Numerical approximation of the flux identification problem for scalar conservation laws

C. Castro (Universidad Politécnica de Madrid)

Joint work with E. Zuazua (Basque Center of Applied Mathematics)

CIRM, February 16-20, 2009

Statement

We consider the 1-d scalar conservation law:

$$\begin{cases} \partial_t u + \partial_x(f(u)) = 0, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), & x \in \mathbb{R} \end{cases} \tag{1}$$

Given an initial datum $u^0 \in L^2(\mathbb{R})$ and target $u^d \in L^2(\mathbb{R})$ we consider the cost functional $J : \mathcal{U}_{ad} \to \mathbb{R}$, defined by

$$J(f) = \int_{\mathbb{R}} |u(x,T) - u^d(x)|^2 \, dx, \tag{2}$$

where $u(x,t)$ is the unique entropy solution.

Flux identification problem: Find $f^{\min} \in \mathcal{U}_{ad}$ such that

$$J(f^{\min}) = \min_{f \in \mathcal{U}_{ad}} J(f). \tag{3}$$

(James and Sepúlveda, 1999)

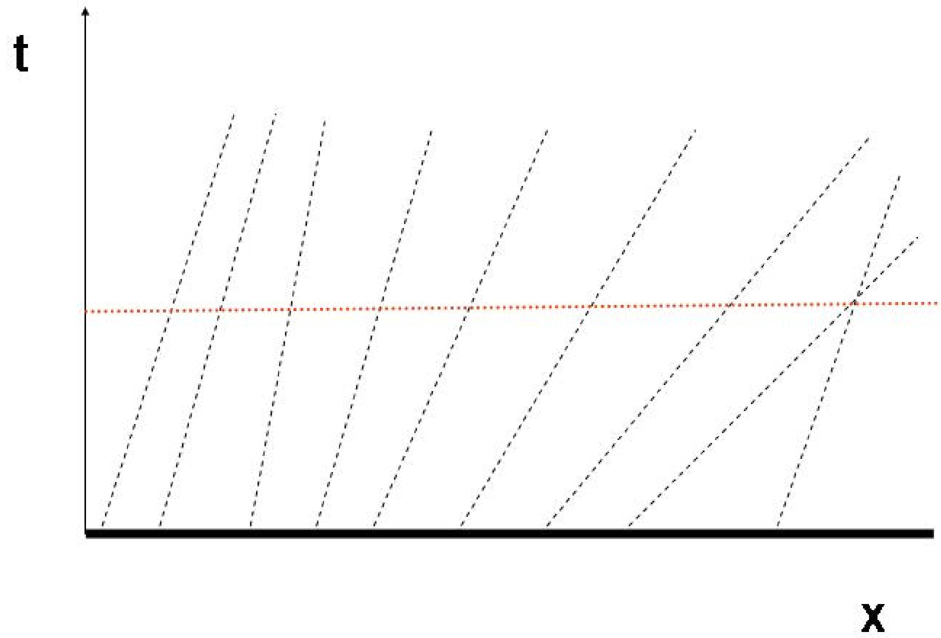


Figure 1: Characteristics lines for the scalar conservation law.

Characteristic lines

$$\frac{dx}{dt} = f'(u^0(x)).$$

Main questions

1. Existence of minimizers. We include conditions on the admissible set to guarantee:

   - Continuity in some topology (Lucier, 1986)

     $$\|u_f(\cdot,t) - u_g(\cdot,t)\|_{L^1(\mathbb{R})} \leq t\|f-g\|_{Lip}\|u^0\|_{BV}.$$

   - Compactness of minimizing sequences. We can consider

     $$\mathcal{U}_{ad} = W^{2,\infty}.$$

2. Uniqueness. A unique minimizer does not exists in general for such problems. Moreover we can have many local minima.

3. Numerical approximation.

   (a) Introduce a suitable discretization for the functional J, J_Δ, the equations, etc.

   (b) Solve the discrete optimization problem: Find $f_\Delta^{\min}$ s.t.

$$J_\Delta(f_\Delta^{\min}) = \min_{f_\Delta \in \mathcal{U}_\Delta} J_\Delta(f_\Delta),$$

4. Convergence of discrete minimizers when $\Delta \to 0$ (conservative monotone schemes).

The discrete problem

Assume that we discretize the conservation law using one of the convergent conservative numerical schemes (Lax-Friedrichs, Godunov, etc.) and we take

$$J_\Delta(f_\Delta) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \tag{4}$$

where $u^0_{\Delta x} = \{u^0_j\}$ and $u^d_\Delta = \{u^d_j\}$ are numerical approximations of $u^0(x)$ and $u^d(x)$ at the nodes x_j, respectively. For example, we can take

$$u^0_j = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u_0(x)dx,$$

where $x_{j\pm1/2} = x_j \pm \Delta x$.

Let us introduce an approximation of the space $\mathcal{U}_{ad}$, $\mathcal{U}^\Delta_{ad}$, as the linear space generated by a set of base functions

$$\mathcal{U}^\Delta_{ad} =< f^1, f^2, ..., f^K > .$$

Problem: Find $f^{\min}_\Delta$ such tha

$$J_\Delta(f^{\min}_\Delta) = \min_{f_\Delta \in \mathcal{U}^\Delta_{ad}} J_\Delta(f_\Delta). \tag{5}$$

Methods to approximate the gradient

- The discrete approach: differentiable schemes.
- The discrete approach: non-differentiable schemes.
- The continuous approach.
- The continuous approach: The alternating descent method.

