Flux identification problems for conservation laws. A numerical approach

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Benasque, August 25th, 2009

Statement

Le us consider the 1-d scalar conservation law:

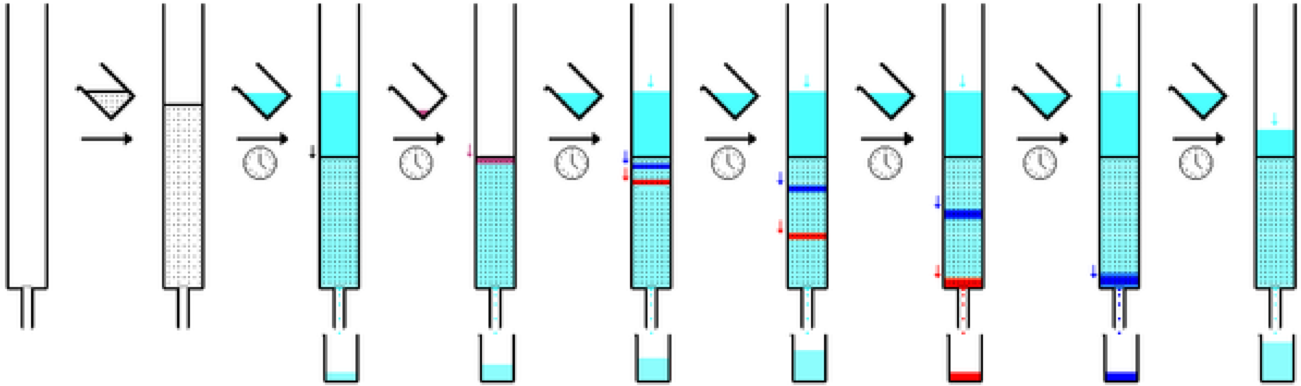
$$\begin{cases} \partial_t u + \partial_x(f(u)) = 0, & \textbf{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), & x \in \mathbb{R} \end{cases} \tag{1}$$

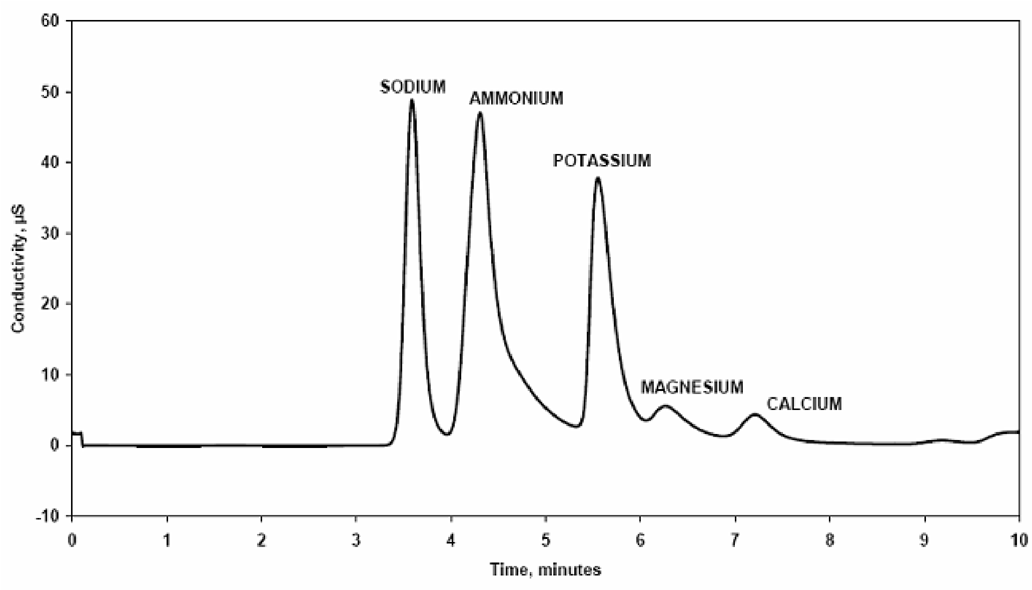
where the nonlinear flux $f(u)$ is unknown.

Identification problem: Assume that we know the solution at time $t = T$, $u(x,T)$ for a given initial datum $u^0 \in L^2(\mathbb{R})$. Can we determine f?

1 Motivation: a problem in chromatography

”Chromatography is the collective term for a set of laboratory techniques for the separation of mixtures. It involves passing a mixture dissolved in a ”mobile phase” through a stationary phase, which separates the analyte to be measured from other molecules in the mixture and allows it to be isolated.”





Typical chromatogram: conductivity of the liquid at the bottom

Mathematical modelling (James and Postel, 09)

We consider a mixture of p components and denote by $\mathbf{c^1}, \mathbf{c^2} \in \mathbb{R}^\mathbf{p}$ the concentrations in phases 1 and 2 of the p chemical components.

Assume that equilibrium is modelled by the **isotherm**

$$\mathbf{h} : \mathbb{R}^p \longrightarrow \mathbb{R}^p$$

such that $\mathbf{c^2} = \mathbf{h}(\mathbf{c^1})$

If we assume constant temperature (no energy equation) and constant velocity (no momentoum equation) the only equation is the mass conserving one.

Phase 1 moves downward with constant velocity u.

