Optimal control for conservation laws

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An optimal control problem for Burgers equation

We consider the inviscid Burgers equation:

$$\begin{cases} \partial_t u + \partial_x(\frac{u^2}{2}) = 0, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), & x \in \mathbb{R} \end{cases} \tag{1}$$

Given a target $u^d \in L^2(\mathbb{R}))$ we consider the cost functional to be minimized $J : L^1(\mathbb{R}) \to \mathbb{R}$, defined by

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

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

We also introduce the set of admissible initial data $\mathcal{U}_{ad} \subset L^1(\mathbb{R})$.

We consider the inverse design problem: Find $u^{0,\min} \in \mathcal{U}_{ad}$ such that

$$J(u^{0,\min}) = \min_{u^0 \in \mathcal{U}_{ad}} J(u^0). \tag{3}$$

Main questions

1. Existence of minimizers. We include conditions on the admissible set to guarantee compactness of minimizing sequences. We can consider

$$\mathcal{U}_{ad} = \{f \in L^\infty,\ supp(f) \subset K,\ \|f\|_{L^\infty} \leq C\}.$$

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 $u_\Delta^{0,\min}$ s.t.

$$J_\Delta(u_\Delta^{0,\min}) = \min_{u_\Delta^0 \in \mathcal{U}_\Delta} J_\Delta(u^0),$$

4. Convergence of discrete minimizers when $\Delta \to 0$ (conservative monotone schemes satisfying the discrete one-side Lipschitz condition OSLC).

Main difficulty: numerical approximation of minimizers

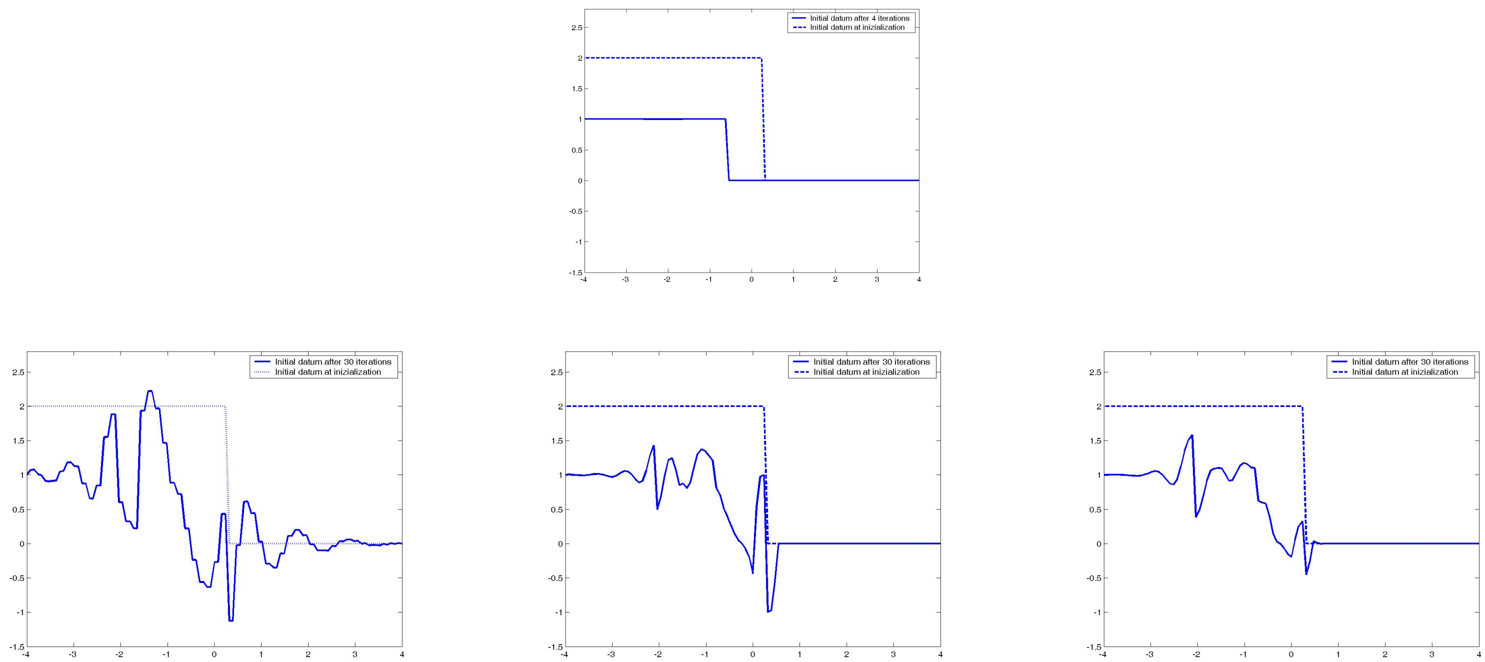
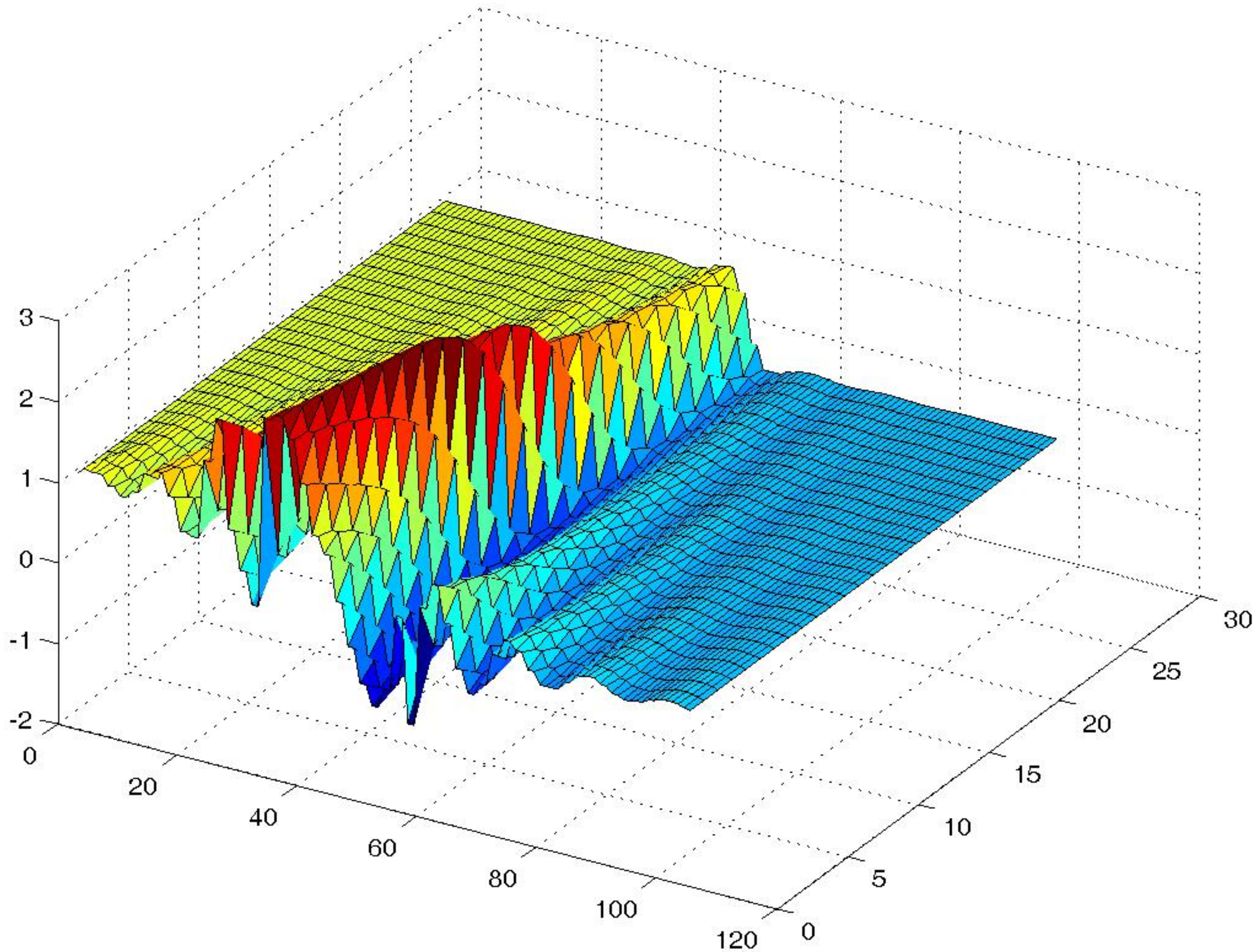


Figure 1: upper figure: $u0$ (dashed line) and uT. Initialization (dashed line) and initial data obtained after 30 iterations (solid line) with Lax-Friedrichs (left) , Engquist-Osher (medium), Roe (right)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Discrete problem

Assume that we discretize the Burgers equation using one of the convergent conservative numerical scheme (Lax-Friedrichs, upwind, etc.) and we take

$$J_\Delta(u^0_\Delta) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \tag{4}$$

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

Let us introduce an approximation of the space $\mathcal{U}_{ad}$, $\mathcal{U}^\Delta_{ad}$ constituted by sequences $u_\Delta = \{v_j\}_{j\in\mathbb{Z}}$ for which the function obtained by piecewise constant interpolation u_Δ, defined by

$$u_\Delta(x) = u_j, \quad x_{j-1/2} < x < x_{j+1/2},$$

satisfies $u_\Delta \in \mathcal{U}_{ad}$.

