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SOLVING SOME NON LINEAR PDES INVERSE PROBLEMS USING VARIATIONAL DATA ASSIMILATION

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Abstract: We present a practical technique for calculating adjoint codes arising in variational methods for data assimilation. Our aim is to bring a more to the automatic differentiation in the MatLab langage. It is used to identify the initial condition of the problem governed by a non linear partial differential equation. The cost function gradient's is derived by using the discrete adjoint model. Numerical examples are presented for Kardar-Parisi-Zhang equation using explicit Euler discretisation in time and pseudo-spectral discretisation in the 2D space dimension. The numerical results obtained from the MatLab environment allow us to verify the efficient of this scheme.

Key Words: tangent linear model, adjoint model, pseudo-spectral method, optimal control

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1. Introduction

Data assimilation is a set of mathematical optimization methods that combine information from observation and numerical simulation of a physical system to improve its description [11]. Assimilation methods are in two main families:

- the stochastic methods based on the theory of optimal statistical estimation the most famous is the Kalman filter [10], and
- the variational methods based on optimal control theory [7, 8, 9, 14].

This second class of methods, which we are interested in, requires the calculation of the cost function gradient's for solutions determination. In most cases, the direct calculation of this gradient is difficult. One often uses adjoint models that involve the tangent linear models. The numerical simulation needs to write associated adjoint code. Such code can be generated by automatic differentiation, but it often contains steps that are not necessary and must be $''cleaned''$ before their use [21, 22]. It can be generated manually. This procedure is considered to be too long, expensive, and it is the source of errors. In this work, we developed a very practical technique for calculating adjoint codes. We apply it to an identification problem of the initial condition in a nonlinear system of partial differential equations.

The section 2 of this work is devoted to the formulation of a model problem and the overall presentation of the principle of variational data assimilation. A discrete adjoint method and our approach are presented in section 3. An application of this technique on a nonlinear system of partial differential equations and also the numerical results are presented in the section 4. The section 5 focuses on the conclusion.

2. Problem Formulation

Let Ω be an open set of $\mathbb{R}^2$. We consider the mathematical model where the state $h = h(x, y, t)$ is governed by the following boundary value problem:

$$\begin{cases} \frac{\partial h}{\partial t} + A(h) & = p & \text{in } \Omega\times]0,+\infty[\\ h & = 0 & \text{on } \partial\Omega\times]0,+\infty[\\ h(0) & = H_0 & \text{in } \Omega, \end{cases} \tag{1}$$

where A is an operator that we assumed to be nonlinear, $h(0)$ denotes the initial state, and p is the source function. In general, for to ensure the existence,

uniqueness and positivity of the solution, it is further assumed that the operator A is monotone, that is

$$\langle Ah, h\rangle_{\mathcal{E}} \geq 0, \ \forall h \in \mathcal{E}, \tag{2}$$

where $\langle ., .\rangle_{\mathcal{E}}$ denotes inner product on a functional space $\mathcal{E}$ suitably chosen [4].

This model translates a wide range of physical phenomena including diffusion problems, fluid flow, draining lakes, rivers and others. We focus particularly on the problem of identifying the initial condition H_0. A best estimation of this, results in looking for H_0^* that minimizes, subject to (1), the following cost function

$$J(H_0) = \frac{1}{2}\int_0^T \int_\Theta (\Lambda h(H_0) - h^{obs})^2 + \frac{\lambda}{2}\int_\Omega (H_0 - h^b)^2, \tag{3}$$

where h^{obs} is an observation function defined in an observation domain Θ, h^b denotes a priori the initial condition estimation, λ is a regularization parameter and Λ is an observation operator's that maps the state variable $h(t)$ of the model in an observation space.

More generally, the determination of the solution of (3) requires calculation of its gradient. Frequently, one uses an adjoint model via tangent linear model of the problem (1) called direct problem. This process constitutes the key point of variational assimilation methods. For a good understanding of them, we present a theoretical result which is applied to our problem. The adjoint model allows us to calculate the gradient, and it may be determined in two differences ways [15, 17, 18, 20, 23]:

- to determine the adjoint model from a discrete direct model. It is called discrete adjoint model,
- or to find the adjoint from the continuous direct model and to discretize it. It's known as continuous adjoint model.