Phase 2 has velocity $v = 0$.

$$\partial_t(\mathbf{c^1} + \mathbf{c^2}) + \partial_{\mathbf{x}}(\mathbf{uc^1}) = \mathbf{0}.$$

If we use the isotherm and write $\mathbf{c} = \mathbf{c^1}$ then

$$\begin{cases} \partial_x \mathbf{c} + \partial_t \mathbf{F}(\mathbf{c}) = 0, & t \in (0,T), \quad x \in [0,L], \\ \mathbf{c}(0,t) = \mathbf{c}_{injected}(t), & t \in (0,T), \\ \mathbf{c}(x,0) = 0. \end{cases}$$

where

$$\mathbf{F}(\mathbf{c}) = \frac{1}{u}\left(\mathbf{c} + \frac{1-\varepsilon}{\varepsilon}\mathbf{h}(\mathbf{c})\right)$$

$\varepsilon =$ void fraction of the column

If we change x by t a classical conservation law is obtianed.

Main problem: Find the isotherm h. This can be obtained as a solution of an optimal control problem. Consider the cost functional

$$J(h) = \frac{1}{2}\int_0^T \sum_{i=1}^{p} \left| c_i(L,T) - c_i^{obs}(t) \right|^2 dt$$

Usually h is obtained from a parametric model. A classical example of isotherm is the Langmuir isotherm which is determined by $p + 1$ parameters

$$h(\mathbf{c}) = N^* \frac{K_i c_i}{1 + \sum_{i=1}^{p} K_i c_i},$$

with $\mathbf{c} = (c_1, ..., c_p)$.

Statement

We consider the 1-d scalar conservation law:

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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

$$J(f) = \int_{\mathbb{R}} |u(x,T) - u^d(x)|^2 \, dx, \tag{3}$$

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

We consider the inverse problem: Find $f^{\min} \in \mathcal{U}_{ad}$ such that

$$J(f^{\min}) = \min_{f \in \mathcal{U}_{ad}} J(f). \tag{4}$$

(James and Sepúlveda, 1999)

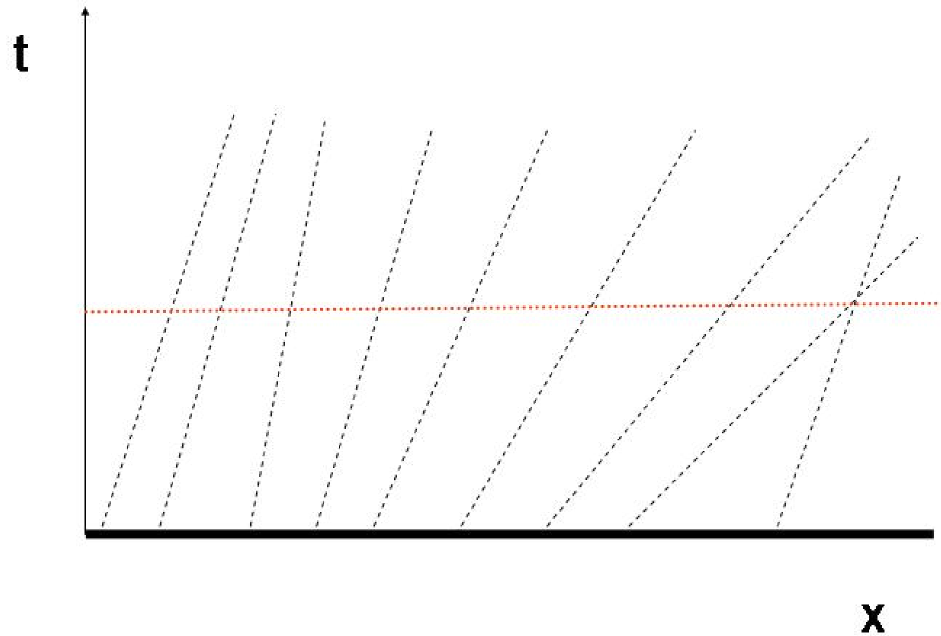


Figure 1: Characteristics lines for the scalar conservation law.

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 scheme (Lax-Friedrichs, Godunov, etc.) and we take

$$J_\Delta(f_\Delta) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \tag{5}$$

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

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

where $x_{j\pm 1/2} = x_j \pm \Delta x$.

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

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

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

$$J_\Delta(f_\Delta^{\min}) = \min_{f_\Delta \in \mathcal{U}_{ad}^\Delta} J_\Delta(f_\Delta). \tag{6}$$

Methods to obtain descent directions

- The discrete approach. We compute the gradient of the discrete system. Discontinuities are ignored.
- The continuous approach. We discretize the gradient of the continuous functional. Discontinuities must be taken into account.