Problem: Find $u^{0,\min}_\Delta$ such that

$$J_\Delta(u^{0,\min}_\Delta) = \min_{u^0_\Delta \in \mathcal{U}^\Delta_{ad}} J_\Delta(u^0_\Delta). \tag{5}$$

Methods to approximate the gradient

- The discrete approach.
- The continuous approach.

Solutions of scalar conservation laws

The linear advection equation

$$\partial_t u + a\partial_x u = 0, \quad x \in \mathbb{R},\ t > 0 \tag{6}$$

where a is a given constant. For a given initial datum

$$u(0,x) = u^0(x), \quad x \in \mathbb{R},$$

the Cauchy problem is well-defined and the solution is simply

$$u(t,x) = u^0(x - at),\ t \geq 0.$$

The solution u at time $t = t_0$ is a pure translation of the initial datum u^0. In fact, if we define the *characteristic lines* of (6) as

$$x'(t) = a,\ x(0) = x_0 \in \mathbb{R},$$

the solution u satisfies

$$\frac{d}{dt}u(t,x(t)) = 0,$$

Two important properties:

1. Finite speed of propagation.
2. Characteristics allow to define a natural notion of weak solution for such cases.

The inviscid Burgers equation

$$\begin{cases} \partial_t u + \partial_x(\frac{u^2}{2}) = 0, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), \end{cases}$$

Our main objective is to study the main properties of the solutions of this problem and their numerical approximation.

Characteristics

Let $u(x,t)$ be a smooth solution of the Burgers equation

$$\partial_t u + \partial_x(\frac{u^2}{2}) = 0$$

Then,

$$\partial_t u + u\partial_x u = 0.$$

We introduce the characteristics as the integral curves $x(t)$ of the differential equation

$$\frac{dx}{dt} = u(x,t).$$

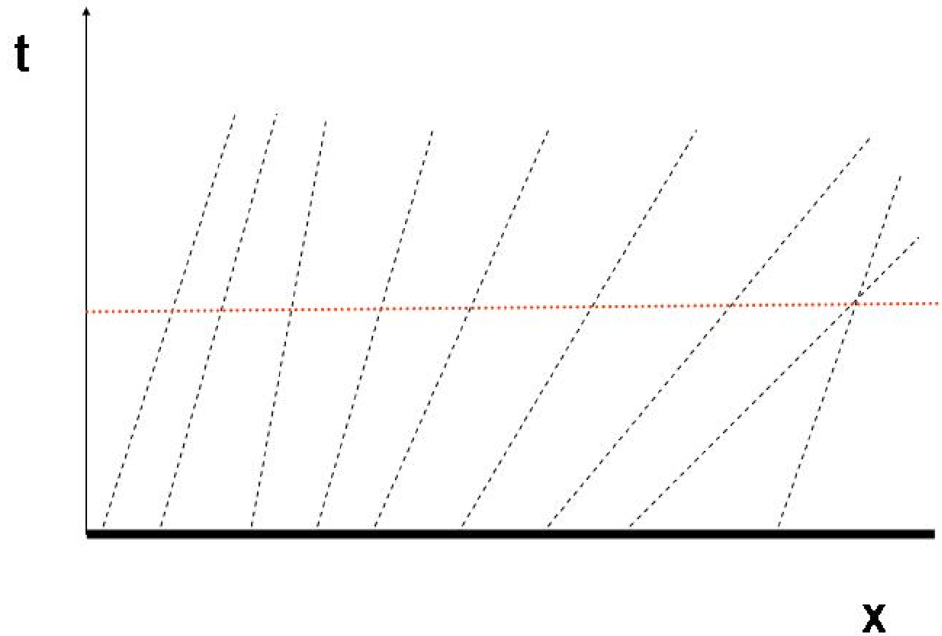
Along these curves the solution is constant since

$$\begin{aligned} \frac{d}{dt}u(x(t),t) &= \partial_t u(x(t),t) + \partial_x (u(x(t),t))\frac{dx}{dt} \\ &= \partial_t u(x(t),t) + \partial_x (u(x(t),t))u(x(t),t) = 0. \end{aligned}$$

Therefore

$$\frac{dx}{dt} = u(x,t) = u^0(x(0),0),$$

and the characteristics are straight lines whose slopes depend on the initial data.



Note that, for some initial data (even for smooth ones) two different characteristics lines may possibly meet at some time $t = t_0$. In this case, the solution cannot be continuous for $t > t_0$ and classical solutions will not exist.

Weak solutions

Let u be a smooth solution of Burgers equation and let $\varphi \in C_0^1(\mathbb{R} \times [0,T))$ be a test function. Multiplying the equation of u by φ and integrating we obtain

$$
\begin{aligned}
0 &= \int_0^\infty \int_{\mathbb{R}} \left(\partial_t u + \partial_x \left(\frac{u^2}{2}\right) \right) \varphi \\
&= -\int_0^\infty \int_{\mathbb{R}} \left(\partial_t \varphi + \frac{u^2}{2} \partial_x \varphi \right) - \int_{\mathbb{R}} u(x,0)\varphi(x,0).
\end{aligned}
$$

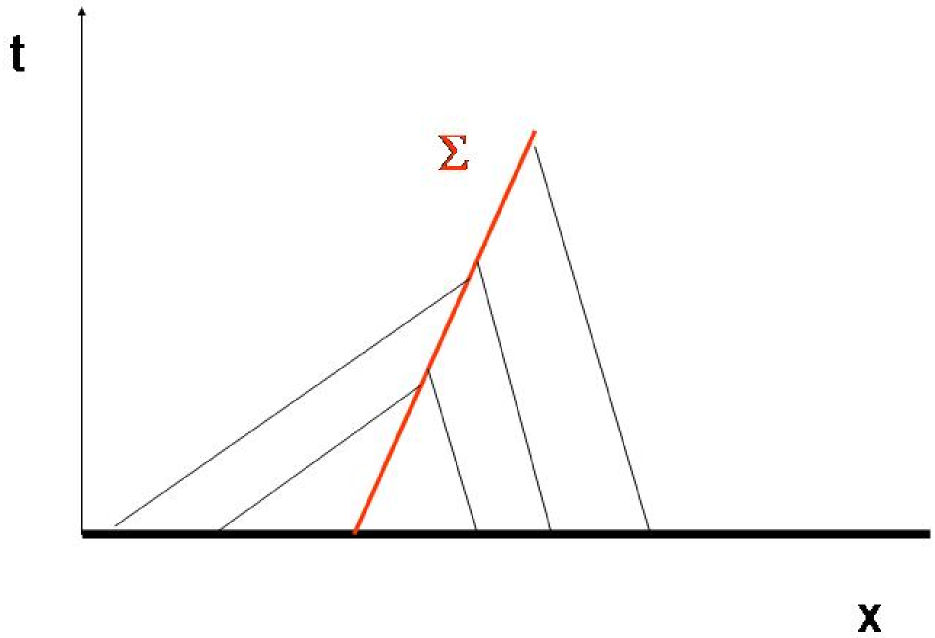
We adopt this identity as the definition of **weak solution**.

The following characterization of weak solutions is easily proved:

1. u is a classical solution when smooth (C^1).
2. u satisfies the Rankine-Hugoniot conditions

$$[u]_\Sigma n_t + [u^2/2]_\Sigma n_x = 0$$

along discontinuities Σ.



If we parametrize the discontinuity Σ with a function $s(t)$ by

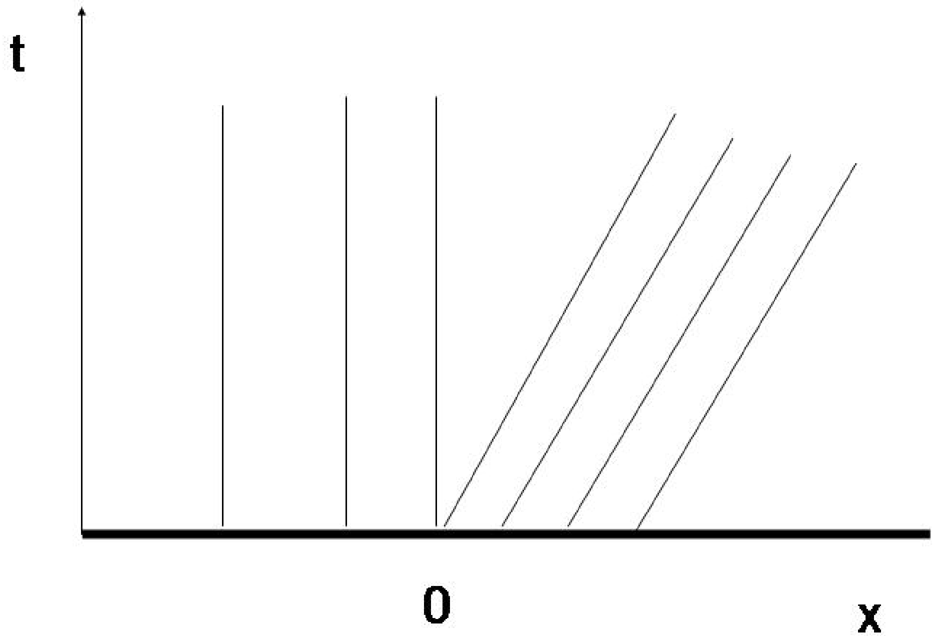
$$\Sigma = \{(t, s(t)),\ t \in (0, T)\}$$

then $s(t)$ must satisfy

$$s'(t) = \frac{[u^2/2]_{(t,s(t))}}{[u]_{(t,s(t))}}.$$

Weak solutions allows us to determine the physically relevant solution when characteristics intersect. However, this definition does not provide unicity for some initial data.