However, these two models are not equivalent. Indeed, the use of discrete adjoint in minimizing the functional J gives its gradient while the continuous adjoint can lead to poor approximation of the cost function gradient's. This leads us to choose the discrete adjoint method.

3. Numerical Scheme

We are developing here a discrete model based on computation of a discrete adjoint operator for computing the numerical solution of the problem (3). Furthermore we assume that explicit discretization scheme of the system (1) can

be expressed as follows

$$\begin{cases} \dfrac{S_{k+1}(\underline{u}) - S_k(\underline{u})}{\Delta t} &= F(S_k(\underline{u})), \quad k = 0, ..., M-1 \\ \\ S_0 &= \underline{u}, \end{cases} \tag{4}$$

where $\underline{u}$ is a $\mathbb{R}^N$ vector that is a discrete approximation of the initial state, S_k is an operator on $\mathbb{R}^N$ such that

$$S_k(\underline{u}) = \underline{h}_k \tag{5}$$

is a discrete approximation of the state system at the time t_k. In addition we assume that the applications

$$\underline{u} \longmapsto (S_k(\underline{u})) \text{ and } \underline{u} \longmapsto F(S_k(\underline{u})), \ k = 0, 1, ..., M-1$$

are differentiable. Moreover the discrete functional can be formulated as follows

$$J_N(\underline{u}) = \frac{1}{2}\Delta t \sum_{k=0}^{M-1} \parallel \Lambda_N S_{k+1}(\underline{u}) - \underline{h}_{k+1}^{0bs} \parallel^2 + \frac{\lambda}{2} \parallel \underline{u} - \underline{u}^b \parallel^2, \tag{6}$$

where Λ_N denotes a discrete observation operator, $\underline{h}_{k+1}^{0bs}$ is a observed state vector at time t_{k+1}, $\underline{u}^b$ represents an *a priori* estimation of $\underline{u}$ in the discrete case and $\|\|$ denotes the euclidian norm.

Our aim is to solve the system

$$\nabla J_N(\underline{u}) = 0, \tag{7}$$

where ∇J_N is the gradient of J_N. Next we focus our attention on computing the best expression of ∇J_N. Under differentiability hypothesis we can obtain the following discrete system

$$\begin{cases} \widehat{h}_{k+1} &= \widehat{h}_k + \Delta t \widehat{F}_k.\widehat{h}_k, \quad k = 0, ..., M-1 \\ \\ \widehat{h}_0 &= \widetilde{u} \end{cases} \tag{8}$$

where we have set

$$\widehat{h}_k = \lim_{\xi \to 0} \frac{S_k(\underline{u} + \xi\widetilde{\underline{u}}) - S_k(\underline{u})}{\xi} \quad \text{and} \quad \widehat{F}_k.\widehat{h}_k = \lim_{\xi \to 0} \frac{F(S_k(\underline{u} + \xi\widetilde{\underline{u}})) - F(S_k(\underline{u}))}{\xi} \tag{9}$$

for any perturbation vector $\widetilde{\underline{u}}$. Also it is easy to see that the gradient in the direction $\widetilde{\underline{u}}$ is given by

$$\nabla J_N(\underline{u})[\widetilde{\underline{u}}] = \sum_{k=0}^{M-1} \Delta t \langle \widehat{h}_{k+1}, \Lambda_N^T(\Lambda_N S_{k+1}(\underline{u}) - \underline{h}_{k+1}^{0bs})\rangle + \lambda\langle \widetilde{u}, \underline{u} - \underline{u}^b\rangle, \quad (10)$$

where $\langle .,. \rangle$ denotes euclidian inner product. Using equation (8), we can write

$$\sum_{k=0}^{M-1} \langle \widehat{h}_{k+1}, q_k\rangle = \sum_{k=0}^{M-1} \langle \widehat{h}_k, q_k\rangle + \sum_{k=0}^{M-1} \langle \Delta t \widehat{F}_k.\widehat{h}_k, q_k\rangle, \quad (11)$$

where $(q_k)_{k=0,...,M}$ is a sequence of vectors in $\mathbb{R}^N$. Thus, equation (11) can be rewritten as

$$0 = \sum_{k=0}^{M-1} \langle \widehat{h}_{k+1}, q_k - q_{k+1} - \Delta t \widehat{F}_{k+1}^*.q_{k+1}\rangle - \langle \widetilde{u}, q_0 + \Delta t \widehat{F}_0^*.q_0\rangle + \langle \widehat{h}_M, q_M + \Delta t \widehat{F}_M^*.q_M\rangle, \quad (12)$$