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,

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

A characteristic change of variables allows us to write

$$\delta u(x,t) = -t\partial_x(\delta f(u(x,t))).$$

Then, δJ can be written as,

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

If we assume that

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

Then

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

and an obvious descent direction is given by

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

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

$$\varphi'(t)[u]_{\varphi(t)} = [f(u)]_{\varphi(t)} \,. \tag{7}$$

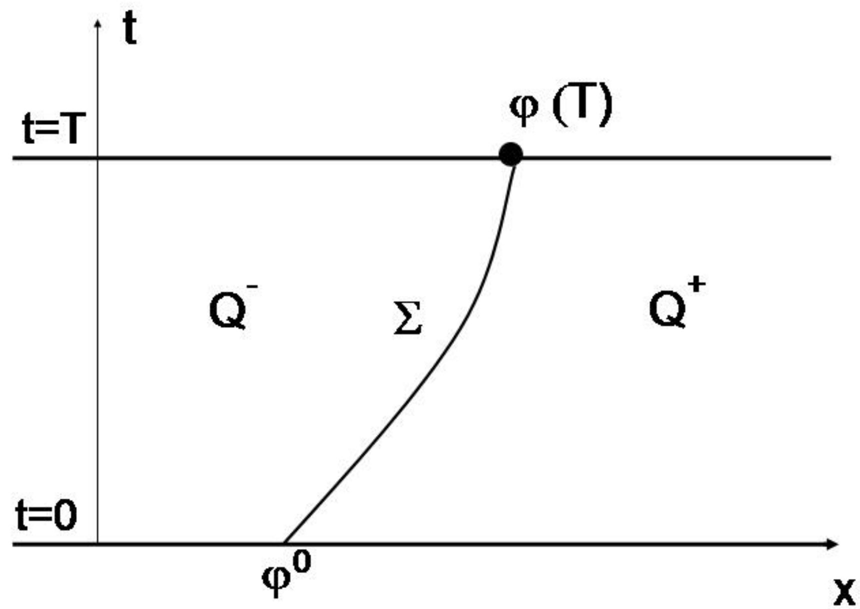
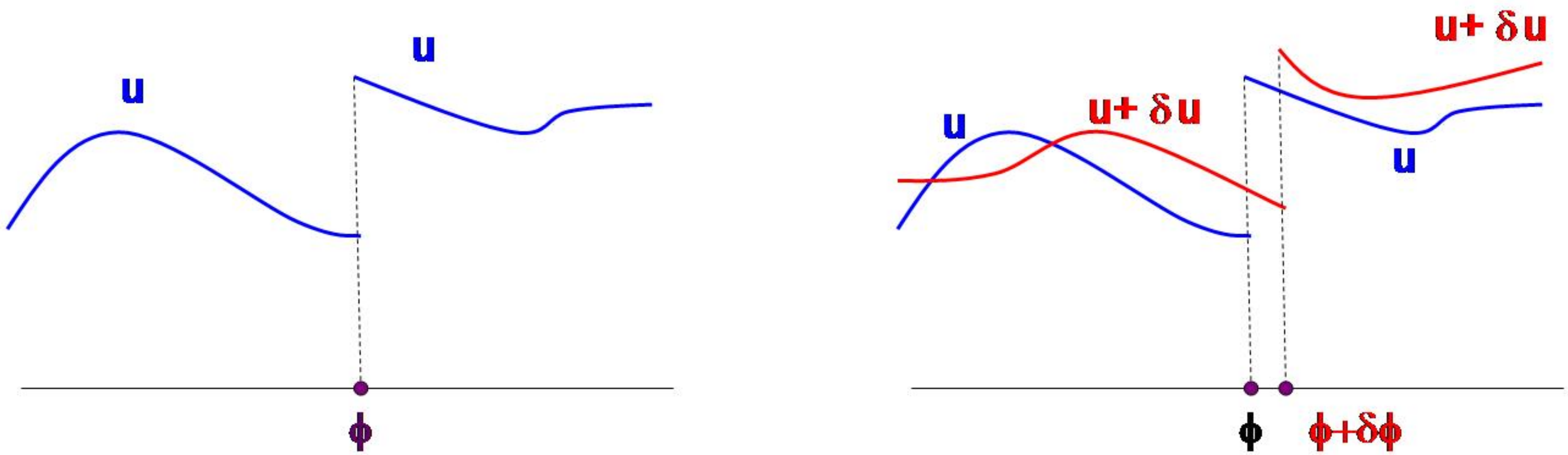


Figure 2: Subdomains Q^- and Q^+.

Then the pair (u, φ) satisfies the system

$$\begin{cases} \partial_t u + \partial_x(f(u)) = 0, & \text{in } Q^- \cup Q^+, \\ \varphi'(t)[u]_{\varphi(t)} = [f(u)]_{\varphi(t)}\,, & t \in (0,T), \\ \varphi(0) = \varphi^0, & \\ u(x,0) = u^0(x), & \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}. \end{cases} \tag{8}$$



We call generalized tangent vector at u to the pair $(\delta u, \delta\varphi)$ which describes an infinitesimal perturbation of the function u, i.e.

$$u^\varepsilon = u + \varepsilon\delta u - [u]_\varphi \chi_{[\varphi, \varphi+\delta\varphi]}$$