A situation where characteristics do not fill the domain



In general, the physical relevant solution is obtained by defining a new class of solutions, known as *entropy solutions*, for which unicity holds. Entropy solutions can also be characterized as limits, as $\varepsilon \to 0$, of solutions of the Burgers equations with viscosity:

$$\left\{ \begin{array}{ll} \partial_t u + \partial_x(\frac{u^2}{2}) = \varepsilon \partial_{xx} u, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), & \end{array} \right.$$

Numerical approximation of scalar conservation laws

A first example

Consider the advection equation

$$\left\{\begin{array}{ll} \partial_t u + a\partial_x u = 0, & \text{in } \mathbb{R}\times(0,T), \\ u(x,0) = u^0(x). & \end{array}\right.$$

We introduce a uniform discretization in space and time. We take $\Delta t, \Delta x > 0$.

$$\left\{\begin{array}{ll} t^n = n\Delta t, & n \in \mathbb{N} \\ x_j = j\Delta x, & j \in \mathbb{Z} \end{array}\right.$$

Our objective is to compute $u_j^n \sim u(x_j, t^n)$.

The simplest scheme:

$$\frac{u_j^{n+1} - u_j^n}{\Delta t} + a\frac{u_{j+1}^n - u_{j-1}^n}{\Delta x} = 0,$$

does not converge!!

Teorema (Lax) A consistent and stable numerical scheme is convergent.

Consistent schemes

The order of accuracy of a difference scheme is the largest number $p \geq 1$ such that any smooth solution u and for $\lambda = \Delta t/\Delta x$ constant, the numerical scheme evaluated on it provides a rest of the order

$$\mathcal{O}(\Delta t^{p+1}), \quad \text{as } \Delta t \to 0.$$

A numerical scheme is **consistent** if its order of accuracy is at lest 1.

The above scheme is consistent.

Stability

A numerical scheme is stable if it satisfies a discrete maximum principle: If $m \leq u_j^0 \leq M$ for all $j \in \mathbb{Z}$ then $m \leq u_j^n \leq M$ for all $n \in \mathbb{N}$ y $j \in \mathbb{Z}$

The above numerical scheme is not stable. To see that we can perform the von Neumann analysis. We consider solutions of the type

$$u_j^n = A^n e^{ikj\Delta x}$$

and we see that the amplification factor is $|A| > 1$.

Conservative schemes

$$\partial_t u + \partial_x f(u) = 0,\ x \in \mathbb{R},\ t > 0, \quad (7)$$
$$u(x,0) = u^0(x). \quad (8)$$

We assume that f is a C^2 function, $u^0 \in L^\infty(\mathbb{R})$ and we set

$$a(u) = f'(u).$$

We set

$$\lambda = \frac{\Delta t}{\Delta x}.$$

General 3-point explicit difference scheme:

$$v_j^{n+1} = H(v_{j-1}^n, v_j^n, v_{j+1}^n),\ \forall n \geq 0, j \in \mathbb{Z}, \quad (9)$$

where $H : \mathbb{R}^3 \to \mathbb{R}$ is a continuous function and v_j^n denotes an approximation of the exact solution u at the grid point $(x_j = j\Delta x, t_n = n\Delta t)$.

Definition 1 *The above difference scheme can be put in conservation form if there exists a continuous function $g : \mathbb{R}^2 \to \mathbb{R}$ such that*

$$H(v_{-1}, v_0, v_1) = v^0 - \lambda[g(v_{-1}, v_0) - g(v_0, v_1)]. \tag{10}$$

The function g is called the numerical flux.

If we define

$$g^n_{j+1/2} = g(v^n_j, v^n_{j+1})$$

then, the numerical scheme (9) reads

$$v^{n+1}_j = v^n_j - \lambda(g^n_{j+1/2} - g^n_{j-1/2}). \tag{11}$$

The difference scheme (11) is consistent with equation (7) if

$$g(v, v) = f(v), \ \forall v \in \mathbb{R}. \tag{12}$$

Concerning the initial datum (8) we will consider any *suitable* discretization. A common choice is to take

$$v_{j,0} = \frac{1}{\Delta x} \int_{x_{j-1/2}}^{x_{j+1/2}} u^0(x)\, dx, \qquad (13)$$

where $x_{j+1/2} = (x_j + x_{j+1})/2$.

Finally the approximation by a conservative scheme of (7)-(8) is

$$v_j^{n+1} = v_j^n - \lambda(g_{j+1/2}^n - g_{j-1/2}^n), \; j \in \mathbb{Z}, \; n \geq 0 \qquad (14)$$

$$v_j^0 = v_{j,0}. \qquad (15)$$

The Lax-Wendroff theorem

For a given sequence (v_j^n) we introduce the piecewise constant function v_Δ defined in $(0,\infty)\times\mathbb{R}$ by

$$v_\Delta(t,x) = v_j^n, \quad t\in[t_n,t_{n+1}), \; x\in(x_{j-1/2},x_{j+1/2}). \tag{16}$$

Theorem 2 *(Lax-Wendroff) Assume that the difference scheme (11) is consistent with (7) and let $v^0 = (v_{j,0})$ be given by (13). Assume that there exists a sequence $\Delta x\to 0$ such that if $\Delta t = \lambda\Delta x$ (with λ constant)*

$$\|v_\Delta\|_{L^\infty((0,\infty)\times\mathbb{R}))} \leq C,$$
$$v_\Delta \text{ converges in } L^1_{loc}((0,\infty)\times\mathbb{R})) \text{ and a.e. to a function } u$$

Then u is a weak solution of (7)-(8).

The above theorem tell us that a difference scheme in conservation form which converges always converges to a weak solution.

The main questions now are:

- Find sufficient conditions to convergence.
- Find criteria which ensure that the limit is the unique entropy solution.
- Determine the order of accuracy of the difference scheme.

Some examples

Lax-Friedrichs scheme

$$\frac{u_j^{n+1} - \frac{1}{2}(u_{j+1}^n + u_{j-1}^n)}{\Delta t} + v\frac{u_{j+1}^n - u_{j-1}^n}{\Delta x} = 0,$$

which can be put in conservation form with the numerical flux

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

In the linear case, $q = 1$ and this scheme is L^2-stable under the CFL condition

$$|v|\frac{\Delta t}{\Delta x} \leq 1.$$

Upwind scheme

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+v\frac{u_{j+1}^n-u_j^n}{\Delta x}=0, \qquad \text{si } v<0,$$

$$\frac{u_j^{n+1}-u_j^n}{\Delta t}+v\frac{u_j^n-u_{j-1}^n}{\Delta x}=0, \qquad \text{si } v>0,$$

In the linear case, $q=|a\lambda|=|\nu|$ and the scheme is L^2-stable under the CFL condition.

Godunov scheme

The Godunov scheme is based on the exact solution of local Riemann problems. The numerical flux is given by

$$g(u,v)=\begin{cases}\min_{w\in[u,v]} f(w), & \text{if } u\le v\\ \max_{w\in[u,v]} f(w), & \text{if } v\le u\end{cases}$$

In the linear case, it coincides with the upwind difference scheme.

Optimization methods

1. Newton method.
2. Gradient methods.
   (a) Steepest descent.
   (b) Conjugate gradient.
   (c) Others (homogenization method, Level sets, etc.)
3. Others (Genetic algorithms, etc.)

Remark. Constraints are included by using Lagrange multipliers.

Gradient methods

We use the fact that the gradient of a functional J provides a local descent direction.

Let V be a Hilbert space and $J : V \rightarrow R$ a smooth cost function. Then $J'(v) : V \rightarrow R$ is linear and

$$\begin{aligned} J(v + \delta v) &= J(v) + J'(v)\, \delta v + o(\|\delta v\|) \\ &= J(v) + < Grad_v J, \delta v > + o(\|\delta v\|), \end{aligned}$$

where $\| \cdot \|$ and $< \cdot, \cdot >$ represents the norm and scalar product on V respectively.

The vector $Grad_v J \in V$ is knows as the gradient of J in $v \in V$.

In particular, taking $\delta v = -\lambda Grad_v J$ with $\lambda << 1$ we have

$$J(v - \lambda Grad_v J) - J(v) = -\lambda \|Grad_v J\|^2 + o(\lambda \|Grad_v J\|),$$

that must be negative if λ is sufficiently small.

Thus, the following sequence makes $J(v_n)$ to be a decreasing sequence:

$$v^{n+1} = v^n - \lambda Grad_{v_n} J$$

Descent method with optimal step

- Step 0: Choose $v_0 \in V$
- For $n = 1 : n$
  - Compute $w = -Grad_{v_n} J$,
  - Compute $\lambda_n =$ argmin $J(v_n + \lambda w)$
  - Take $v_{n+1} = v_n + \lambda_n w$
- end

Remark: The choice of λ_n requires to solve a one-dimension optimization problem.

Computing the gradient

We have to solve a finite dimensional optimización problem which comes from a suitable discretization of a continuous optimization problem.

In general we have to compute the gradient of a function

$$F_h(x, u_h(x)), \qquad x \in R^N, \quad \text{(discretization of the a functional F)}$$

where $u_h(x)$ satisfies

$$A_h(x, u_h(x)) = 0, \quad \text{(discretization of the fluid equations)}$$

In practice, there are three different method:

1. Finite differences.
2. Adjoint method for the discrete system.
3. Adjoint method for the continuous system.

1. Finite differences

It consists in computing the partial derivatives of F which respect to each one of the free variables $x \in R^N$. In this way,

$$(Grad_x F_h)_i = \frac{F_h(x + \alpha e_i, u_h(x + \alpha e_i)) - F_h(x, u_h(x))}{\alpha}, \qquad \alpha << 1, \quad i = 1, ..., N$$

$$A_h(x + \alpha e_i, u_h(x + \alpha e_i)) = 0, \quad \alpha << 1, \quad i = 1, ..., N.$$

where

$$e_i = (0, ..., 0, \underset{i}{1}, 0, ..., 0)$$

Advantages: Easy to implement numerically.