The discrete approach: Differentiable numerical schemes

Assume that the Burgers equation is approximated by a differentiable conservative numerical scheme

$$u_j^{n+1} = u_j^n - \lambda(g_{j+1/2}^n - g_{j-1/2}^n), \quad j \in \mathbb{Z}, \quad n = 0, ..., N.$$

$$u_j^0 = u_{j,0}, \qquad \lambda = \Delta t/\Delta x$$

where

$$g_{j+1/2}^n = g(u_j^n, u_{j+1}^n)$$

and the numerical flux $g(u,v)$ is differentiable. For example,

$$g^{LF}(u,v) = \frac{f(u)+f(v)}{2} - \frac{v-u}{2\lambda}.$$

The linearized scheme is well-defined as

$$\delta u_j^{n+1} = \delta u_j^n - \lambda\left(\partial_1 g_{j+1/2}^n \delta u_j^n + \partial_2 g_{j+1/2}^n \delta u_{j+1}^n - \partial_1 g_{j-1/2}^n \delta u_{j-1}^n - \partial_2 g_{j-1/2}^n \delta u_j^n\right) = 0,$$
$$j \in \mathbb{Z}, \quad n = 0, ..., N.$$

The derivative of the cost functional

$$J_\Delta = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \tag{6}$$

is given by

$$\delta J_\Delta = \Delta x \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d) \delta u_j^{N+1}, \tag{7}$$

where δu_j^n solves the above linearized system. If we introduce the following adjoint system

$$\begin{aligned} p_j^n &= p_j^{n+1} + \lambda \left(\partial_1 g_{j+1/2}^n (p_{j+1}^{n+1} - p_j^{n+1}) + \partial_2 g_{j-1/2}^n (p_j^{n+1} - p_{j-1}^{n+1}) \right), \\ p_j^{N+1} &= (u_j^{N+1} - u_j^d), \quad j \in \mathbb{Z}, \quad n = 0, ..., N. \end{aligned}$$

it is easy to check that

$$\delta J_\Delta = \Delta x \sum_{j \in \mathbb{Z}} (u_j^{N+1} - u_j^d) \delta u_j^{N+1} = \Delta x \Delta t \sum_{j \in \mathbb{Z}} \sum_{n=0,...,N+1} p_j^n \frac{\delta f(u_j^n) - \delta f(u_{j+1}^n)}{\Delta x}.$$

Thus, if we assume that

$$f = \sum_{k=1}^{K} \alpha_k f_k(x),$$

then

$$\delta f = \sum_{k=1}^{K} \delta\alpha_k f_k(x).$$

We have

$$\delta J_\Delta = \sum_{k=1}^{K} \left(\Delta x \Delta t \sum_{j\in\mathbb{Z}} \sum_{n=0,\dots,N+1} p_j^n \frac{\delta f_k(u_{j+1}^n) - \delta f_k(u_j^n)}{\Delta x} \right) \delta\alpha_k$$

and we obtain a descent direction by choosing,

$$\delta\alpha_k = -\Delta x \Delta t \sum_{j\in\mathbb{Z}} \sum_{n=0,\dots,N+1} p_j^n \frac{\delta f_k(u_j^n) - \delta f_k(u_{j+1}^n)}{\Delta x}.$$

Lax-Friedrichs

$$\begin{cases} \frac{u_j^{n+1} - \frac{u_{j-1}^n + u_{j+1}^n}{2}}{\Delta t} + \frac{f(u_{j+1}^n) - f(u_{j-1}^n)}{2\Delta x} = 0, & n = 0, ..., N, \\ u_j^0 = u_{0,j}, & j \in \mathbb{Z}, \end{cases} \tag{8}$$

Adjoint:

$$\begin{cases} \frac{p_j^n - \frac{p_{j+1}^{n+1} + p_{j-1}^{n+1}}{2}}{\Delta t} + f'(u_j^n) \frac{p_{j-1}^{n+1} - p_{j+1}^{n+1}}{2\Delta x} = 0, & n = 0, ..., N \\ p_j^{N+1} = p_j^T, & j \in \mathbb{Z}, \end{cases} \tag{9}$$

with $p_j^T = (u_j^{N+1} - u_j^d)$.

The discrete approach: Non-differentiable numerical schemes

Assume now that the conservation law is approximated by a non-differentiable conservative numerical scheme

$$u_j^{n+1} = u_j^n - \lambda(g_{j+1/2}^n - g_{j-1/2}^n), \quad j \in \mathbb{Z}, \quad n = 0, ..., N.$$

$$u_j^0 = u_{j,0}$$

where

$$g_{j+1/2}^n = g(u_j^n, u_{j+1}^n)$$

and the numerical flux $g(u,v)$ is non-differentiable. For example,

$$g^{Roe}(u,v) = \frac{1}{2}(f(u) + f(v) - |A(u,v)|(v-u))$$

where

$$A(u,v) = \begin{cases} (f(v) - f(u))/(v-u), & \text{if } u \neq v, \\ f'(u), & \text{if } u = v, \end{cases}$$

In this case non-smooth optimization techniques are necessary.