where $\widehat{F}_k^*$ denotes the adjoint of $\widehat{F}_k$. Finally, this leads to a discrete adjoint model that consists in determining a sequence $(q_k)_{k=0,...,M}$ satisfying

$$\begin{cases} \dfrac{q_k - q_{k+1}}{\Delta t} - \widehat{F}_{k+1}^*.q_{k+1} &= \Lambda_N^T(\Lambda_N S_{k+1}(\underline{u}) - \underline{h}_{k+1}^{0bs}), \quad k = 0, ..., M-1 \\ \\ q_M &= 0. \end{cases} \quad (13)$$

Substituting $\Lambda_N^T(\Lambda_N S_{k+1}(\underline{u}) - \underline{h}_{k+1}^{0bs})$ in (10) by its expression to equation (13) and using equation (12), we obtain

$$\nabla J_N(\underline{u}) = \lambda(\underline{u} - \underline{u}^b) + q_0 + \Delta t \widehat{F}_0^*.q_0. \quad (14)$$

From this, we see that the determination of the gradient requires the calculation of the discrete adjoint model (13). In practice, a calculation of adjoint operators can be very tedious. We try in this work to provide some transformations that facilitate the determination of $\widehat{F}_k^*$ and establish a matrix programming in order to reduce iteration loops.

We carry out a practical case to clarify our technique. Moreover we assume that $F(.)$ can be written as

$$F(\underline{h}_k) = L_1\underline{h}_k + Q(\underline{h}_k), \quad (15)$$

where $L_1\underline{h}_k$ and $Q(\underline{h}_k)$ represent respectively its linear and nonlinear parts.

For simplicity, let us also assume that

$$Q(\underline{h}_k) = L_2(h_k).h_k, \tag{16}$$

where $(v, w) \longmapsto L_2(v).w$ is a bilinear application.

Similar operations to those used for determining the linear tangent model are required to calculate the linear tangent operator $\widehat{F}_k$ associated to F. We have

$$\widehat{F}_k.\widehat{h}_k = L_1\widehat{h}_k + L_2(\widehat{h}_k).\underline{h}_k + L_2(\underline{h}_k).\widehat{h}_k, \tag{17}$$

and the following result.

Proposition 3.1. *Let $B = (b_{ij})_{1\leq i,j\leq N}$ be a square matrix of order N and assume that for any vectors $\underline{v}$ and $\underline{w}$ in $\mathbb{R}^N$,*

$$(L_2(\underline{v}).\underline{w})_i = (\sum_{j=1}^{N} b_{ij}\underline{v}_j)\underline{w}_i. \tag{18}$$

Then the adjoint of $\widehat{F}_k$ is given by

$$\widehat{F}_k^*.q_k = L_1^T q_k + diag(\underline{h}_k)B^T q_k + L_2(h_k).q_k \tag{19}$$

In fact, we have

$$\begin{aligned}
\langle \widehat{F}_k.\widehat{h}_k, q_k\rangle &= \langle L_1\widehat{h}_k + L_2(\widehat{h}_k).h_k + L_2(h_k).\widehat{h}_k, q_k\rangle \\
&= \langle L_1\widehat{h}_k, q_k\rangle + \langle L_2(\widehat{h}_k).h_k, q_k\rangle + \langle L_2(h_k).\widehat{h}_k, q_k\rangle \\
&= \langle \widehat{h}_k, L_1^T q_k\rangle + \langle \widehat{h}_k, diag(h_k)B^T q_k\rangle + \langle \widehat{h}_k, L_2(h_k).q_k\rangle \\
&= \langle \widehat{h}_k, L_1^T q_k + diag(h_k)B^T q_k + L_2(h_k).q_k\rangle,
\end{aligned}$$

where $diag(\underline{h}_k)$ is a diagonal matrix whose diagonal elements are components of vector $\underline{h}_k$. □