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

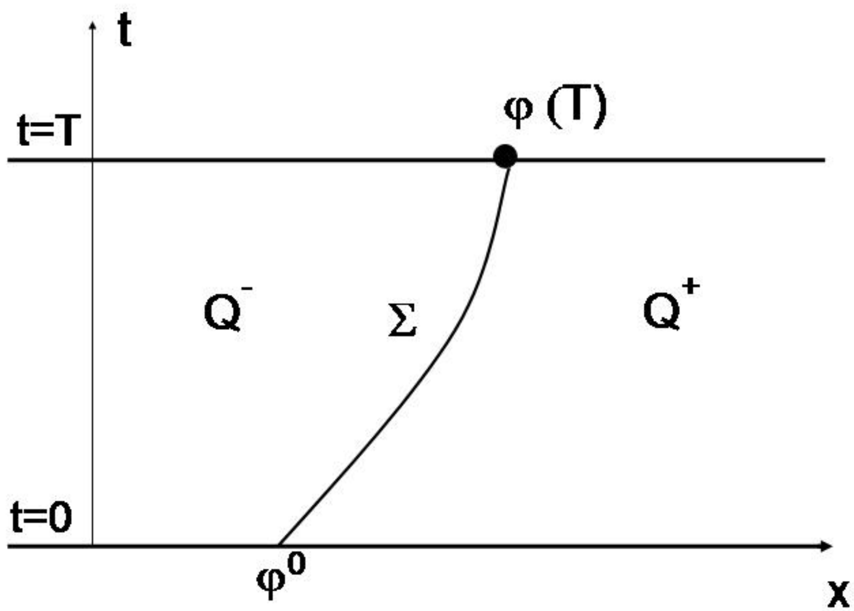
$$\left\{\begin{array}{l} \partial_t \delta u + \partial_x (f'(u)\delta u) = -\partial_x(\delta f(u)), \quad \text{in } Q^- \cup Q^+, \\ \delta\varphi'(t)[u]_{\varphi(t)} + \delta\varphi(t)\left(\varphi'(t)[u_x]_{\varphi(t)} - [f'(u)u_x]_{\varphi(t)} - [\delta f(u)]_{\varphi(t)}\right) \\ \quad +\varphi'(t)[\delta u]_{\varphi(t)} - [u\delta u]_{\varphi(t)} = 0, \quad \text{in } (0,T), \\ \delta u(x,0) = 0, \quad \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}, \\ \delta\varphi(0) = 0, \end{array}\right. \tag{9}$$

This linearization has been obtained by different authors in similar problems: Bressan and Marson (95), Ulbrich (03), Bardos and Pironneau (03), Godlewski and Raviart (99), etc.

A heuristic derivation of the linearized Rankine Hugoniot condition

$$\varphi'(t)[u]_{\varphi(t)} = [f(u)]_{\varphi(t)}$$

is obtained by considering it as a inner Dirichlet boundary condition for which the classical shape derivative applies.



This also applies for systems and higher dimensions. However a rigorous proof is much more difficult. It requires to prove that the solution u^ε with flux $f + \epsilon\delta f$ can be represented with the generalized tangent vector $(\delta u, \delta\varphi)$ at any time $t \in (0, T)$.

The linearized system is well-defined

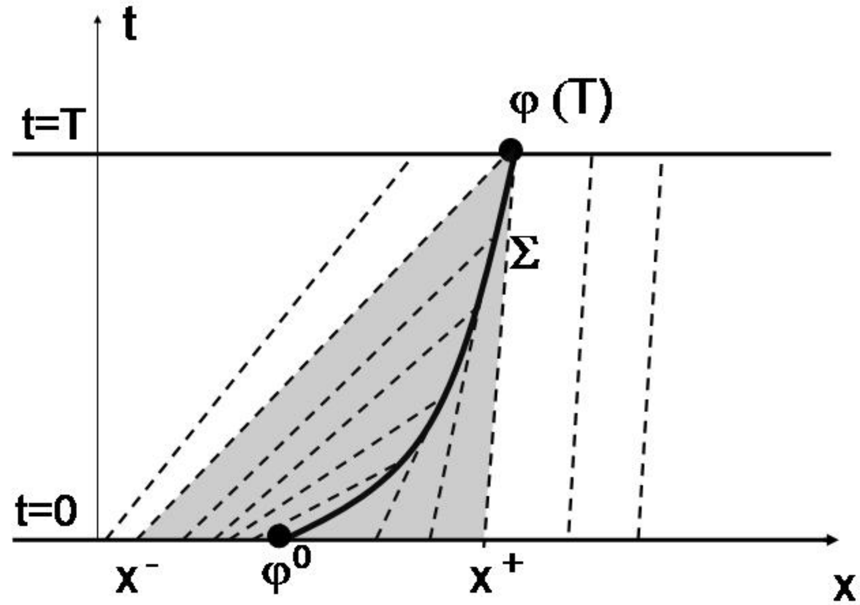


Figure 3: Characteristic lines entering on a shock

Variation of the functional J:

$$J(f) = \frac{1}{2}\int_{\mathbb{R}} |u(x,T) - u^d|^2 dx$$

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

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

$$\eta = \begin{cases} \frac{1}{2}\left[(u(\cdot,T) - u^d(\varphi(T)^+))^2\right]_{\varphi(T)}, & \text{if } \delta\varphi(T) > 0, \\ \frac{1}{2}\left[(u(\cdot,T) - u^d(\varphi(T)^-))^2\right]_{\varphi(T)}, & \text{if } \delta\varphi(T) < 0, \end{cases} \tag{10}$$