The continuous approach for smooth solutions

Let δJ be the Gateaux derivative of J at f in the direction δf. We have

$$\delta J = \int_{\mathbb{R}} (u(x,T) - u^d(x))\delta u(x,T)\, dx,$$

where δu solves the linearized system,

$$\begin{cases} \partial_t \delta u + \partial_x \left(f'(u)\delta u\right) = -\partial_x(\delta f(u)), \\ \delta u(x,0) = 0. \end{cases}$$

The solution δu of this system is given by

$$\delta u(x(t),t) = -\int_0^t \exp\left(-\int_s^t \partial_x(f'(u))(x(r),r)\, dr\right) \partial_x(\delta f(u))(x(s),s)\, ds = -t\partial_y(\delta f(u(y,t))).$$

and then,

$$\delta J \quad = \quad -T\int_{\mathbb{R}} \partial_y(\delta f(u(y,T)))\,(u(y,T) - u^d(y))\, dy.$$

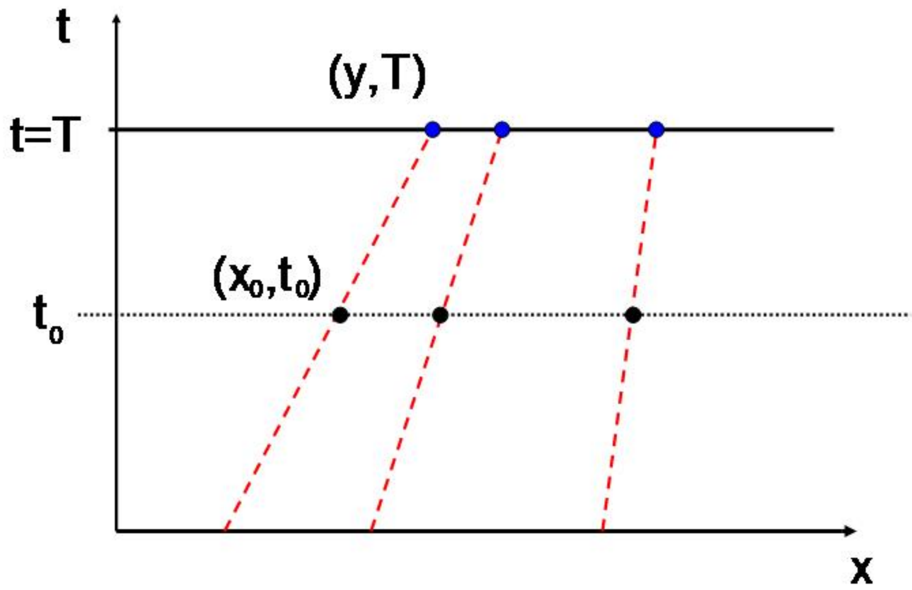


Figure 2: Change of variables.

If we assume that

$$f(s) = \sum_{k=1}^{K} \alpha_k f_k(s)$$

Then

$$\delta J = -\sum_{k=1}^{K} \delta\alpha_k T \int_{\mathbb{R}} \partial_x(\delta f_k(u(x,T)))\,(u(x,T) - u^d(x))\,dx$$

and an obvious descent direction is given by

$$\delta\alpha_k = T \int_{\mathbb{R}} \partial_x(\delta f_k(u(x,t)))\,(u(x,T) - u^d(x)\,dx.$$

The continuous approach in presence of shocks

Several difficulties: 1. Define solutions of the linearized system

$$\begin{cases} \partial_t \delta u + \partial_x \left(f'(u) \delta u \right) = -\partial_x (\delta f(u)), \\ \delta u(x,0) = 0. \end{cases}$$

2. Is this product well-defined?

$$\delta J = \int_{\mathbb{R}} (u(x,T) - u^d(x)) \delta u(x,T) \, dx,$$

3. The derivative of J does not exists, in general. For example, consider the one parameter family of nonlinearities $f_k(u) = ku^2$. Associated to this family we have the solutions

$$u_k(x,t) = \begin{cases} 1 \text{ if } x \geq kt, \\ 0 \text{ otherwise.} \end{cases}$$

If $u^{obj} = u_{k_0}(x,T)$ then,

$$J(f_k) = T|k - k_0|,$$

which is not differentiable.

