{cal}-d_{obs},J(m)dm)+o(\|dm\|^2) \\ & & \frac{1}{2}\|d_{cal}(m)-d_{obs}\|^2+\left(J(m)^T\left(d_{cal}-d_{obs}\right),dm\right)+o(\|dm\|^2) \end{array}$$

Therefore

$$f(m+dm)-f(m)=\left(J(m)^T\left(d_{cal}-d_{obs}\right),dm\right)+o(\|dm\|^2)$$

Gradient computation of a nonlinear least-squares function

For a perturbation *dm* we have

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Therefore

$$f(m+dm)-f(m)=\left(J(m)^T(d_{cal}-d_{obs}),dm\right)+o(\|dm\|^2)$$

$$\nabla f(m)=J(m)^T(d_{cal}-d_{obs})$$

Gradient computation of a nonlinear least-squares function

Implementation for large-scale applications

- The size of $J(m)$ can be problematic for large scale applications
- After discretization it is a matrix with N rows and M columns where
  1. N is the number of discrete data
  2. M is the number of discrete model parameters
- For Full Waveform Inversion for instance, we can have approximately

$$N \simeq 10^{10}, \quad M \simeq 10^{9}$$

- This prevents from
  1. Computing $J(m)$ at each iteration of the inversion
  2. Storing $J(m)$ (or on disk but then expensive I/O and the performance severely decreases)

Gradient computation of a nonlinear least-squares function

Can we avoid computing the Jacobian matrix?

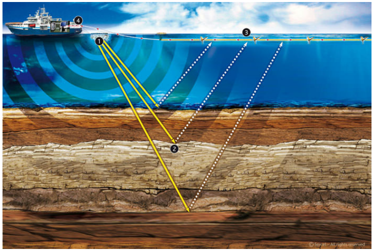
Yes, using adjoint state methods

Outline

First-order adjoint state method

Specializing the forward problem

- Now the problem is specialized such that
$$d_{cal}(m) = Ru(m)$$
where $u(m)$ satisfies
$$A(m, \partial_x, \partial_y, \partial_z)u = s,$$
- u is the solution of the PDE (wavefield for instance) in all the volume
- R is an extraction operator as, most of the time, only partial measurements are available



First-order adjoint state method

References

- Adjoint state method come from optimal control theory and preliminary work of (Lions, 1968)
- It has been first applied to seismic imaging by (Chavent, 1974)
- A nice review of its application in this field has been proposed by (Plessix, 2006)

First-order adjoint state method

The Lagrangian function

From constrained optimization, we introduce the function

$$L(m, u, \lambda) = \frac{1}{2}\|Ru - d\|^2 + (A(m, \partial_x, \partial_y, \partial_z)u - s, \lambda)$$

First-order adjoint state method

The Lagrangian function

From constrained optimization, we introduce the function

$$L(m,u,\lambda)=\frac{1}{2}\|Ru-d\|^2+(A(m,\partial_x,\partial_y,\partial_z)u-s,\lambda)$$

Link with the misfit function

Let $\overline{u}(m)$ be the solution of the forward problem for a given m, then

$$L(m,\overline{u}(m),\lambda)=\frac{1}{2}\|R\overline{u}(m)-d\|^2=f(m)$$

First-order adjoint state method

The Lagrangian function

From constrained optimization, we introduce the function

$$L(m,u,\lambda)=\frac{1}{2}\|Ru-d\|^2+(A(m,\partial_x,\partial_y,\partial_z)u-s,\lambda)$$

Link with the misfit function

Let $\overline{u}(m)$ be the solution of the forward problem for a given m, then

$$L(m,\overline{u}(m),\lambda)=\frac{1}{2}\|R\overline{u}(m)-d\|^2=f(m)$$

Link with the gradient of the misfit function

Therefore

$$\frac{\partial L(m,\overline{u}(m),\lambda)}{\partial m}=\nabla f(m)$$

First-order adjoint state method

Expending

This means that

$$\left(\frac{\partial A(m,\partial_x,\partial_y,\partial_z)}{\partial m}\overline{u}(m),\lambda\right)+\frac{\partial L(m,\overline{u}(m),\lambda)}{\partial u}\frac{\partial \overline{u}(m)}{\partial m}=\nabla f(m)$$

First-order adjoint state method

Expending

This means that

$$\left(\frac{\partial A(m,\partial_x,\partial_y,\partial_z)}{\partial m}\overline{u}(m),\lambda\right)+\frac{\partial L(m,\overline{u}(m),\lambda)}{\partial u}\frac{\partial\overline{u}(m)}{\partial m}=\nabla f(m)$$