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 ,

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

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

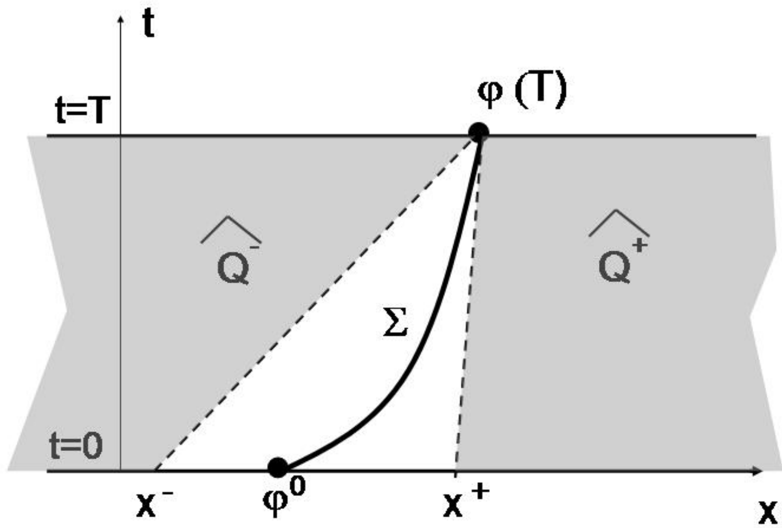


Figure 4: Subdomains $\hat{Q}^-$ and $\hat{Q}^+$

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

$$[\delta f(u(x,T))]_{\varphi(T)} = \delta f(u(\varphi(T)^+,T)) - \delta f(u(\varphi(T)^-,T)) = 0. \tag{11}$$

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

$$\delta J = -T \int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} \partial_x(\delta f(u))(x,T)(u(x,T) - u^d(x))\, dx. \tag{12}$$

Moreover, if we choose δf such that

$$[\delta f(u(x,T))]_{\varphi(T)} = \delta f(u(\varphi(T)^+,T)) - \delta f(u(\varphi(T)^-,T)) \neq 0, \tag{13}$$

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

We are assuming that the fluxes f are taken in the finite dimensional space. We decompose the finite dimensional space of variations of f

$$T_\alpha = T_\alpha^1 \oplus T_\alpha^2,$$

where T_α^1 is the subspace of elements $(\alpha_1, ..., \alpha_M) \in \mathbb{R}^M$ for which

$$\sum_{m=1}^{M} \alpha_m [\delta f_m(u(\cdot,T))]_{\varphi(T)} = 0,$$

and we consider alternatively descent directions in T_1^α and T_2^α.

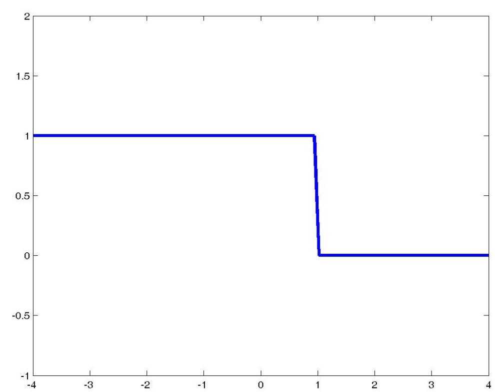
Numerical experiments

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

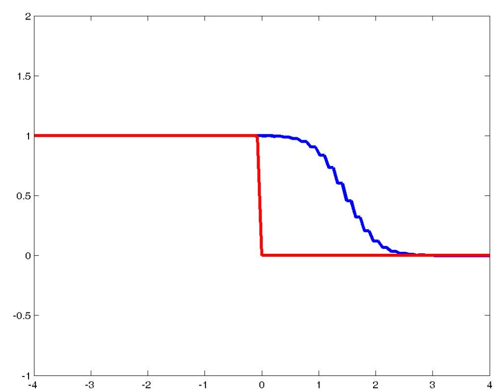
$$u^{0,min} = \begin{cases} 1 \text{ if } x < -1/2, \\ 0 \text{ if } x \geq 0. \end{cases} \tag{14}$$

$$u^d = \begin{cases} 1 \text{ if } x < 0, \\ 0 \text{ if } x \geq 0, \end{cases} \tag{15}$$

and the time $T = 1$.



u^0



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

The nonlinearity is assumed to be a linear combination of the Legendre polinomials in $[0,1]$

$$
\begin{aligned}
&P_1(u) = 1,\\
&P_2(u) = \sqrt{12}(u-1/2),\\
&P_3(u) = \sqrt{80}(3/2u^2 - 3/2u + 1/4),\\
&P_4(u) = \sqrt{448}(5/2u^3 - 15/4u^2 + 3/2u - 1/8),\\
&P_5(u) = \sqrt{2304}(35/8u^4 - 35/4u^3 + 45/8u^2 - 5/4u + 1/16),\\
&P_6(u) = \sqrt{11264}(63/8u^5 - 315/16u^4 + 35/2u^3 - 105/16u^2 + 15/16u - 1/32).
\end{aligned}
$$

If no restriction is included on the size of the nonlinearities then, different solutions are obtained for different courant numbers