The continuous approach in presence of a single shock

Assume that $u(x,t)$ is a weak entropy solution of the conservation law with a discontinuity along a regular curve $\Sigma = \{(t, \varphi(t)), t \in [0,T]\}$. It satisfies the Rankine-Hugoniot condition on Σ

$$\varphi'(t)[u]_{\varphi(t)} = [f(u)]_{\varphi(t)} \,. \tag{10}$$

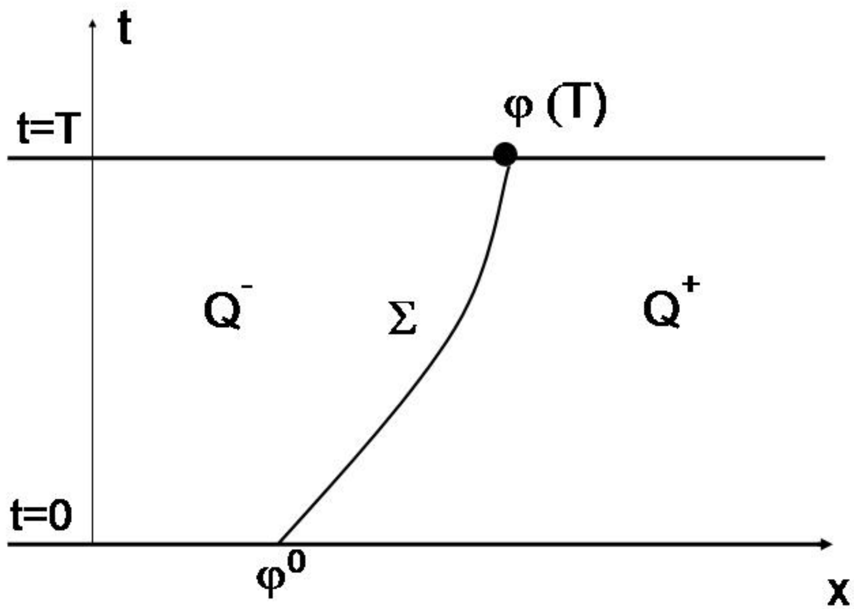
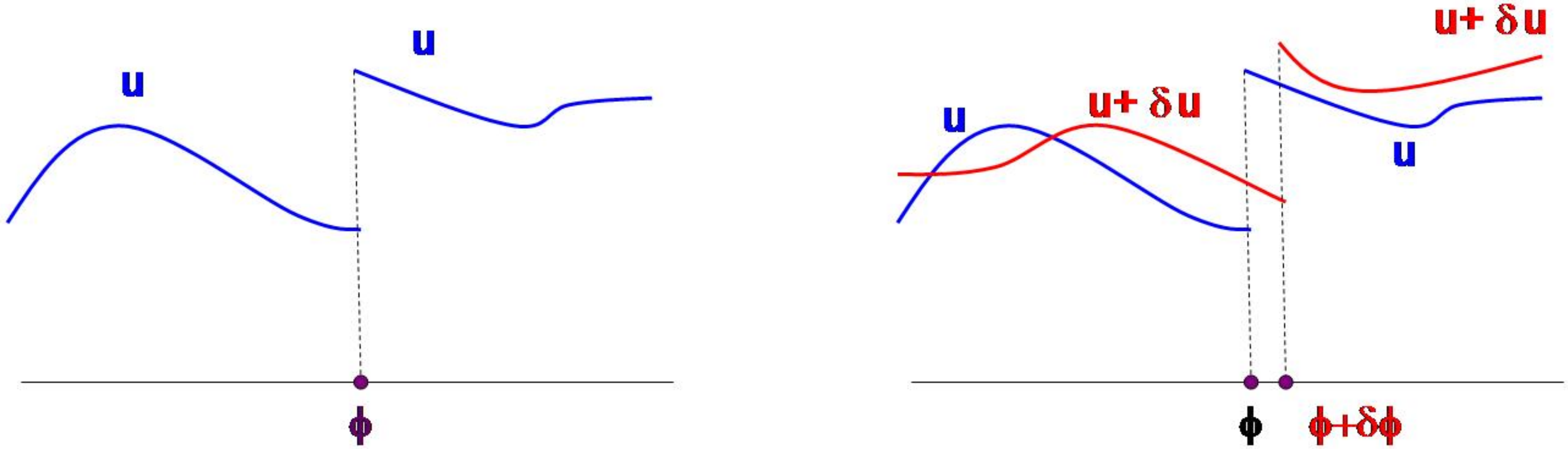


Figure 3: Subdomains Q^- and Q^+.

Then the pair (u, φ) satisfies the system

$$\begin{cases} \partial_t u + \partial_x (f(u)) = 0, & \text{in } Q^- \cup Q^+, \\ \varphi'(t)[u]_{\varphi(t)} = [f(u)]_{\varphi(t)}\,, & t \in (0,T), \\ \varphi(0) = \varphi^0, & \\ u(x,0) = u^0(x), & \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}. \end{cases} \tag{11}$$



$(\delta u, \delta \varphi)$ is a generalized tangent vector (A. Bressan, 95)

Theorem. The generalized tangent vector $(\delta u, \delta\varphi)$ satisfies the following linearized system:

$$\left\{\begin{array}{l} \partial_t \delta u + \partial_x (f'(u)\delta u) = -\partial_x(\delta f(u)), \quad \text{in } Q^- \cup Q^+, \\ \delta\varphi'(t)[u]_{\varphi(t)} + \delta\varphi(t)\left(\varphi'(t)[u_x]_{\varphi(t)} - [f'(u)u_x]_{\varphi(t)} - [\delta f(u)]_{\varphi(t)}\right) \\ \quad +\varphi'(t)[\delta u]_{\varphi(t)} - [u\delta u]_{\varphi(t)} = 0, \quad \text{in } (0,T), \\ \delta u(x,0) = 0, \quad \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}, \\ \delta\varphi(0) = 0, \end{array}\right. \tag{12}$$

with the initial data $(\delta u^0, \delta\varphi^0)$.