4. Numerical Simulation

For our numerical simulation we have considered the operator A of the problem (1) defined by

$$A(h) = -\Delta h - a \mid \nabla h \mid^2, \tag{20}$$

where $a \in \mathbb{R}, a \neq 0$. With this operator, the problem (1) is a Cauchy-Direchlet problem for Hamilton-Jacobi equation

$$\frac{\partial h}{\partial t} - \Delta h - a \mid \nabla h \mid^2 = 0 \tag{21}$$

which is called generalized Kardar-Parisi-Zhang (KPZ) equation. It describes certain physics models like the ballistic deposition processes: the evolution of the profile of growing surfaces (such as a flame, a chemical deposit or a tumor) due to a variety of mechanisms [5, 12, 13]. This problem has been intensively studied (see for example [2, 3, 16, 19]). For $a = -1$, Barles and Da Lio [1] prove a strong comparison result that allows to get the existence and the uniqueness of a continuous solution which is defined globally in time.

Considering $a = -1$ and $\Omega =]-1,\ 1[^2$, the problem (1) is approached by using explicit Euler in time and pseudo-spectral in space. therefore we have

$$\frac{S_{k+1}(\underline{u}) - S_k(\underline{u})}{\Delta t} = L_1(S_k(\underline{u})) + Q(S_k(\underline{u})),\ k = 0, ..., M-1, \tag{22}$$

where the linear and non linear parts are given as follows

$$L_1(S_k(\underline{u})) = D_{xx}S_k(\underline{u}) + D_{yy}S_k(\underline{u}) \tag{23}$$

$$Q(S_k(\underline{u})) \quad = \quad -diag(D_xS_k(\underline{u}))D_xS_k(\underline{u}) - diag(D_yS_k(\underline{u}))D_yS_k(\underline{u}) \tag{24}$$

with D_x and D_{xx} (resp. D_y and D_{yy}) are the first and second order differentiation matrices according to variables x (resp. y).

The similar calculations which lead to the system (13) gives the adjoint model

$$\begin{cases} q_k - q_{k+1} - \Delta t[(D_{xx} + D_{yy})^T + 2D_x^T diag(D_xS_{k+1}(\underline{u})) \\ +2D_y^T diag(D_yS_{k+1}(\underline{u}))]q_{k+1} = \Delta t\Lambda_N^T.(\Lambda_N.S_{k+1}(\underline{u}) - U_{k+1}^{obs}) \\ q_M = 0 \end{cases} \tag{25}$$

and, the cost function gradient's becomes

$$\begin{aligned} \nabla_{\underline{u}}J = \lambda(\underline{u} - \underline{u}^b) + q_0 \\ + \Delta t[(D_{xx} + D_{yy})^T - 2D_x^T diag(D_x\underline{u}) - 2D_y^T diag(D_y\underline{u})]q_0. \end{aligned} \tag{26}$$

Our simulation is based on the synthetic experiments, because they help to understand the success of the method. In this end we have considered the interval $[0, 1]$ for the time's variable and the step $\Delta t = 0.0002$.

Gradient Test. Before using the minimization process, we verify, by gradient test [6], if the numerical scheme for computing the gradient is exact. The following relation is established by using the Taylor series of one order.

$$\rho(\xi) = \frac{J(\underline{u} + \xi\widetilde{u}) - J(\underline{u})}{\xi\langle\nabla J(\underline{u}), \widetilde{u}\rangle} \tag{27}$$

where $\widetilde{u}$ denotes a vector in $\mathbb{R}^N$ such that $\| \widetilde{u} \| = 1$. The test consists in seeing, for any direction, if $\lim_{\xi \to 0} \rho(\xi) = 1$. In practice, we try to verify it for some directions. For example, Figure 1 gives us the gradient test for our scheme.

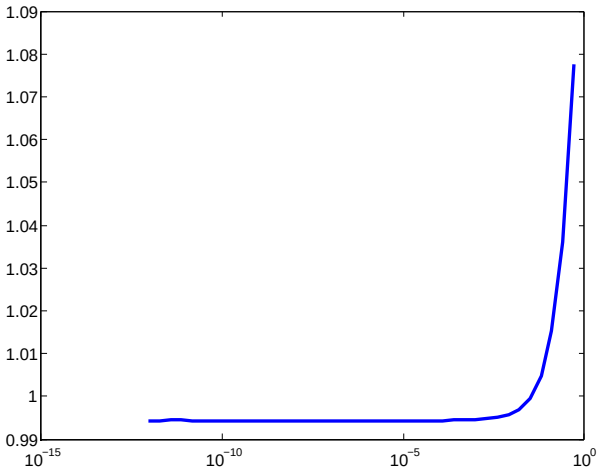


Figure 1: Gradient test with $\xi \to 0$

After this verification, we proceed to estimate the initial condition following four experiments relative to observations types.