Thus, we effectively minimize the functional

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

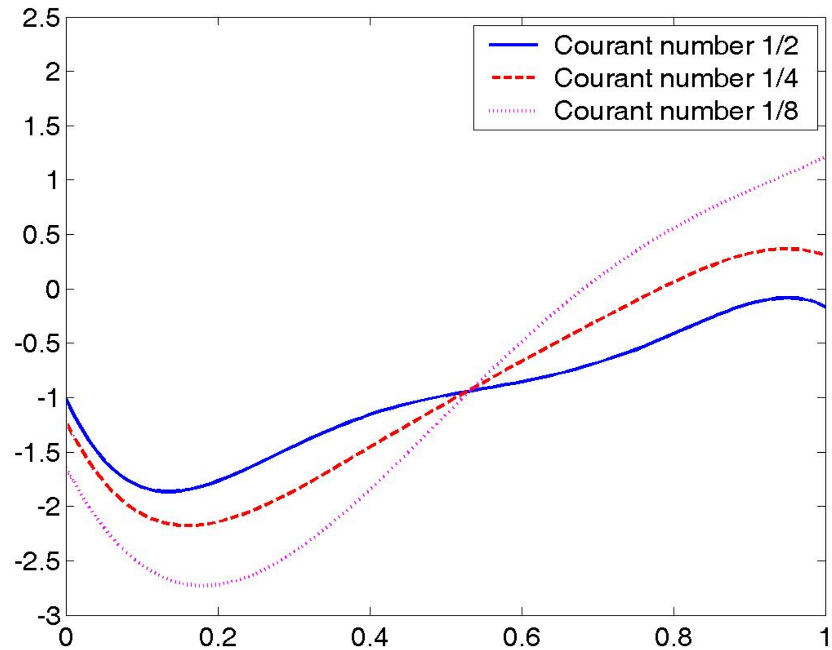


Figure 5: Experiment 1. $f'(s)$ obtained after 30 iterations of the gradient method, for the unpenalized functional (5), with the Lax-Friedrichs scheme and for different values of the Courant number $\Delta x/\Delta t = 1/2, 1/4, 1/8$. The algorithm is initialized with $f = 0$.

$\Delta x = 1/20, f_{ini} = 0$	α_1	α_2	α_3	α_4	α_5	α_6	$f(0) - f(1)$
Lax-Friedrichs	-0.9082	0.2149	0.2014	-0.1127	0.0675	-0.0268	0.9082
Roe	-0.9354	0.1347	0.1797	-0.1048	0.0176	0.0059	0.9354
Continuous	-0.9240	0.1575	0.2299	-0.2108	0.0226	-0.0139	0.9240
Alternating	-0.9832	0.3000	0.0054	-0.0046	-0.0029	0.0078	0.9832

$\Delta x = 1/40, f_{ini} = 0$	α_1	α_2	α_3	α_4	α_5	α_6	$f(0) - f(1)$
Lax-Friedrichs	-0.9176	0.0681	0.1997	-0.1167	0.0656	0.0237	0.9176
Roe	-0.9648	0.0171	0.0797	-0.1415	0.0183	0.0480	0.9354
Continuous	-0.9465	0.0234	0.1304	-0.2533	-0.0136	0.1058	0.9465
Alternating	-0.9865	0.1227	0.0831	-0.1129	-0.0407	0.0404	0.9865

$\Delta x = 1/20, f_{ini} = u^2/2$	α_1	α_2	α_3	α_4	α_5	α_6	$f(0) - f($
Lax-Friedrichs	-0.9136	0.2220	0.1907	-0.1070	0.0666	-0.0320	0.9136
Roe	-0.9536	0.1403	0.1201	-0.0611	0.0241	-0.0318	0.9536
Continuous	-0.9125	0.1879	0.3727	-0.1332	-0.0488	-0.1111	0.9125
Alternating	-0.9782	0.3017	0.0404	-0.0288	0.0169	-0.0267	0.9782

Table 1: Experiment 1. Values for the parameters found after 12 iterations of the descent algorithm with the different methods. The last column contains the value $f(0) - f(1)$, which must be 1 for the minimizers of the continuous functional without penalization. We assume that the Courant number is $\Delta t/\Delta x = 0.5$ and the algorithm is initialized with the indicated $f = f_{ini}$.