Linearization of similar problems have been obtained by Bressan (95), Ulbrich (03), Bardos and Pironneau (03), Godlewski and Raviart (99), etc.

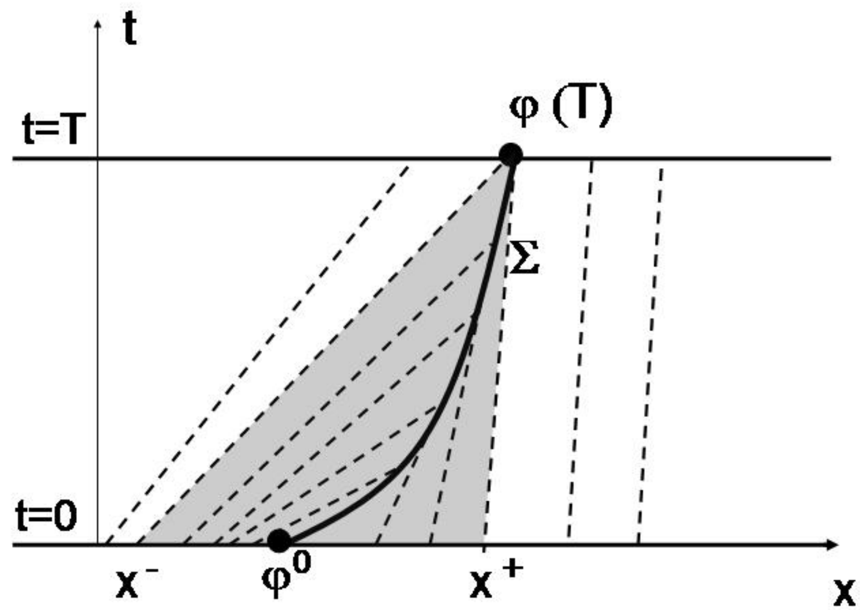


Figure 4: Characteristic lines entering on a shock

Variation of the functional J:

$$J(u^0) = \int_{\mathbb{R}} |u(x,T) - u^d|^2 dx$$

$$\delta J = \int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} (u(x,T) - u^d(x))\delta u(x,T) - \left[\frac{(u(x,T) - u^d(x))^2}{2}\right]_{\varphi(T)} \delta\varphi(T).$$

Lemma The Gateaux derivative of J can be written as

$$\begin{aligned} \delta J &= -T \int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} \partial_x(\delta f(u))(x,T)\ (u(x,T) - u^d(x))\ dx \\ &\quad -T\eta \frac{[\delta f(u(x,T))]_{\varphi(t)}}{[u(x,T)]_{\varphi(t)}}, \end{aligned}$$

where

$$\eta = \begin{cases} \frac{1}{2}\left[(u(\cdot,T) - u^d(\varphi(T)^+))^2\right]_{\varphi(T)}, & \text{if } \delta\varphi(T) > 0, \\ \frac{1}{2}\left[(u(\cdot,T) - u^d(\varphi(T)^-))^2\right]_{\varphi(T)}, & \text{if } \delta\varphi(T) < 0, \end{cases} \tag{13}$$

The alternating descent method (C. Castro F. Palacios and E. Zuazua, 07)

Let

$$x^- = \varphi(T) - u^-(\varphi(T))T, \qquad x^+ = \varphi(T) - u^+(\varphi(T))T,$$

and consider the following subsets ,

$$\hat{Q}^- = \{(x,t) \in \mathbb{R} \times (0,T) \text{ such that } x < \varphi(T) - u^-(\varphi(T))t\},$$

$$\hat{Q}^+ = \{(x,t) \in \mathbb{R} \times (0,T) \text{ such that } x > \varphi(T) - u^+(\varphi(T))t\}.$$

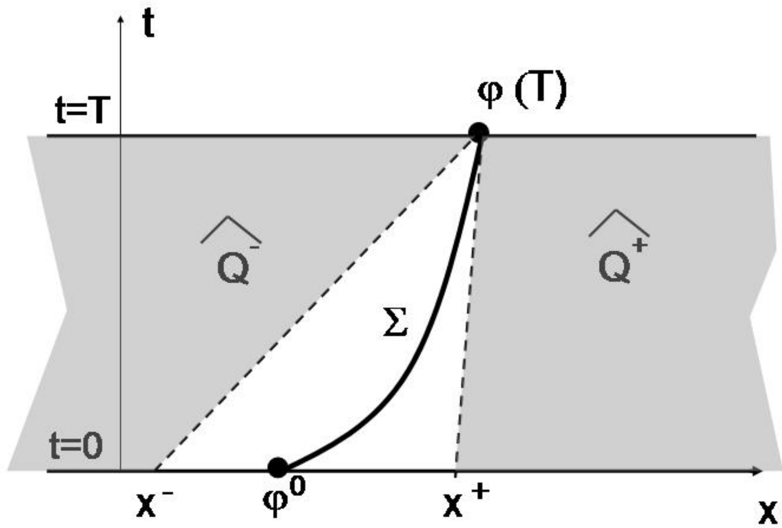


Figure 5: Subdomains $\hat{Q}^-$ and $\hat{Q}^+$

Theorem 1 *Assume that we restrict the variations δf to those that satisfy,*

$$[\delta f(u(x,T))]_{\varphi(T)} = \delta f(u(\varphi(T)^+,T)) - \delta f(u(\varphi(T)^-,T)) = 0. \tag{14}$$