Drawbacks:

1. Choice of the parameter α. It must be sufficiently small but not too small to avoid numerical errors.
2. Very costly. It requires $N + 1$ evaluations of the objective function. In real applications, it can not be used.

2. Discrete adjoint

It is like the continuous adjoint method that we show below but applied to the discrete optimization problem.

Drawbacks:

1. It requires to differentiate the numerical algorithm (automatic differentiation).
2. The equations and their particularities are hidden in the numerical scheme.

3. Continuous adjoint

We compute the gradient of the continuous optimization problem and discretize it to obtain a *descent direction*.

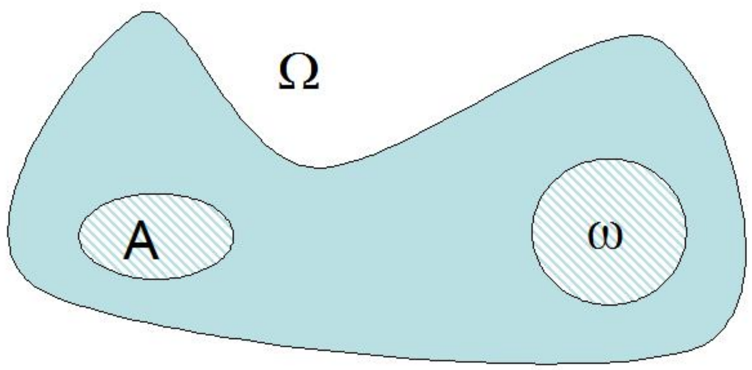
Example (optimal control problem)

Let $\Omega \subset \mathbb{R}^n$ be C^2 and $\omega \subset \Omega$ an open nonempty subset. We consider the following system:

$$\begin{cases} -\Delta u(x) = g(x)\chi_\omega(x), \text{ en } \Omega \\ u = 0, \text{ en } \partial\Omega, \end{cases} \tag{17}$$

where $\chi_\omega(x)$ is the characteristic function of the subset ω.

Problem 1: *Given $A \subset \Omega$ and $h \in L^2(A)$, compute $g \in L^2(\Omega)$ such that $u(x)\chi_A(x) = h(x)$ in A.*



In general, this problem has no solution. For instance, if A is not a subset of ω a necessary condition is to take h an harmonic function in $A\backslash\omega$.

Problem 2: *Given $A \subset \Omega$ and $h \in L^2(A)$, compute $g \in L^2(\Omega)$ such that $u(x)\chi_A(x)$ is as close as we want to $h(x)$ in A.*

To solve this problem we introduce the functional $J_k : L^2(\omega) \longrightarrow \mathbb{R}$ defined by

$$J_k(g) = \frac{1}{2}\int_A |u-h|^2 dx + \frac{k}{2}\int_\omega |g|^2 dx$$

and we look for

$$\min_{g\in L^2(\omega)} J_k(g), \qquad k \text{ suficiently large.}$$

We observe that J_k is a continuous, coercive and convex functional. Thus, it has a minimizer g_k.

We now illustrate the adjoint method to compute the gradient of J_k,

$$grad\ J_k(g) \in L^2(\omega)$$

.

Let us define δJ_k the derivative of the cost function J_k in a generic direction δg. Then,

$$\delta J_k = \int_A (u-h)\delta u \; dx + k \int_\omega g\delta g \; dx,$$

where δu solves the linearized problem,

$$\begin{cases} -\Delta\delta u(x) = \delta g(x)\chi_\omega(x), \text{ in } \Omega \\ \delta u = 0, \text{ on } \partial\Omega. \end{cases} \tag{18}$$

We want to write the expression of δJ_k like

$$\delta J_k = (grad\; J_k(g), \delta g)_{L^2(\omega)} = \int_\omega grad\; J_k(g)\; \delta g \; dx$$

To eliminate δu we introduce the adjoint to the linearized problem

$$\begin{cases} -\Delta p = (u-h)\chi_A(x), & x \in \Omega \\ p = 0, & x \in \partial\Omega, \end{cases}$$

Multiplying the equations of δu by p and integrating by parts we obtain

$$\int_\omega \delta g \; p = -\int_\Omega \Delta\delta u p = -\int_\Omega \delta u \Delta p = \int_A (u-h)\delta u$$

Therefore,

$$grad\ J_k(g) = p\chi_\omega + kg$$

and we can write

$$\delta J_k = \int_\omega (p\chi_\omega + kg)\delta g$$

Discrete problem

Assume that we discretize the Burgers equation using one of the convergent conservative numerical scheme (Lax-Friedrichs, upwind, etc.) and we take

$$J_\Delta(u^0_\Delta) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \tag{19}$$

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

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

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

Let us introduce an approximation of the space $\mathcal{U}_{ad}$, $\mathcal{U}_{ad}^\Delta$ constituted by sequences $u_\Delta = \{v_j\}_{j\in\mathbb{Z}}$ for which the function obtained by piecewise constant interpolation u_Δ, defined by

$$u_\Delta(x) = u_j, \quad x_{j-1/2} < x < x_{j+1/2},$$

satisfies $u_\Delta \in \mathcal{U}_{ad}$.

Problem: Find $u_\Delta^{0,\min}$ such that

$$J_\Delta(u_\Delta^{0,\min}) = \min_{u^0_\Delta \in \mathcal{U}_{ad}^\Delta} J_\Delta(u^0_\Delta). \tag{20}$$

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,

$$g^{LF}(u,v) = \frac{u^2 + v^2}{4} - \frac{v-u}{2\lambda}, \qquad \text{or} \quad g^{EO}(u,v) = u\frac{u+|u|}{4} + v\frac{v-|v|}{4}$$

The derivative of the cost functional

$$J_\Delta(u_j^0) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \qquad (21)$$

is given by

$$\delta J_\Delta = \Delta x \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d) \delta u_j^{N+1}, \qquad (22)$$

where δu_j^n solves the linearized system

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

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

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

Thus, the gradient of J_Δ is given by p_j^0.

Lax-Friedrichs

1. Start with u^0_Δ.
2. Solve

$$\left\{ \begin{array}{l} \frac{u_j^{n+1} - \frac{u_{j-1}^n + u_{j+1}^n}{2}}{\Delta t} + \frac{f(u_{j+1}^n) - f(u_{j-1}^n)}{2\Delta x} = 0, \qquad n = 0, ..., N, \\ u_j^0 = u_{0,j}, \qquad j \in \mathbb{Z}, \end{array} \right. \tag{23}$$

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

$$\left\{ \begin{array}{l} \frac{p_j^n - \frac{p_{j+1}^{n+1} + p_{j-1}^{n+1}}{2}}{\Delta t} + u_j^n \frac{p_{j-1}^{n+1} - p_{j+1}^{n+1}}{2\Delta x} = 0, \qquad n = 0, ..., N \\ p_j^{N+1} = p_j^T, \quad j \in \mathbb{Z}, \end{array} \right. \tag{24}$$

4. Find the step of descent α
5. Take $u_j^0 = u_j^0 - \alpha p_j^0$
6. Return to 1

Algorithm 1: **solve** Burgers eq. with initial datum $\{u_j^0\}_{j=1,\ldots,N}^k \rightarrow \{u_j^n\}_{j=1,\ldots,N}^{n=1,\ldots,M}$

1 **input** Δx, Δt, $\{u_j^0\}_{j=1,\ldots,N}$
2 **set** $\lambda = \Delta t / \Delta x$
3 **for** $n = 0(1)M-1$ **repeat**
4   **set** $u_1^{n+1} = u_1^0$, $u_N^{n+1} = u_N^0$
5   **for** $j = 2(1)N-1$ **repeat**
6   **set** $u_j^{n+1} = u_j^n + \lambda(g(u_j^n, u_{j+1}^n) - g(u_{j-1}^n, u_j^n))$
7   **end**
8 **end**

Line	Comments
2	λ satisfies the CFL condition.
6	g is the numerical convective flux.

Algorithm 2: **solve** adjoint eq. with final datum $\{p_j^T\}_{j=1,\dots,N} \longrightarrow \{p_j^0\}_{j=1,\dots,N}$

1 **input** Δx, Δt, $\{u_j^n\}_{j=1,\dots,N}$
2 **set** $\lambda = \Delta t / \Delta x$
2 **for** $n = 0(1)M$ **repeat**
3   **set** $p_1^{n-1} = p_1^M$, $p_N^{n-1} = p_N^M$,
4   **for** $j = 2(1)N-1$ **repeat**
5   **set** $p_j^{n-1} = p_j^n + \lambda(\partial_1 g(u_j^{n-1}, u_{j+1}^{n-1}) * (p_j^n - p_{j+1}^n)$
6             $+\partial_2 g(u_{j-1}^{n-1}, u_j^{n-1}) * (p_{j-1}^n - p_j^n))$
7   **end**
8 **end**

Line	Comments
2	λ satisfies the CFL condition.
6	g is the numerical convective flux.