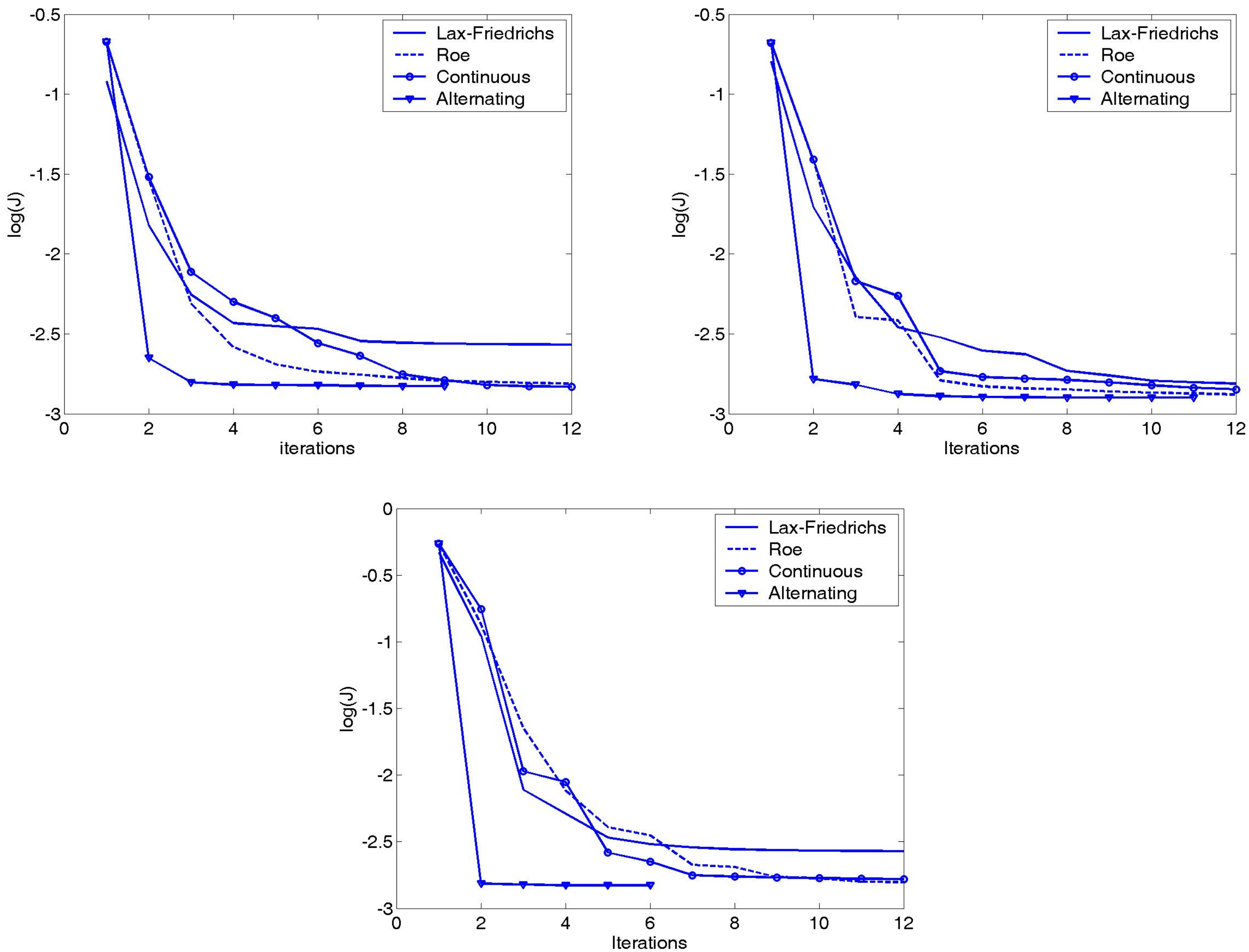
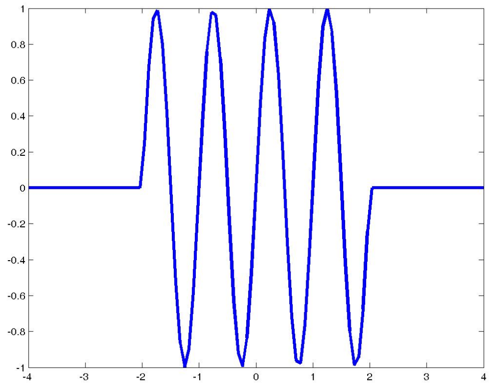
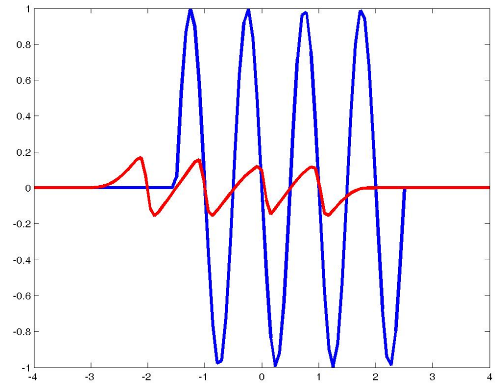


Figure 6: Experiment 1. Log of the functional versus the number of iterations for the different methods. $\Delta t/\Delta x = 1/20$ (upper left) and $1/40$ (upper right) with initialization $f = 0$. The lower figure correspond to the initialization $f(u) = u^2/2$ and $\Delta x = 1/20$.



u^0



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

parameters	α_1	α_2	α_3	α_4	α_5	α_6
Lax-Friedrichs	0.4601	0.5786	0.0016	-0.0954	-0.0034	-0.0383
Roe	-0.5497	1.4065	-0.0901	0.1191	-0.0165	0.0446
Continuous	-0.5326	1.0487	-0.0246	0.0244	-0.0020	0.0030
Alternating	0.4902	0.1256	0.0276	-0.0804	0.0037	-0.0110

Table 2: Experiment 3. Optimal values for the parameters with the different methods