Then, the solution $(\delta u, \delta\varphi)$ of the linearized system satisfies $\delta\varphi(T) = 0$ and the generalized Gateaux derivative of J in the direction $(\delta u^0, \delta\varphi^0)$ can be written as

$$\delta J = -T \int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} \partial_x(\delta f(u))(x,T)(u(x,T) - u^d(x))\, dx. \tag{15}$$

Moreover, if we choose δf such that

$$[\delta f(u(x,T))]_{\varphi(T)} = \delta f(u(\varphi(T)^+,T)) - \delta f(u(\varphi(T)^-,T)) \neq 0, \tag{16}$$

then $\delta\varphi(T) \neq 0$ and this produce a change in the shock position.

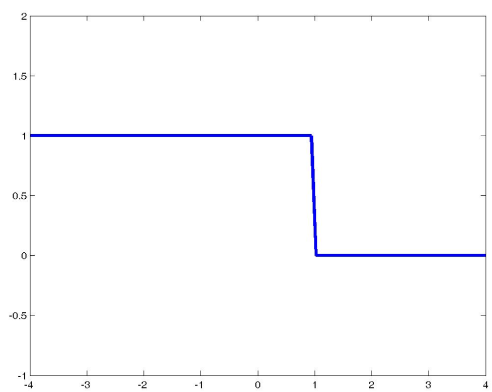
Numerical experiments

Experiment 1. We first consider a piecewise constant initial datum u^0 and target profile u^d given by

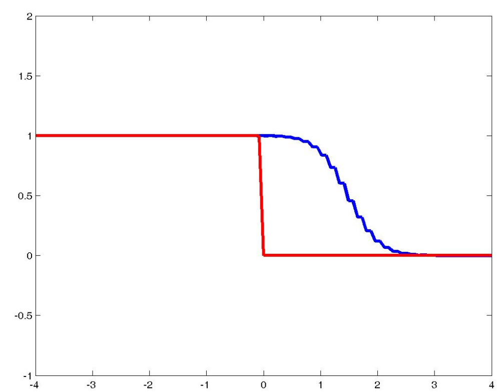
$$u^{0,min} = \begin{cases} 1 \text{ if } x < -1/2, \\ 0 \text{ if } x \geq 0. \end{cases} \tag{17}$$

$$u^d = \begin{cases} 1 \text{ if } x < 0, \\ 0 \text{ if } x \geq 0, \end{cases} \tag{18}$$

and the time $T = 1$.