Algorithm 3: Discrete approach

STEP 0: initialization

1 **input** Δx, Δt, $\{u_j^0\}_{j=1,\ldots,N}$, $\{u^d\}_{j=1,\ldots,N}$

2 **set** $\lambda = \Delta t / \Delta x$

STEP 1: optimization loop

1 **input** ε

2 **for** $k = 0, 1, \ldots$ **repeat**

3   **solve** Burgers eq. with initial datum $\{u_j^0\}_{j=1,\ldots,N}^k \longrightarrow \{u_j^n\}_{j=1,\ldots,N}^{n=1,\ldots,M}$

4   **for** $j = 1(1)N$ **repeat**

5   **set** $p_j^T = u_j^M - u_j^d$

6   **end**

7   **solve** adjoint eq. with final datum $\{p_j^T\}_{j=1,\ldots,N} \longrightarrow \{p_j^0\}_{j=1,\ldots,N}$

8   **set** $g_k = \{p_j^0\}_{j=1,\ldots,N}$,

9   **compute** α_k

10   **set** $\{u_j^0\}_{j=1,\ldots,N}^{k+1} = \{u_j^0\}_{j=1,\ldots,N}^k - \alpha_k * g_k$

11 **end until** $||g_{k+1}|| < \varepsilon$

Line	Comments
1	ε is the tolerance.
9	Compute the descent step α_k arg min. $J(\{u_j^0\}_{j=1,\ldots,N}^k - \alpha_k * g_k)$.
11	$\|\| \cdot \|\|$ is the Euclidean norm in $\mathbb{R}^N$.

The discrete approach: Non-differentiable numerical schemes

Assume now that the Burgers equation 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,

$$g^{Up}(u, v) = \frac{1}{4}(u^2 + v^2 - |u + v|(v - u))$$

In this case non-smooth optimization techniques are necessary.

A proposed linearization (Godlewski-Raviart, 1995),

$$\delta g(u,v) = \frac{1}{4}((2u+2v)(\delta u + \delta v) - |u+v|(\delta v - \delta w))$$

The continuous approach in presence of a single shock

Assume that $u(x,t)$ is a weak entropy solution of Burgers equation with a discontinuity along a regular curve $\Sigma = \{(t,\varphi(t)), t \in [0,T]\}$, which is Lipschitz continuous outside Σ. In particular, it satisfies the Rankine-Hugoniot condition on Σ

$$\varphi'(t)[u]_{\varphi(t)} = \left[u^2/2\right]_{\varphi(t)} . \tag{25}$$

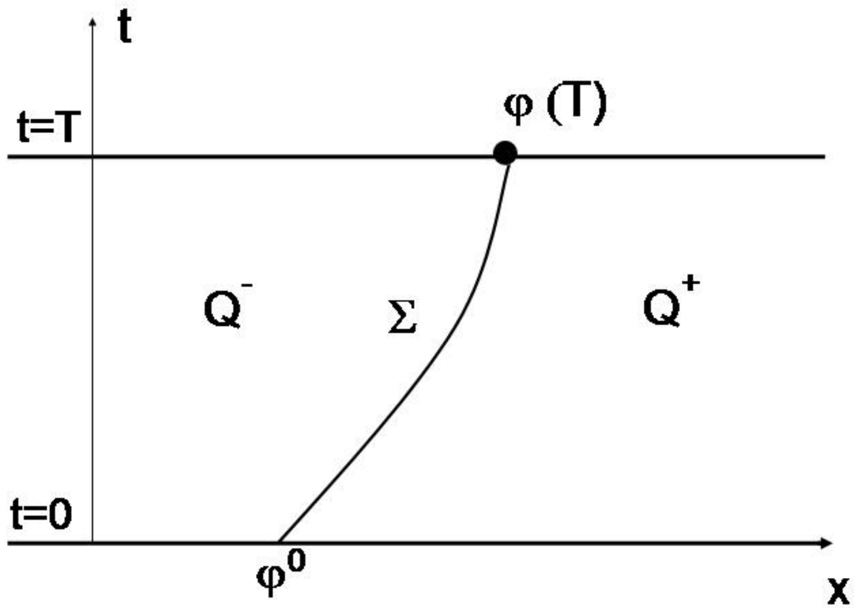
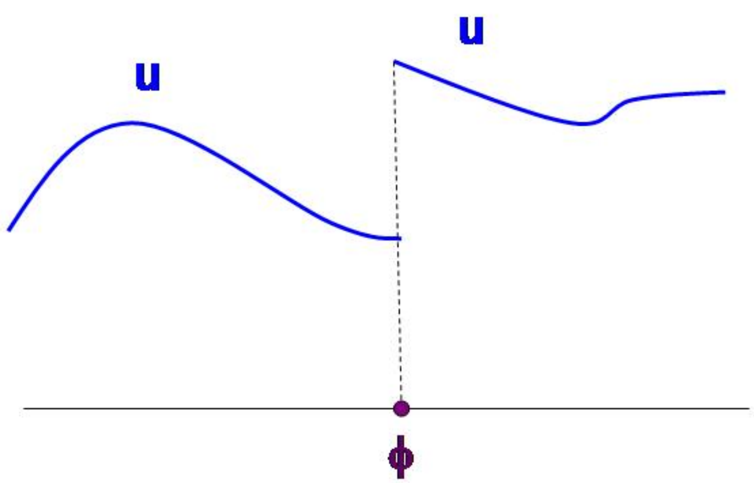
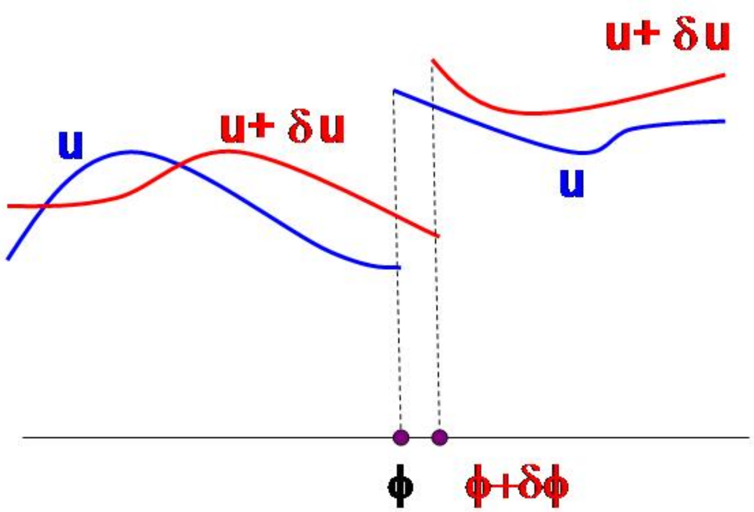


Figure 2: Subdomains Q^- and Q^+.

Then the pair (u, φ) satisfies the system

$$\left\{\begin{array}{ll} \partial_t u + \partial_x(\frac{u^2}{2}) = 0, & \text{in } Q^- \cup Q^+, \\ \varphi'(t)[u]_{\varphi(t)} = [u^2/2]_{\varphi(t)}\,, & t \in (0,T), \\ \varphi(0) = \varphi^0, & \\ u(x,0) = u^0(x), & \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}. \end{array}\right. \quad (26)$$





The **generalized tangent vector** $(\delta u, \delta\varphi)$ satisfies the following linearized system (Bressan and Marson, Ulbrich, Godlewski and Raviart, etc.):

$$\left\{ \begin{array}{l} \partial_t \delta u + \partial_x (u \delta u) = 0, \quad \text{in } Q^- \cup Q^+, \\ \delta\varphi'(t)[u]_{\varphi(t)} + \delta\varphi(t) \left(\varphi'(t)[u_x]_{\varphi(t)} - [u_x u]_{\varphi(t)} \right) \\ \quad + \varphi'(t)[\delta u]_{\varphi(t)} - [u \delta u]_{\varphi(t)} = 0, \quad \text{in } (0,T), \\ \delta u(x,0) = \delta u^0, \quad \text{in } \{x < \varphi^0\} \cup \{x > \varphi^0\}, \\ \delta\varphi(0) = \delta\varphi^0, \end{array} \right. \tag{27}$$

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

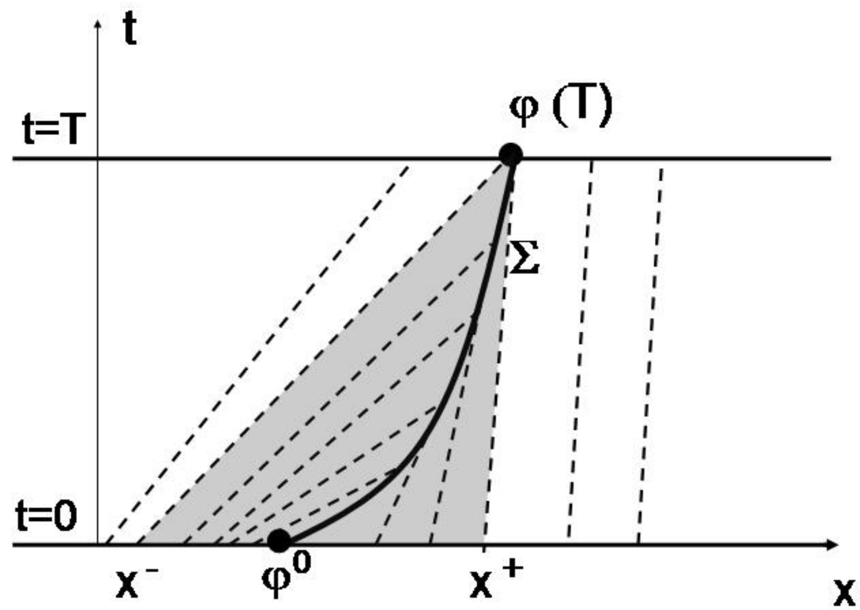


Figure 3: Characteristic lines entering on a shock

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

$$\delta J = \int_{\{x<\varphi^0\}\cup\{x>\varphi^0\}} p(x,0)\delta u^0(x)\, dx + q(0)[u^0]_{\varphi^0}\delta\varphi^0, \tag{28}$$

where the adjoint state pair (p, q) satisfies the system

$$\begin{cases} -\partial_t p - u\partial_x p = 0, \quad \text{in } Q^- \cup Q^+, \\ [p]_\Sigma = 0, \\ q(t) = p(\varphi(t), t), \ \text{in } t \in (0,T) \\ q'(t) = 0, \ \text{in } t \in (0,T) \\ p(x,T) = u(x,T) - u^d, \quad \text{in } \{x < \varphi(T)\} \cup \{x > \varphi(T)\} \\ q(T) = \dfrac{\frac{1}{2}\left[(u(x,T) - u^d)^2\right]_{\varphi(T)}}{[u]_{\varphi(T)}}. \end{cases} \tag{29}$$