Potential simplification

Therefore, if we define $\overline{\lambda}(m)$ such that

$$\frac{\partial L\left(m,\overline{u}(m),\overline{\lambda}(m)\right)}{\partial u}=0$$

we have

$$\left(\frac{\partial A(m,\partial_x,\partial_y,\partial_z)}{\partial m}\overline{u}(m),\overline{\lambda}(m)\right)=\nabla f(m)$$

First-order adjoint state method

Adjoint state formula

What does mean

$$\frac{\partial L\left(m, \overline{u}(m), \overline{\lambda}(m)\right)}{\partial u} = 0?$$

First-order adjoint state method

Consider a perturbation du. We have

$$\begin{array}{rcl} L(m,u+du,\lambda) & = & \frac{1}{2}\|Ru-d_{obs}+Rdu\|^2+(A(m)u-s+A(m)du,\lambda) \\ & = & \frac{1}{2}\|Ru-d_{obs}\|^2+(Ru-d_{obs},Rdu)+(A(m)u-s,,\lambda) \\ & & +(A(m)du,\lambda)+o(\|du\|^2) \\ & = & L(m,u,\lambda)+\left(R^T(Ru-d_{obs}),du\right) \\ & & +\left(du,A(m)^T\lambda\right)+o(\|du\|^2) \\ & = & L(m,u,\lambda)+\left(A(m)^T\lambda+R^T(Ru-d_{obs}),du\right)+o(\|du\|^2) \end{array}$$

First-order adjoint state method

Consider a perturbation du. We have

$$\begin{array}{rcl} L(m, u+du, \lambda) & = & \frac{1}{2}\|Ru - d_{obs} + Rdu\|^2 + (A(m)u - s + A(m)du, \lambda) \\ & = & \frac{1}{2}\|Ru - d_{obs}\|^2 + (Ru - d_{obs}, Rdu) + (A(m)u - s, , \lambda) \\ & & + (A(m)du, \lambda) + o(\|du\|^2) \\ & = & L(m, u, \lambda) + \left(R^T(Ru - d_{obs}), du\right) \\ & & + \left(du, A(m)^T \lambda\right) + o(\|du\|^2) \\ & = & L(m, u, \lambda) + \left(A(m)^T \lambda + R^T(Ru - d_{obs}), du\right) + o(\|du\|^2) \end{array}$$

Therefore

$$\frac{\partial L\left(m, \overline{u}(m), \overline{\lambda}(m)\right)}{\partial u} = A(m)^T \lambda + R^T(Ru - d_{obs})$$

First-order adjoint state method

Adjoint state equation

Remember we are looking for $\overline{\lambda}(m)$ such that

$$\frac{\partial L\left(m, \overline{u}(m), \overline{\lambda}(m)\right)}{\partial u} = 0$$

This simply means that $\overline{\lambda}(m)$ should be the solution of the adjoint PDE

$$A(m)^T \lambda + R^T (R\overline{u}(m) - d_{obs}) = 0$$

First-order adjoint state method

Adjoint state equation

Remember we are looking for $\overline{\lambda}(m)$ such that

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$$A(m)^T \lambda + R^T(R\overline{u}(m) - d_{obs}) = 0$$

Self-adjoint case

- In some cases, the forward problem is self adjoint, and the adjoint state $\overline{\lambda}(m)$ is the solution of the same equation than $\overline{u}(m)$ except that the source term is different
- In addition, the source term implies $\overline{u}(m)$ has been computed before hand, as it depends on this field

First-order adjoint state method

Summary

- We have seen that we can compute the gradient of the misfit function following the formula

$$\nabla f(m) = \left(\frac{\partial A(m, \partial_x, \partial_y, \partial_z)}{\partial m} \overline{u}(m), \overline{\lambda}(m) \right)$$

where $\overline{u}(m)$ satisfies

$$A(m, \partial_x, \partial_y, \partial_z) u = s,$$

and $\overline{\lambda}(m)$ satisfies

$$A(m, \partial_x, \partial_y, \partial_z)^T \lambda + R^T (R\overline{u}(m) - d_{obs}) = 0$$

First-order adjoint state method

Implementation issues

What are the benefits of the adjoint-state approach?

To compute the gradient, we first have to compute $\overline{u}(m)$: first PDE solve

Then we compute $\overline{\lambda}(m)$: second PDE solve

Finally we form the gradient through the formula

$$\nabla f(m) = \left(\frac{\partial A(m, \partial_x, \partial_y, \partial_z)}{\partial m} \overline{u}(m), \overline{\lambda}(m) \right)$$

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The Jacobian matrix has never to be formed nor stored explicitly!