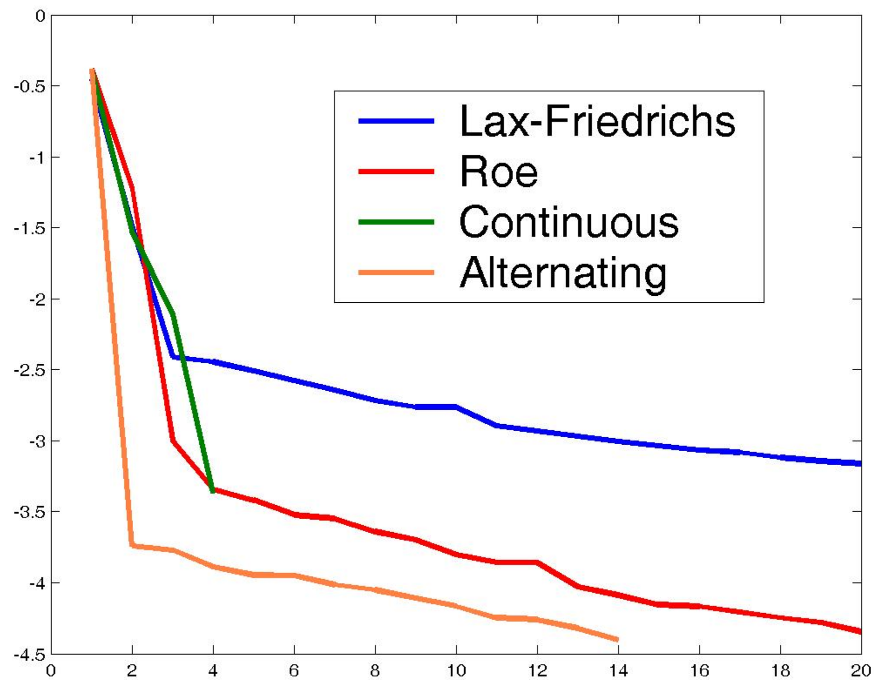
u^0



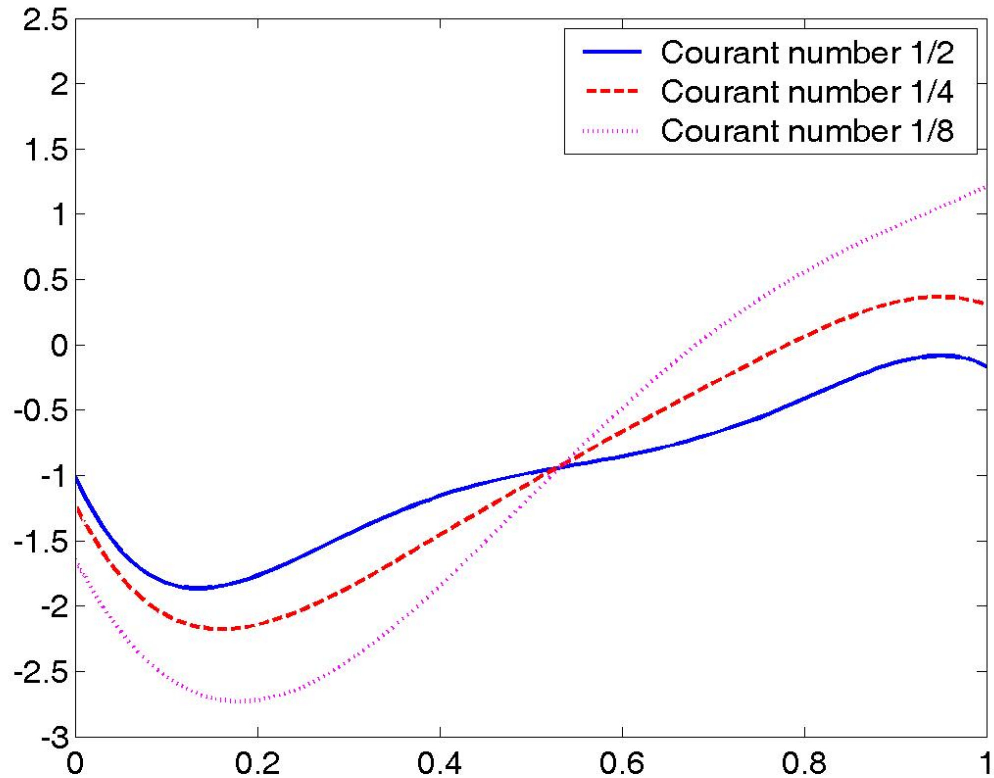
u^d and $u(x, T)$ at initialization

$$f(u) = \alpha_1 u + \alpha_2 u^2 + ... + \alpha_6 u^6$$

$\Delta x = 1/20$

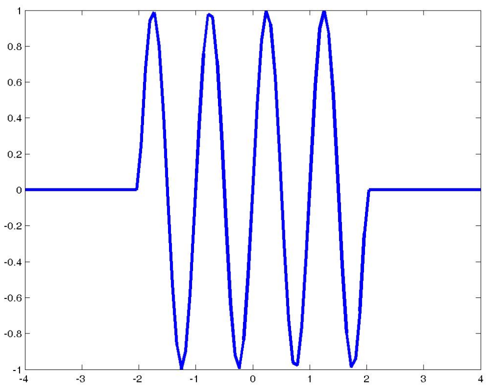


Optimal nonlinearities $f'(u)$ for the Lax-Friedrichs method with different Courant numbers

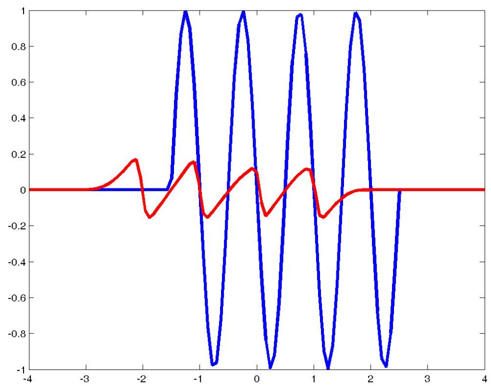


We have considered the new functional,

$$J(u) = \int_{\mathbb{R}} |u(x,T) - u^d(x)|^2 \, dx + \frac{1}{10} \int_0^1 |f'(s)|^2 ds.$$