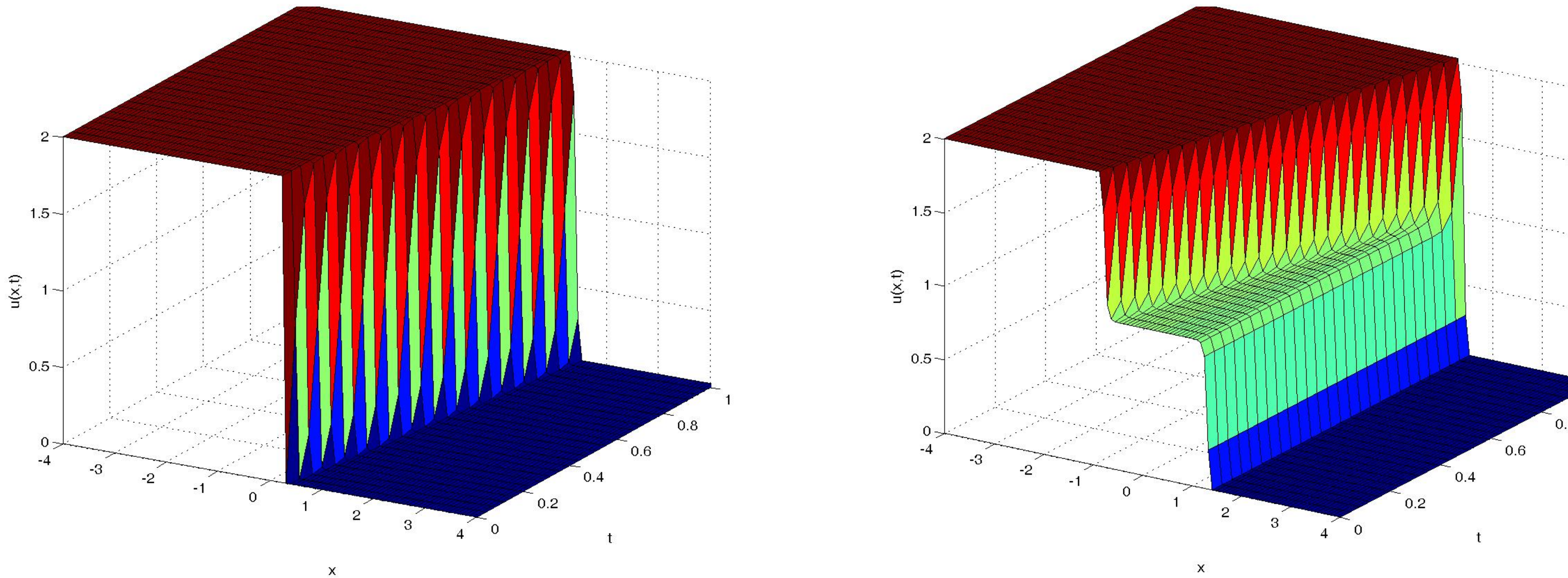


Figure 4: Solution $u(x,t)$ of the Burgers equation with an initial datum having a discontinuity (left) and adjoint solution which takes a constant value in the region occupied by the characteristics that meet the shock (right).

The new initial datum is $(\delta\varphi^0 > 0)$

$$u_j^{0,new} = \begin{cases} u_j^0 + \varepsilon\delta u_j^0, & \text{if } j < \varphi^0 \text{ or } j > \varphi^0 + \varepsilon\delta\varphi^0/\Delta x, \\ u_j^0 + \varepsilon\delta u_j^0 + [u_j^0]_{\varphi^0}, & \text{if } \varphi^0 \le j \le \varphi^0 + \varepsilon\delta\varphi^0/\Delta x. \end{cases}$$

The main drawbacks of this approach are the following:

1. At any step of the descent algorithm, a numerical approximation of the position of the shock is required.
2. The first component in $(p(x,0), q(0))$ has two discontinuities which are not at the same place at the discontinuity of u^0. Thus, an iterative gradient method based on this gradient generates increasingly complex initial data. Numerical experiments confirm that this actually occurs.
3. A pure displacement of the discontinuity will never be a descent direction computed by this method.

The alternating descent method

Let

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

and consider the following subsets ,

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

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

Theorem 3 *Assume that we restrict the generalized tangent vectors* $(\delta u^0, \delta\varphi^0) \in T_{u^0}$ *to those that satisfy,*

$$\delta\varphi^0 = \frac{\int_{x^-}^{\varphi^0} \delta u^0 + \int_{\varphi^0}^{x^+} \delta u^0}{[u]_{\varphi^0}}. \tag{30}$$

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*

$$\delta J = \int_{\{x<x^-\}\cup\{x>x^+\}} p(x,0)\delta u^0(x)\, dx, \tag{31}$$

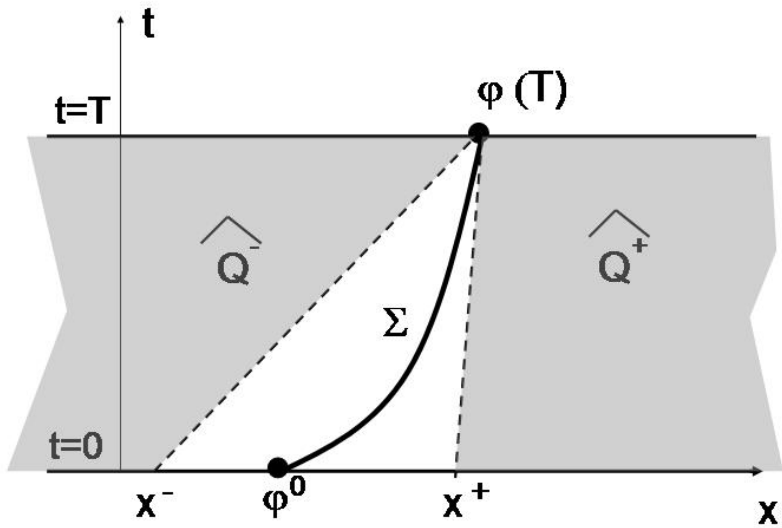


Figure 5: Subdomains $\hat{Q}^-$ and $\hat{Q}^+$

where p satisfies the system

$$\begin{cases} -\partial_t p - u\partial_x p = 0, & \textit{in } \hat{Q}^- \cup \hat{Q}^+, \\ p(x,T) = u(x,T) - u^d, & \textit{in } \{x < \varphi(T)\} \cup \{x > \varphi(T)\}. \end{cases} \tag{32}$$

Analogously, if we restrict the set of paths in Σ_{u^0} to those for which the associated generalized tangent vectors $(\delta u^0, \delta\varphi^0) \in T_{u^0}$ satisfy $\delta u^0 = 0$, then $\delta u(x,T) = 0$ and the generalized Gateaux derivative of J in the direction

$(\delta u^0, \delta\varphi^0)$ *can be written as*

$$\delta J = -\left[\frac{(u(x,T) - u^d(x))^2}{2}\right]_{\varphi(T)} \frac{[u^0]_{\varphi^0}}{[u(\cdot,T)]_{\varphi(T)}} \delta\varphi^0. \qquad (33)$$

Numerical experiments

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

$$u^d = \begin{cases} 1 \text{ if } x < 0, \\ 0 \text{ if } x \geq 0, \end{cases} \tag{34}$$

and the time $T = 1$. Note that in this case one solution of the optimization problem is obviously given by

$$u^{0,min} = \begin{cases} 1 \text{ if } x < -1/2, \\ 0 \text{ if } x \geq 0. \end{cases} \tag{35}$$

This means that the optimal value $u^{0,min}$ can be attained and the minimum value of J in this case is zero.

$\log(J^\Delta)$	-3	-4	-5	-6	-7
Lax-Friedrichs	14	39	> 1000		
Engquist-Osher	26	85	288	> 1000	
Roe	18	33	54	114	> 1000
Imposing b.c.	5	6	9	21	> 1000
Alternating descent	3	3	3	Not attained	

$\log(J^\Delta)$	-3	-4	-5	-6	-7
Lax-Friedrichs	15	49	> 1000		
Engquist-Osher	115	673	> 1000		
Roe	185	> 1000			
Imposing b.c.	5	6	52	440	> 1000
Alternating descent	3	3	3	3	Not attained

Table 1: Experiment 1. Number of iterations needed for a descent algorithm to obtain the value of $\log(J)$ indicated in the upper row, by the different methods presented above. The upper table corresponds to $\Delta x = 1/20$ and the lower one to $\Delta x = 1/80$. In both cases $\lambda = \Delta t/\Delta x = 1/2$.