1. First experiment is done by taking observations without noisy for all times in each point on a grid of 256 points.

2. For the second experiment we consider observations noisy taken at all times in each point on a grid of 256 points.

3. Third experiment deals with observations without noisy at all times for five grid points chosen on a grid of 256 points.

4. The last one experiment focuses on observations noisy at all times conducted at five points chosen on a grid of 256 points.

The observations are called dense when they are made at all times and on each grid point, otherwise they are not dense.

Figure 2 (a) illustrates the reference initial condition from which the observations are created and the Figure 2 (b) represents the initialization process for minimization.

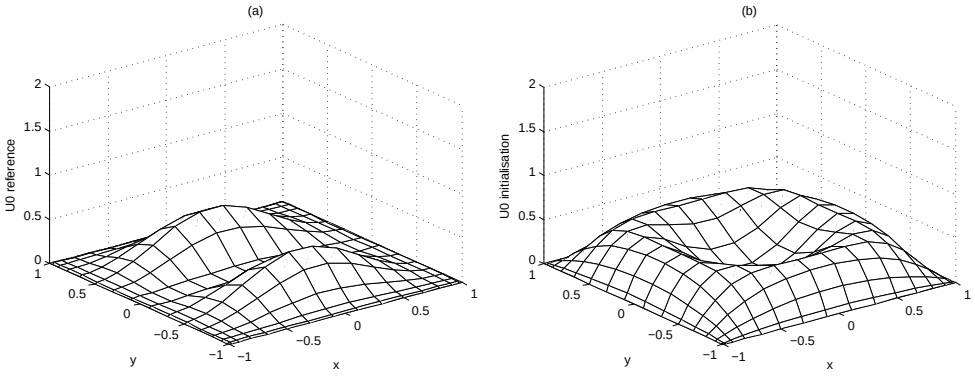


Figure 2: *(a): Initial condition of reference (b): control variable for initialization process*

Simulation of the Cost Function. We discuss the various numerical experiments with the gradient descent method for finding a minimum of the cost function, for various choices of regularization and for different observations types.The following program allows to minimize the cost function.

```
function [X,Y1,J]=U0initialcondition(N,T,M,beta,N2,
lamda1,gamma1,a)

[xx,yy,Dx,Dy,Dxx,Dyy]=matoperatorn(N);
[U0ref,U00,Uobs,U0,Ub,deltaT,U1obs,LAMDAn]=
observation(N,T,M,beta,N2);
tol1=1e-9;
maxinbiter=1000;
normgradJU0=inf;  nbiter=1;  normdU=inf;
Y1=[]; Y2=[]; Z=[]; A=[];
while( normgradJU0>=tol1 && nbiter<=maxinbiter)
   U=zeros((N-1)^2,M);
j=1;
U(:,j)=U0;
for j=2:M-1
   U(:,j+1)= U(:,j) +deltaT*(Dxx + Dyy)*U(:,j)+...
            + deltaT*a*((Dx*U(:,j)).^2 + (Dy*U(:,j)).^2);
end
for j=2:M
```

```
    s=0;
    J1=s+(deltaT/2)*norm(LAMDAn*U(:,j)-Uobs(:,j))^2;
    J=J1+(lamda1/2)*(norm(U(:,1)-Ub))^2;
end
k=M; q(:,k)=zeros((N-1)^2,1);
%t0=tic
for k=(M-1):-1:1
 q(:,k)=q(:,k+1)+deltaT*((Dxx+Dyy)'*q(:,k+1)
   +2*a*(Dx'*diag(Dx*U(:,k+1))+...
   +Dy'*diag(Dy*U(:,k+1)))*q(:,k+1)
   + LAMDAn'*(LAMDAn*U(:,k+1)-Uobs(:,k+1)));
end
%tf=toc(t0)
q0=q(:,1);

% calcul du  gradient
gradJU0=lamda1*(U(:,1)-Ub)+q(:,1)+deltaT*((Dxx+Dyy)'*q(:,1)+...
        +2*a*(Dx'*diag(Dx*U(:,1))+Dy'*diag(Dy*U(:,1)))*q(:,1));

 U0new=U(:,1)- gamma1*gradJU0;
 U0=U0new;

  normgradJU0=norm(gradJU0)
       Y1=[Y1,normgradJU0];

    Z=[Z,J];
    X=1:nbiter;
   nbiter=nbiter+1
end
```