u^0



u^d and $u(x,T)$ at initialization

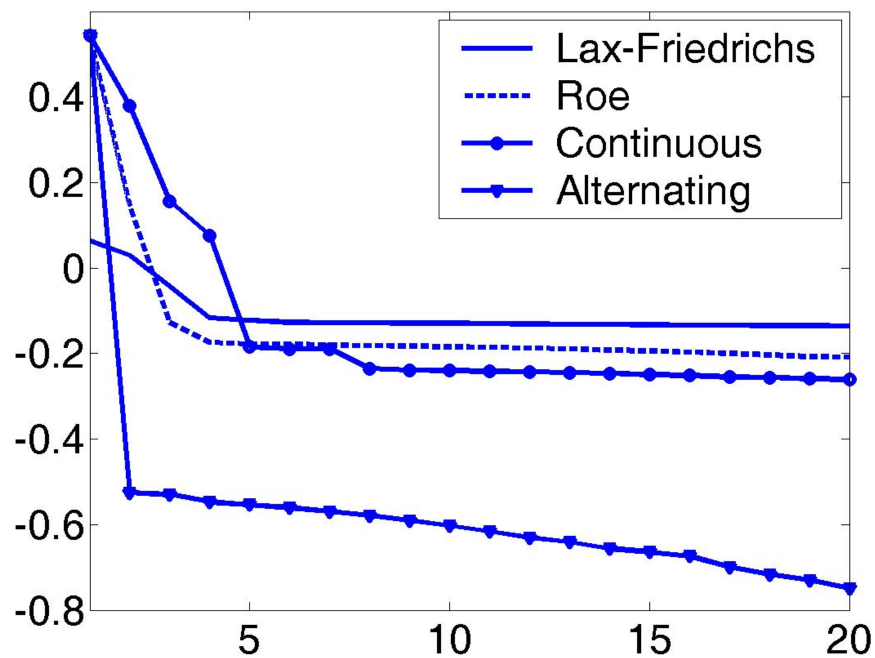


Figure 6: Experiment 2. Log of the functional versus the number of iterations for the different methods.

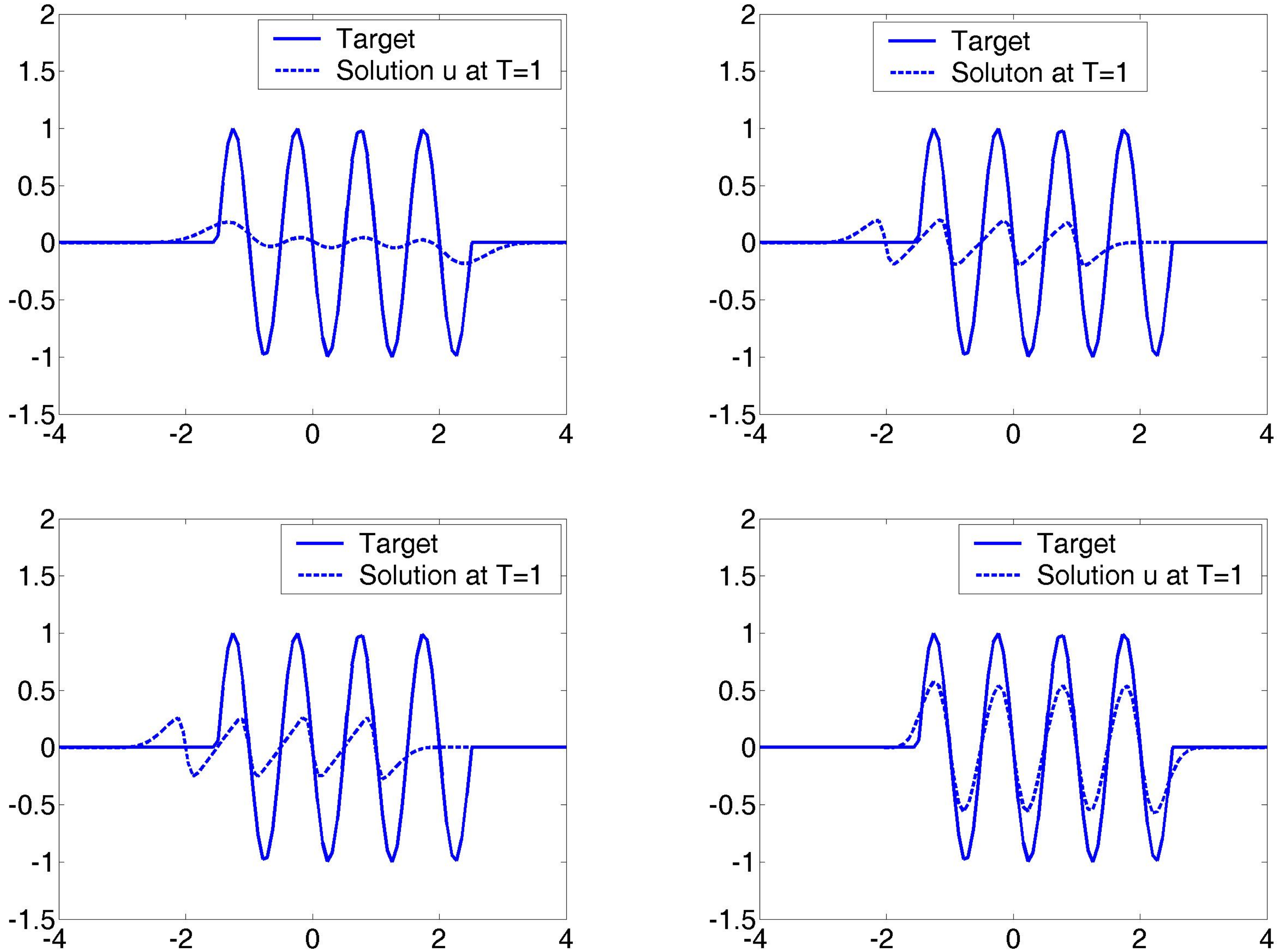


Figure 7: Experiment 2. Target and solution at time $T = 1$ with the optimal f found with the Lax-Friedrichs (upper left), Roe (upper right), continuous (lower left) and Alternating (lower right) methods.