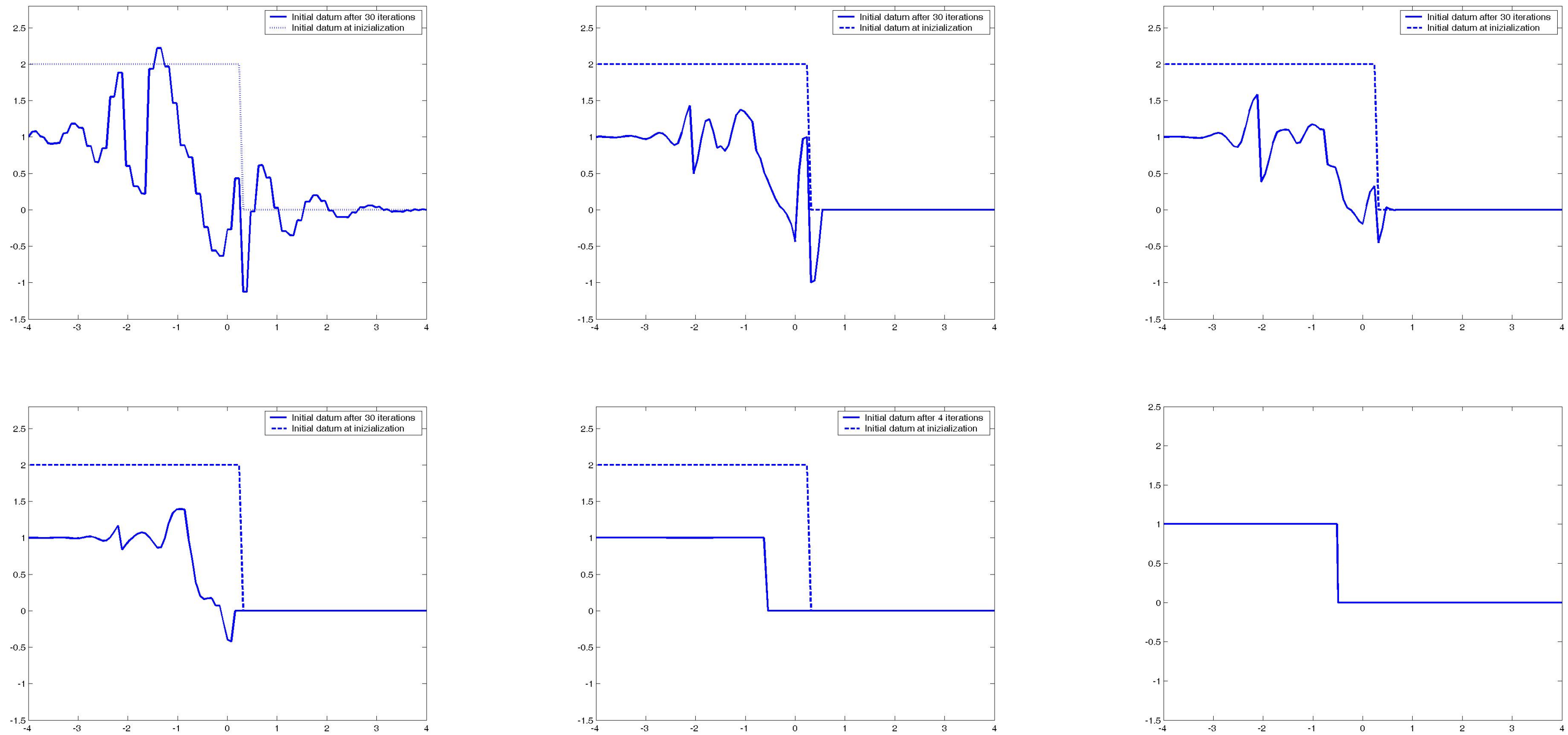


Figure 6: Experiment 1. Initialization (dashed line) and initial data obtained after 30 iterations (solid line) with Lax-Friedrichs (upper left) , Engquist-Osher (upper right), Roe (middle left), the continuous approach imposing a boundary condition on the shock (middle right) and the generalized tangent vectors decomposition method schemes (lower left). A minimizer u^0 of the continuous functional is given in the lower right figure.

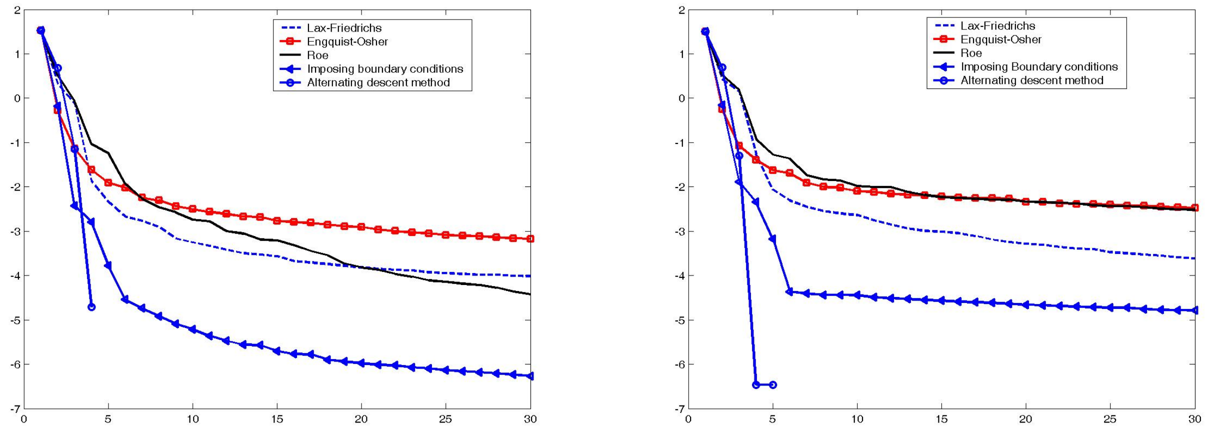


Figure 7: Experiment 1. Log of the value of the functional versus the number of iterations in the descent algorithm for the Lax-Friedrichs, Engquist-Osher and Roe schemes, the continuous approach imposing the internal boundary condition on the shock and the alternating descent method proposed in this article. The upper figure corresponds to $\Delta x = 1/20$ and the lower one to $\Delta x = 1/80$. We see that the last method stabilizes in a few iterations and it is much more efficient when consider small enoughvalues of Δx in order to be able to resolve the shock sufficiently well.

We observe the following:

1. Different numerical approximation and descent methods lead to different solutions.

2. For the first four methods the initial datum u^0 we obtain after the iteration process presents strong oscillations. That is not the case for the alternating descent method.

3. Numerical methods that ignore the presence of the shock (Lax-Friedrichs, Engquist-Osher and Roe) descend more slowly than those that take into account the sensitivity with respect to the shock position (by imposing the boundary condition on the shock or the alternating descent method).

4. For fixed Δx the alternating descent method stabilizes quickly in a few iterations. This is due to the fact that the descent direction is computed for the continuos system and not for the discrete one, and therefore Δx needs to be small for that computation to be valid at the discrete level as well.

5. For smaller values of Δx the only method that remains effective is the alternating descent method. The other methods descent more slowly.

A flux identification problem for scalar conservation laws

Statement

We consider the 1-d scalar conservation law:

$$\begin{cases} \partial_t u + \partial_x (f(u)) = 0, & \text{in } \mathbb{R} \times (0,T), \\ u(x,0) = u^0(x), & x \in \mathbb{R} \end{cases} \tag{36}$$

Given a target $u^d \in L^2(\mathbb{R})$ we consider the cost functional to be minimized $J : \mathcal{U}_{ad} \to \mathbb{R}$, defined by

$$J(f) = \int_{\mathbb{R}} \left| u(x,T) - u^d(x) \right|^2 \, dx, \tag{37}$$

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

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

$$J(f^{\min}) = \min_{f \in \mathcal{U}_{ad}} J(f). \tag{38}$$

(James and Sepúlveda, 1999)

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) Introduce a finite dimensional subspace of $\mathcal{U}_{ad}$, $\mathcal{U}_{ad}^K$, as the linear space generated by a set of base functions

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

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

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

4. Convergence of discrete minimizers when $\Delta \to 0$ (conservative monotone schemes satisfying the discrete one-side Lipschitz condition OSLC).

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

$$J_\Delta(f) = \frac{\Delta x}{2} \sum_{j=-\infty}^{\infty} (u_j^{N+1} - u_j^d)^2, \qquad (39)$$

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

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

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

$$J_\Delta(f_\Delta^{\min}) = \min_{f \in \mathcal{U}_{ad}^K} J_\Delta(f). \qquad (40)$$

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 continuous approach for smooth solutions

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

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

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

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

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

$$\varphi'(t)[u]_{\varphi(t)} = [f(u)]_{\varphi(t)} \,. \tag{41}$$

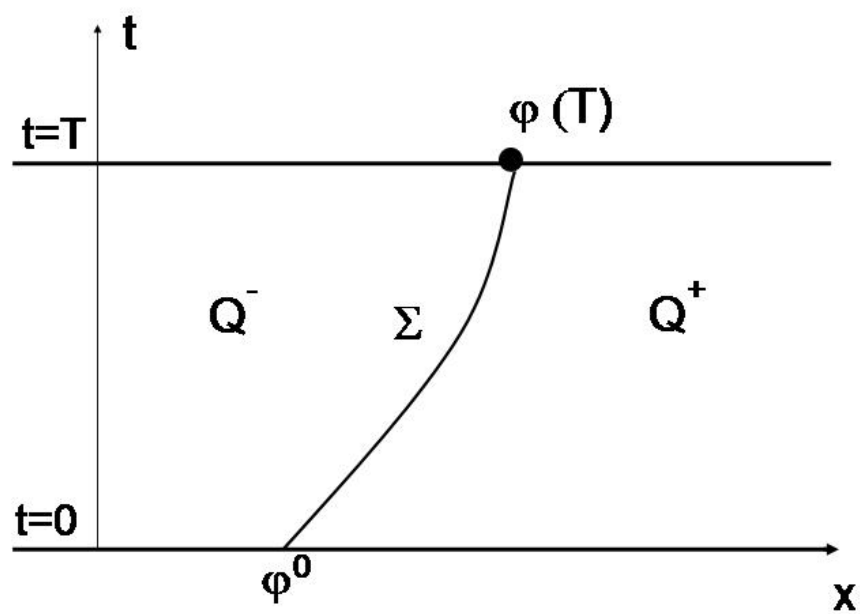


Figure 8: Subdomains Q^- and Q^+.