Outline

Second-order adjoint state method

Computing Hessian-vector product

We have seen that in the particular case of the truncated Newton method, it is required to know how to compute, for any v, the Hessian-matrix product

$$H(m)v,$$

However, as it is the case for the Jacobian matrix $J(m)$ the size of matrix $H(m)$ for large-scale application is such that it cannot be computed explicitly nor stored

Again, the adjoint-state method should allow us to overcome this difficulty see (Fichtner and Trampert, 2011; Epanomeritakis et al., 2008; Métivier et al., 2013)

Second-order adjoint state method

Principle of the method

Consider the function

$$h_v(m) = (\nabla f(m), v)$$

Second-order adjoint state method

Principle of the method

Consider the function

$$h_v(m) = (\nabla f(m), v)$$

For a perturbation *dm* we have

$$\begin{aligned}
h_v(m+dm) &= (\nabla f(m+dm), v) \\
&= (\nabla f(m) + H(m)dm, v) + o(\|dm\|^2) \\
&= (\nabla f(m), v) + (H(m)dm, v) + o(\|dm\|^2) \\
&= (\nabla f(m), v) + (dm, H(m)v) + o(\|dm\|^2) \\
&= h_v(m) + (dm, H(m)v) + o(\|dm\|^2)
\end{aligned}$$

Second-order adjoint state method

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Hv through the gradient of h_v

Therefore

$$\nabla h_v(m) = H(m)v$$

Second-order adjoint state method

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Hv through the gradient of h_v

Therefore

$$\nabla h_v(m) = H(m)v$$

All we have to do is to apply the previous strategy to the function $h_v(m)$!

Second-order adjoint state method

Consider the new Lagrangian function

$$\begin{array}{rcl} L_v(m,u,\lambda,g,\mu_1,\mu_2,\mu_3) & = & (g,v) + \left(\left(\dfrac{\partial A(m)}{\partial m}u\right)^T \lambda - g, \mu_1\right) + \\ & & (A(m)^T\lambda - R^T(Ru-d),\mu_2) + \\ & & (A(m)u - s, \mu_3) \end{array}$$

Second-order adjoint state method

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For $u = \overline{u}(m), \;\; \lambda = \overline{\lambda}(m), \;\; g = \overline{g}(m)$ respectively solutions of

$$A(m)u = s, \;\; A(m)^T\lambda = R^T(R\overline{u}(m) - d_{obs}), \;\; g(m) = \left(\frac{\partial A(m)}{\partial m}\overline{u}(m)\right)^T \overline{\lambda}(m)$$

we have

$$L_v(m,\overline{u}(m),\overline{\lambda}(m),\overline{g}(m),\mu_1,\mu_2,\mu_3) = h_v(m)$$

Second-order adjoint state method

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For $u = \overline{u}(m), \;\; \lambda = \overline{\lambda}(m), \;\; g = \overline{g}(m)$ respectively solutions of

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we have

$$L_v(m, \overline{u}(m), \overline{\lambda}(m), \overline{g}(m), \mu_1, \mu_2, \mu_3) = h_v(m)$$

Hence

$$\frac{\partial L_v(m, \overline{u}(m), \overline{\lambda}(m), \overline{g}(m), \mu_1, \mu_2, \mu_3)}{\partial m} = \nabla h_v(m) = H(m)v$$

Second-order adjoint state method

Again, we develop the previous expression

$$
\begin{array}{l}
\dfrac{\partial L_v(m,\overline{u}(m),\overline{\lambda}(m),\overline{g}(m),\mu_1,\mu_2,\mu_3)}{\partial m} = \\[2ex]
\qquad \left(\left(\dfrac{\partial^2 A(m)}{\partial m^2}\overline{u}(m)\right)^T \overline{\lambda}(m),\mu_1\right) + \\[2ex]
\qquad \left(\dfrac{\partial A(m)}{\partial m}^T \overline{\lambda}(m),\mu_2\right) + \left(\dfrac{\partial A(m)}{\partial m}\overline{u}(m),\mu_3\right) + \\[2ex]
\qquad \dfrac{\partial L_v(m,\overline{u}(m),\overline{\lambda}(m),\overline{g}(m),\mu_1,\mu_2,\mu_3)}{\partial u}\dfrac{\partial \overline{u}}{\partial m} + \\[2ex]
\qquad \dfrac{\partial L_v(m,\overline{u}(m),\overline{\lambda}(m),\overline{g}(m),\mu_1,\mu_2,\mu_3)}{\partial \lambda}\dfrac{\partial \overline{\lambda}}{\partial m} + \\[2ex]
\qquad \dfrac{\partial L_v(m,\overline{u}(m),\overline{\lambda}(m),\overline{g}(m),\mu_1,\mu_2,\mu_3)}{\partial g}\dfrac{\partial \overline{g}}{\partial m}
\end{array}
$$