The Tikhonov regularization is used for the functional (26). For different values of the regularization parameter λ, the minimum of the cost function has been reached (Figure 3), the gradients order are 10^{-10} and an attractive initial condition was obtained. For the simulations, we considered the following values:

$N = 15,\ T = 1,\ M = 5000,\ beta = 1,\ N2 = 10,\ gamma1 = 0.6$ and $a = -1$.

In this condition (16×16 node number), the CPU required for running the adjoint model at one time level is 0.0330. The CPU required 99.9230 for the total in 5000 iterations.

We note that our assimilation algorithm presents similar behavior for two types of observations (noisy and noiseless) in terms of the convergence. This behavior is also confirmed by considering the dense or not dense observations.

The figure 4 shows a good approximation of the initial condition in different experiments. To evaluate the approximation quality in each experiment, we have calculated the relative errors through the following formula

$$E_r = \frac{\| U_{0ref} - U_{0identified} \|}{\| U_{0ref} \|}. \tag{28}$$

Thus, in the first experiment where observations are dense and non noisy (Figure4 (c)) the relative error is $E_r = 1,2493.10^{-4}$. When observations are dense and noisy (second experiment, Figure 4 (e)) we have $E_r = 0,0346$. For non-dense observations and noiseless (third experiment, Figure 4 (f)) $E_r = 0.0036$ and $E_r = 0.0114$ in case of non-dense and noisy observations (fourth experiment, Figure 4 (g)).

From these results, the approximation of the initial condition is much better in the first experiment (Figure 4 (c)). This is explained by the fact that we have considered the ideal conditions created from observations of twin experiments. However, it is very difficult or impossible to be in good conditions in practice, consequently the need is to consider the results of three experiments.

When we consider separately the experiments where observations are dense (Figure 4 (c) and (e)) and the experiments where they are not dense (Figure 4 (f) and (g)), we find that the approximation of the initial condition is better if the observations are not noisy. But taking separately the experiments where observations are not noisy (Figure 4 (c) and (f)) and when they are noisy (Figure 4 (e) and (g)) we find that the approximation is better in the first situation for the Figure 4 (c) while this case happens in the second for the Figure 4 (g). Figure 4 (e) has the greatest relative value ($E_r = 0.0346$) this result is explained by the dense and noisy observations utilization. In fact, the error is due to the observations that are large because they occur at any point and any time.

5. Conclusion

For to estimate the initial condition of the nonlinear partial differential equations model problem, we used the variational data assimilation methods which are based on the optimal control theory. We have developed a technique that allowed us to have very easily the adjoint code. Using a spatial discretization that can lead to a numerical scheme based on column vectors and matrices,