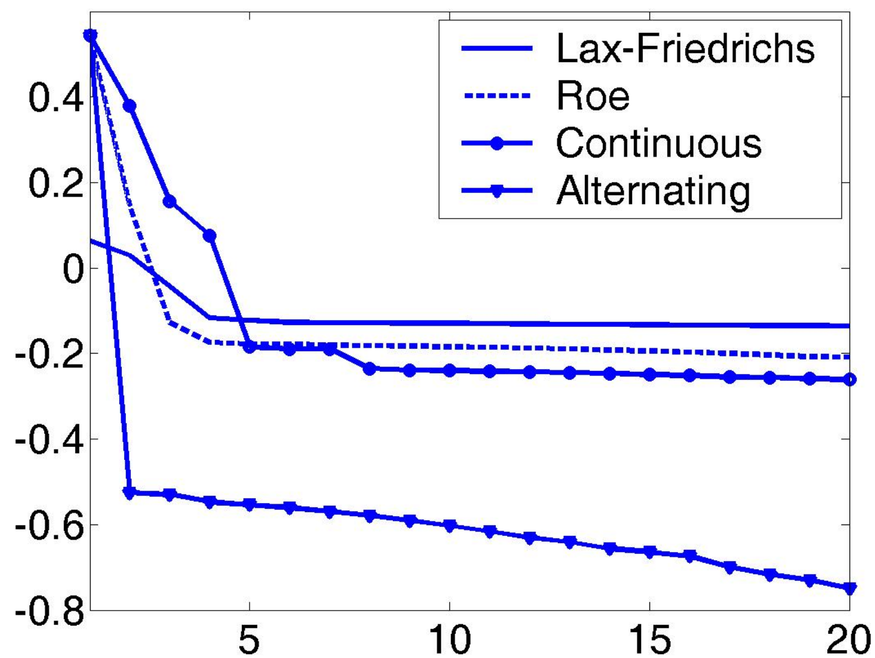


Figure 7: Experiment 2. Log of the functional versus the number of iterations for the different methods.

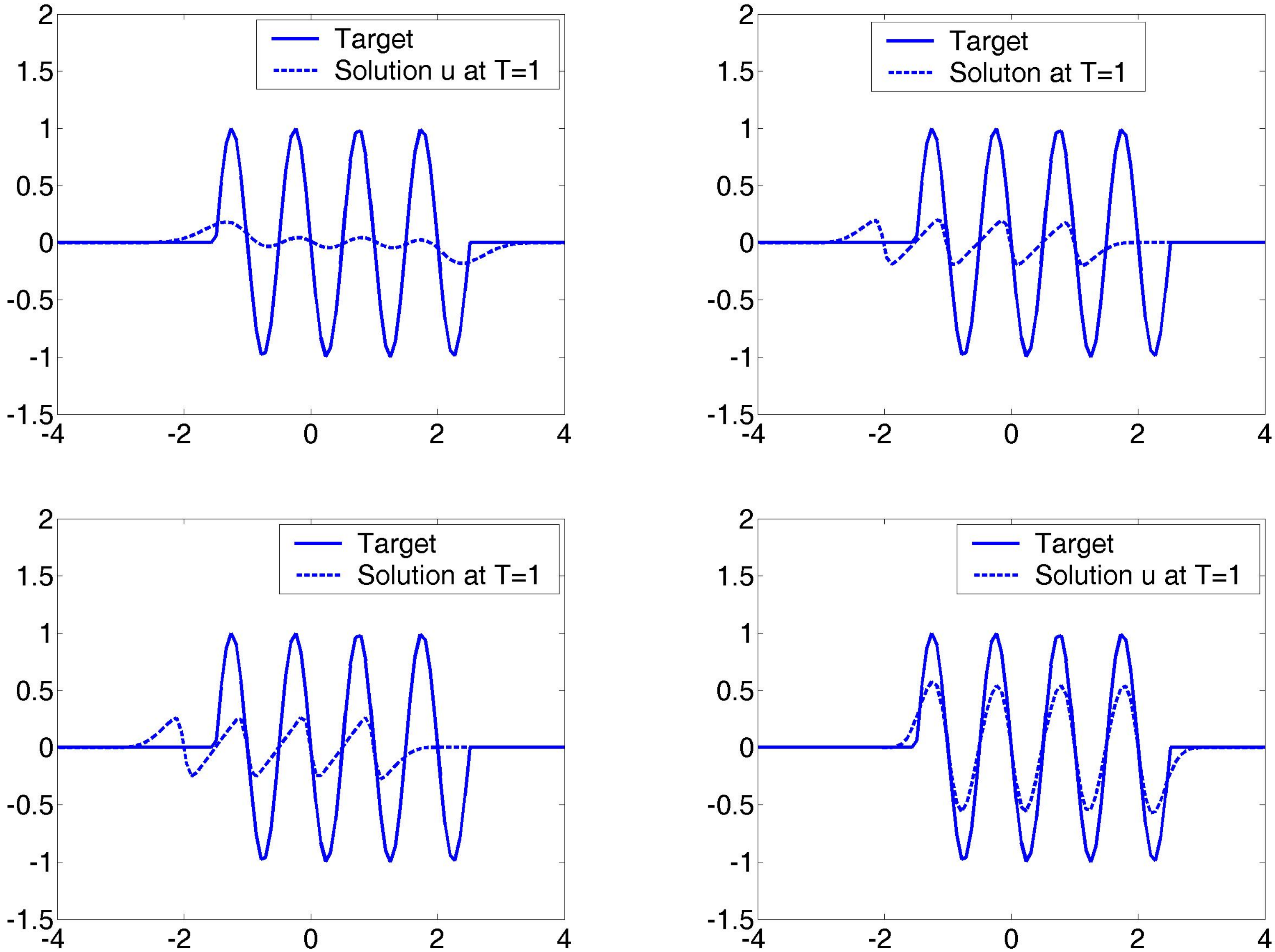


Figure 8: Experiment 2. Target and solution at time $T = 1$ with the optimal f found with the Lax-Friedrichs (upper left), Roe (upper right), continuous (lower left) and Alternating (lower right) methods.