Second-order adjoint state method

Now we look for μ_1, μ_2, μ_3 such that

$$\left\{\begin{array}{l} \dfrac{\partial L_v(m, \overline{u}(m), \overline{\lambda}(m), \overline{g}(m), \mu_1, \mu_2, \mu_3)}{\partial u} = 0 \\ \dfrac{\partial L_v(m, \overline{u}(m), \overline{\lambda}(m), \overline{g}(m), \mu_1, \mu_2, \mu_3)}{\partial \lambda} = 0 \\ \dfrac{\partial L_v(m, \overline{u}(m), \overline{\lambda}(m), \overline{g}(m), \mu_1, \mu_2, \mu_3)}{\partial g} = 0 \end{array}\right.$$

Second-order adjoint state method

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\dfrac{\partial L_v(m, \overline{u}(m), \overline{\lambda}(m), \overline{g}(m), \mu_1, \mu_2, \mu_3)}{\partial g} = 0
\end{array}\right.$$

This is equivalent to

$$\left\{\begin{array}{lcl}
\left(\dfrac{\partial A}{\partial m}\mu_1\right)^T \overline{\lambda}(m) + R^T R\mu_2 + A(m)^T \mu_3 & = & 0 \\[2ex]
\left(\dfrac{\partial A}{\partial m}\overline{u}(m)\right)^T \mu_1 + A(m)\mu_2 & = & 0 \\[2ex]
v - \mu_1 & = & 0
\end{array}\right.$$

Second-order adjoint state method

Reorganizing these equations, we find that

$$\left\{\begin{array}{lcl} \mu_1 = v & & \\ A(m)\mu_2 & = & -\left(\frac{\partial A}{\partial m}\overline{u}(m)\right)^T v \\ A(m)^T\mu_3 & = & -\left(\frac{\partial A}{\partial m}v\right)^T\overline{\lambda}(m) + R^T R\mu_2 \end{array}\right.$$

Second-order adjoint state method

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Implementation

- μ_1 is given for free: it is v
- μ_2 is the solution of a forward problem involving a new source term which depends on v and $\overline{u}(m)$
- μ_3 is the solution of an adjoint problem involving a new source term which depends on b, $\overline{\lambda}(m)$ and μ_2

Second-order adjoint state method

Summary

The computation of $H(m)v$ for a given v can be obtained through the formula

$$\begin{aligned} H(m)v \quad = \quad & \left(\left(\frac{\partial^2 A(m)}{\partial m^2} \overline{u}(m) \right)^T \overline{\lambda}(m), \mu_1 \right) + \\ & \left(\frac{\partial A(m)}{\partial m}^T \overline{\lambda}(m), \mu_2 \right) + \left(\frac{\partial A(m)}{\partial m} \overline{u}(m), \mu_3 \right) \end{aligned} \tag{4}$$

Second-order adjoint state method

Summary

The computation of $H(m)v$ for a given v can be obtained through the formula

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where

Forward and adjoint simulations

- $\overline{u}(m)$ is computed as a solution of the forward problem
- $\overline{\lambda}(m)$ is computed as a solution of the adjoint problem
- μ_2 is computed as a solution of the forward problem for a new source term
- μ_3 is computed as a solution of the adjoint problem for a new source term

Outline

Summary

Optimization methods for nonlinear least-squares problems

$$\min_m f(m) = \frac{1}{2}\|d_{cal}(m) - d_{obs}\|^2$$

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An iterative scheme for local optimization

Local optimization methods are all based on the same iterative scheme

$$m_{k+1} = m_k + \alpha_k \Delta m_k \tag{5}$$

Summary

Optimization methods for nonlinear least-squares problems

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An iterative scheme for local optimization

Local optimization methods are all based on the same iterative scheme

$$m_{k+1} = m_k + \alpha_k \Delta m_k \qquad (5)$$

Four Nonlinear optimization methods

The differences come from the computation of Δm_k

	Steepest descent	$\Delta m_k = -\nabla f(m_k)$
	Nonlinear CG	$\Delta m_k = -\nabla f(m_k) + \beta_k \Delta m_{k-1}$
	l-**BFGS**	$\Delta m_k = -Q_k \nabla f(m_k), \quad Q_k \simeq H_k^{-1}$
	Truncated Newton	$H(m_k)\Delta m_k = -\nabla f(m_k)$ (solved with CG)

Summary

Adjoint methods

The gradient can be computed through the first-order adjoint method at the price

- 1 forward modeling
- 1 adjoint modeling

The Hessian-vector product (only required for truncated Newton) can be computed through second-order adjoint method at the price

- 1 additional forward modeling
- 1 additional adjoint modeling

SEISCOPE Toolbox

A set of optimization routines in FORTRAN90

- Optimization routines for differentiable functions
- Steepest-descent, nonlinear conjugate gradient
- l-BFGS, truncated Newton
- Implemented using a reverse communication protocol: the user is in charge for computing gradient and Hessian-vector product

Open-source code available here

`https://seiscope2.obs.ujf-grenoble.fr/SEISCOPE-OPTIMIZATION-TOOLBOX`

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