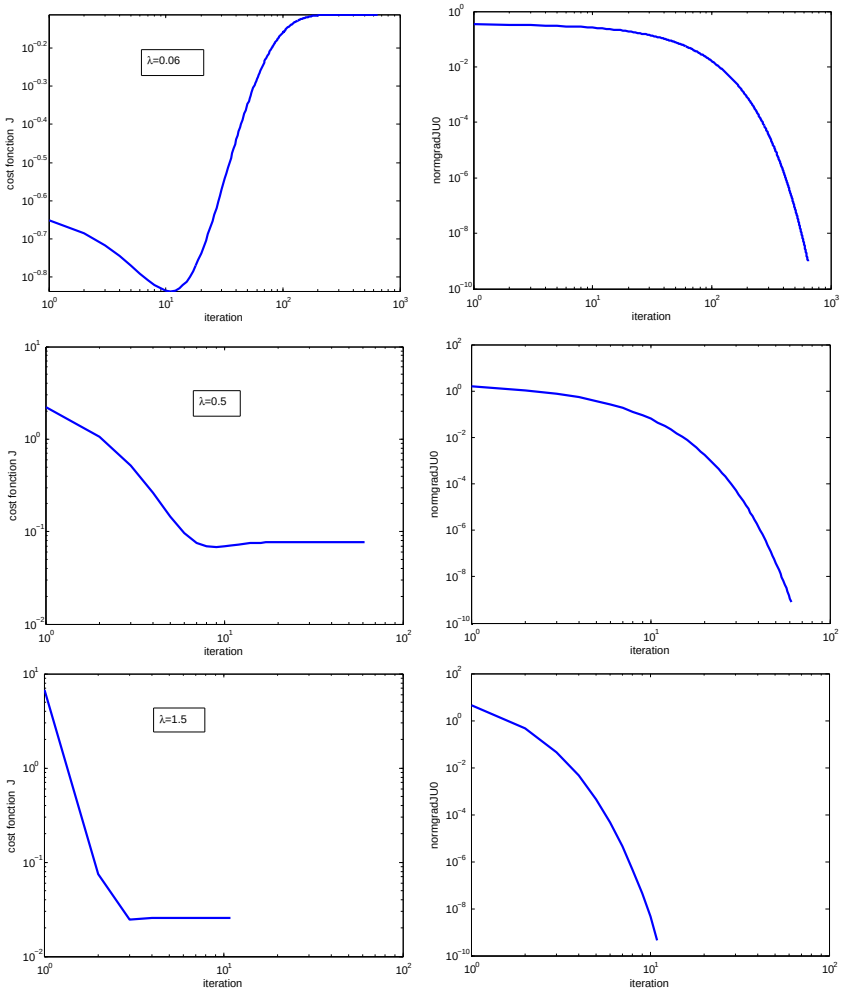


Figure 3: *The cost function (left) and his gradient (right) according to the minimization iteration.*

the technique creates the diagonal matrices that allow to handle the various terms in the adjoint determination. A such approach reveals very efficient in the inverse problem solutions approximation , particularly for the numerical schemes that combine the pseudo-spectral methods and compact approach for determining the adjoint codes.

It is a lot more interest to conduct a comparison of the results with those

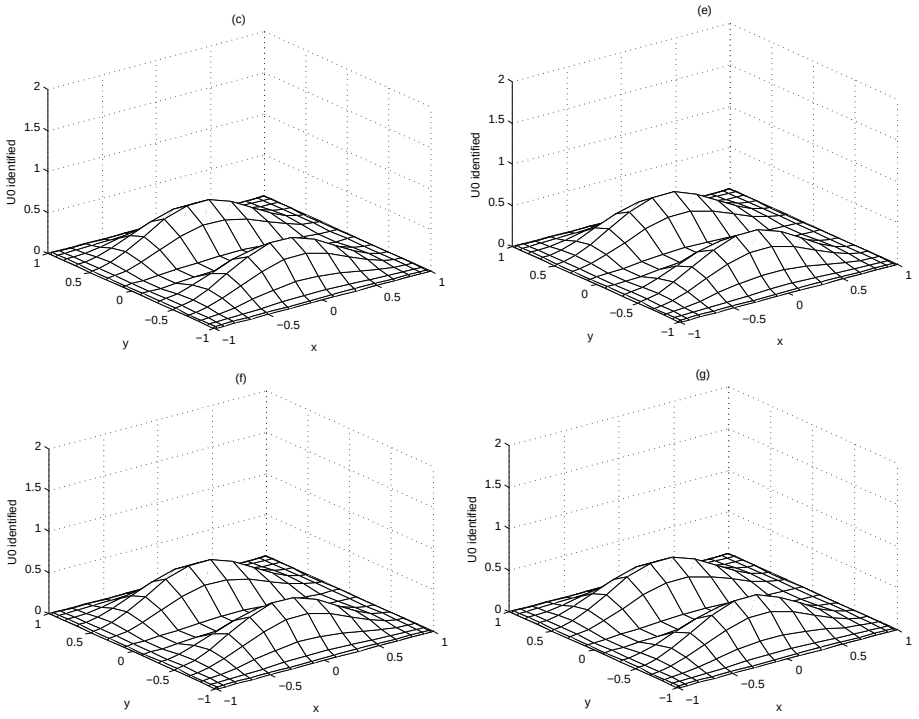


Figure 4: *Initial condition identified according to four experiments*

possibly gotten by automatic differentiation conceived in MatLab language. However, the automatic differentiations in MatLab which we have now (as ADMAT or ADimat) don't permit us to establish this comparisons. We consider to remedy there in our next works.

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