Then

$$J(f) = \int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} |u(x,T) - u^d|^2 dx$$

$$\begin{aligned}\delta J &= -T\int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} \partial_x(\delta f(u))(x,T)(u(x,T) - u^d(x)) \\ &\quad + \frac{\frac{1}{2}\left[(u(x,T) - u^d)^2\right]_{\varphi(T)}}{[u]_{\varphi(T)}}[\partial_x(f(u(x,T)))]_{\varphi(T)}.\end{aligned}$$

The alternating descent method

Let

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

and consider the following subsets ,

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

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

Theorem 4 *Assume that we restrict the variations δf to those that satisfy,*

$$[\delta f(u(x,T))]_{\varphi(T)} dt = 0. \tag{42}$$

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

$$\delta J = -\int_{\{x<\varphi(T)\}\cup\{x>\varphi(T)\}} \partial_x(\delta f(u))(x,t)(u(x,T) - u^d(x))\, dx, \tag{43}$$

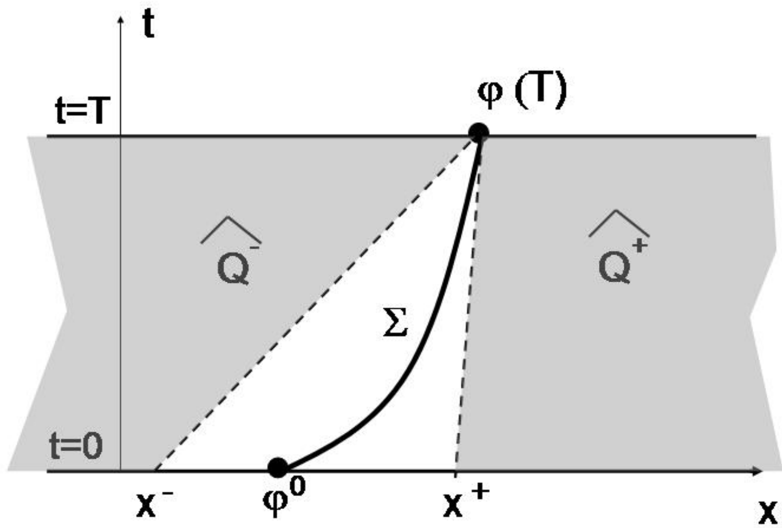


Figure 9: Subdomains $\hat{Q}^-$ and $\hat{Q}^+$

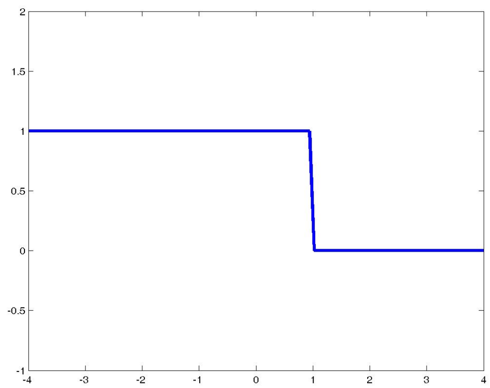
Numerical experiments

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

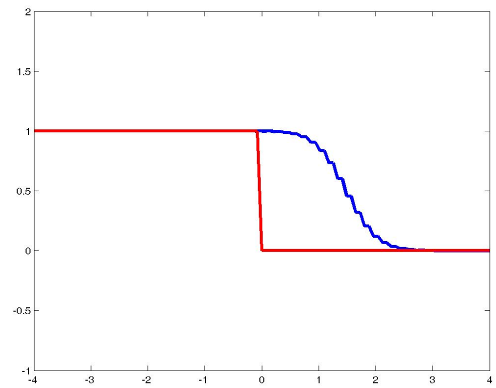
$$u^{0,min} = \begin{cases} 1 \text{ if } x < -1/2, \\ 0 \text{ if } x \geq 0. \end{cases} \tag{44}$$

$$u^d = \begin{cases} 1 \text{ if } x < 0, \\ 0 \text{ if } x \geq 0, \end{cases} \tag{45}$$

and the time $T = 1$.



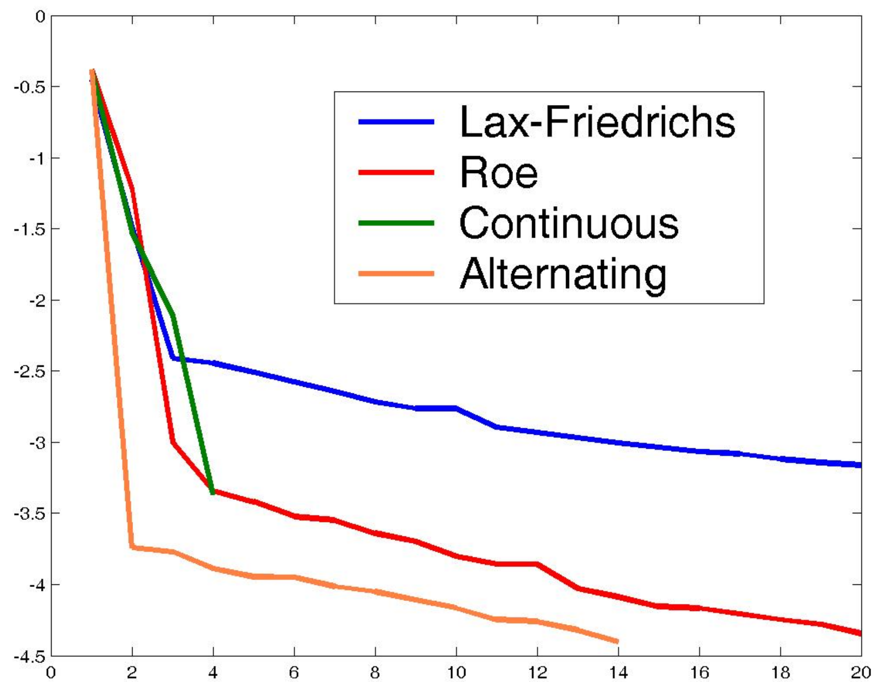
u^0



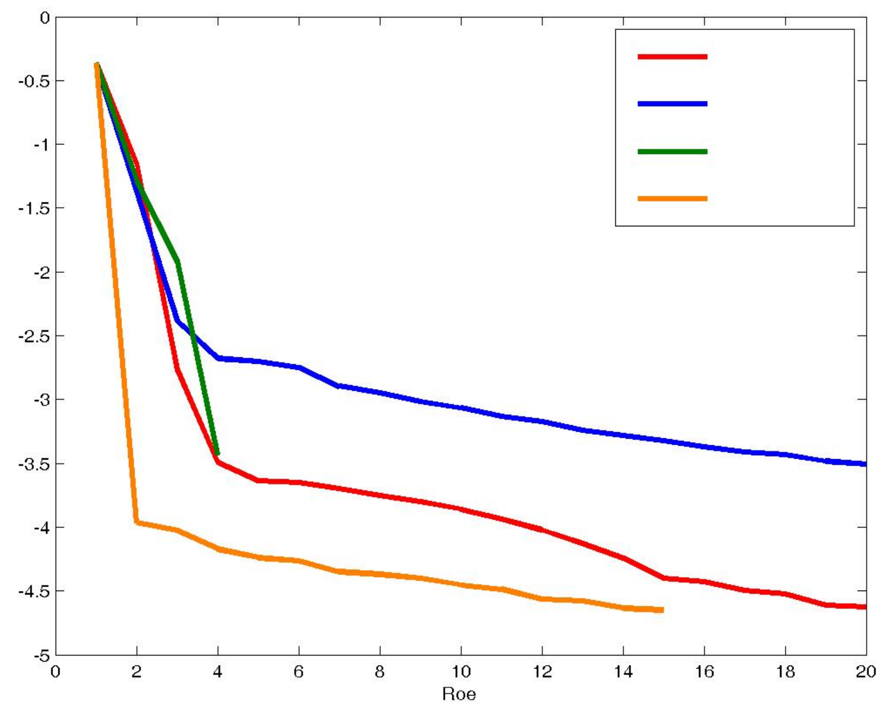
u^d and $u(x, T)$ at initialization

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

$\Delta x = 1/20$



$\Delta x = 1/40$



parameters	α_1	α_2	α_3	α_4	α_5	α_6
Lax-Friedrichs	-1.6171	0.9090	0.1985	0.2527	0.2472	0.2265
Roe	-1.0845	0.6545	-0.1473	-0.0725	-0.0398	-0.0243
Continuous	-0.8162	0.5305	-0.3393	-0.2680	-0.2222	-0.1901
Alternating	-1.0499	0.6524	-0.1520	-0.0729	-0.0354	-0.0159