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Uncertainty propagation of the shock position for hyperbolic PDEs using a sensitivity equation method

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Abstract. In this work, we design a method to provide confidence intervals for the position of a discontinuity arising in hyperbolic conservation laws when some of the parameters of the problem are uncertain. This is based on a sensitivity equation method, therefore can be used only if the variance of the uncertain parameters is small. We illustrate how this method works on a simple one-dimensional conservation law: the inviscid Burgers equation. Multiple test cases are defined, some for which the analytical solution is known, in order to test the method.

Keywords: hyperbolic conservation laws, shock position, uncertainty propagation, sensitivity equation method.

1 Introduction

First order nonlinear hyperbolic partial differential equations (PDEs) are known to develop discontinuities, even when the initial condition is continuous. This adds a challenge if one wants to perform uncertainty propagation studies: a slight change in an input parameter can bring important changes in the output in the neighbourhood of the discontinuity. This translates to a high variance of the output close to the discontinuity [10]. If such variance is then used to compute confidence intervals for the output, this leads to artificially large intervals in the neighbourhood of the discontinuity, sometimes even providing negative values for variables such as the pressure or the density [4]. The use of modified sensitivities in [2, 4] solved the problem of negative values, but is equivalent to neglecting the variance of the position of the discontinuity. In this work, we use a sensitivity equation method to provide a first order estimate of this neglected quantity.

Here we consider a scalar one-dimensional conservation law, for the sake of simplicity. However, this approach can be easily extended to systems. The extension to higher dimension, on the other hand, is more difficult and beyond the scope of this work.

2 State model

In this section, we describe the state model and its analytical solution: this is a well known problem and we use it mainly as an opportunity to introduce the notation. A scalar one dimensional conservation law can be written in the following form:

$$\begin{cases} \partial_t u(x, t) + \partial_x f(u(x, t)) = 0 & x \in \mathbb{R}, t > 0 \\ u(x, 0) = g(x) & x \in \mathbb{R}, \end{cases} \quad (1)$$

where $u(x, t)$ is the conserved variable, f the flux function and g the initial condition. The method of characteristics can be used to solve analytically (1), and one can write the solution implicitly as follows:

$$u(x, t) = g(x - tf'(u(x, t))), \quad (2)$$

where $f' = \frac{df}{du}$. This method is valid as long as there is no intersection among the characteristics: in case of intersection a shock is generated and the solution $u(x, t)$ becomes discontinuous. We can define the *breaking time* t_s as the smallest t for which the characteristics intersect:

$$t_s = -\frac{1}{\min h'(x)}, \quad (3)$$

where $h(x) := f'(g(x))$.

The point $x_{s,0}$ from which the shock originates is known too:

$$x_{s,0} = \bar{x} + h(\bar{x})t_s, \text{ where } \bar{x} := \operatorname{argmin} h'(x).$$

If the initial data g is discontinuous in a point x_d , two scenarios are possible: if $h(x_d^+) < h(x_d^-)$, the initial discontinuity is transported for all $t > 0$ ($t_s = 0$); otherwise the initial discontinuity is smoothed out and a rarefaction wave is generated.

Once the shock is generated, it moves along a curve $x_s(t)$ such that $\frac{dx_s}{dt} = v(t)$, which separates the plane (x, t) into two parts, and in both of them the method of characteristics is valid. We denote with the superscript $+$ (respectively $-$) the quantities in the right (respectively left) part of the plane, i.e. $x > x_s(t)$ (respectively $x < x_s(t)$). The speed of the shock $v(t)$ can be computed using the Rankine-Hugoniot conditions:

$$v(t) = \frac{f(u^+(x_s(t), t)) - f(u^-(x_s(t), t))}{u^+(x_s(t), t) - u^-(x_s(t), t)}. \quad (4)$$

The position of the shock $x_s(t)$ can be then determined by solving the following ODE:

$$\begin{cases} \frac{dx_s}{dt} = v(t), \\ x_s(t_s) = x_{s,0}. \end{cases} \quad (5)$$

Finally, the solution of (1) can be written in the following compact form:

$$u(x, t) = u^+(x, t)H(x - x_s(t)) + u^-(x, t)H(x_s(t) - x), \quad (6)$$

where u^\pm are obtained separately from (2) and H is the Heaviside function.

3 Sensitivity equation

3.1 Derivation of the sensitivity equation

In this section, we apply the continuous sensitivity equation (CSE) method to derive the sensitivity equations. First, we define the sensitivity with respect to a parameter of interest a as the derivative of the state u with respect to a and we use the notation u_a :

$$u_a = \frac{\partial u}{\partial a}. \quad (7)$$

We now apply the CSE method and we differentiate the system (1) with respect to the parameter a , obtaining:

$$\begin{cases} \partial_a(\partial_t u(x, t)) + \partial_a(\partial_x f(u(x, t))) = 0 & x \in \mathbb{R}, t > 0 \\ \partial_a u(x, 0) = \partial_a g(x) & x \in \mathbb{R}, \end{cases}$$

and exchanging the derivatives in space and time with the ones with respect to a one obtains the following equation and initial condition for the sensitivity:

$$\begin{cases} \partial_t u_a + \partial_x(f_a(u, u_a)) = 0 & x \in \mathbb{R}, t > 0 \\ u_a(x, 0) = g_a(x) & x \in \mathbb{R}, \end{cases} \quad (8)$$

where $g_a := \partial_a g$, $f_a(u, u_a) := f'(u)u_a + \partial_a f(u)$ and we dropped the time and space dependence in the equation for simplicity.

3.2 Analytical solution of the sensitivity equation

The analytical solution of (8) can be computed in the regular zones by differentiating (2) with respect to a :

$$u_a(x, t) = g'(x - tf'(u(x, t)))(-tf''(u(x, t))u_a(x, t)) + g_a(x - tf'(u(x, t))),$$

therefore one can obtain an explicit expression for the sensitivity:

$$u_a(x, t) = \frac{g_a(x - tf'(u(x, t)))}{1 + tf''(u(x, t))g'(x - tf'(u(x, t)))} = \frac{g_a(x - tf'(u(x, t)))}{1 + th'(x - tf'(u(x, t)))}. \quad (9)$$

Let us observe that the denominator is zero if and only if there is an intersection between two characteristics, therefore only along the shock.

If the state u is discontinuous, (9) is still valid on both sides of the shock. Along the shock the state u is not differentiable in the classical sense; however, it admits a Dirac distribution as weak derivative. Therefore, by differentiating the compact expression (6) one obtains:

$$\begin{aligned} u_a(x, t) = u_a^+(x, t)H(x - x_s(t)) + u_a^-(x, t)H(x_s(t) - x) \\ + (u^- - u^+)\partial_a x_s(t)\delta(x_s(t) - x), \end{aligned} \quad (10)$$

where δ is the Dirac delta function and u_a^\pm are computed from (9) on either sides of the shock.

3.3 Correction term

In previous works [1–4], a correction to the sensitivity systems was proposed in the case of discontinuous state, resulting in sensitivity solutions which do not exhibit spikes that mimic the Dirac distribution. To obtain such sensitivities, a source term is added, which should compensate the last term of (10). The corrected sensitivity equation is:

$$\partial_t u_a^c + \partial_x f_a(u, u_a^c) = S(u) \quad x \in \mathbb{R}, t > 0, \quad (11)$$

where the source term has the following form:

$$S(u) = \partial_a v(u^+ - u^-) \delta(x_s(t) - x).$$

We use the superscript c to indicate the corrected sensitivity. For more details on the derivation of the source term, see [3, 4] and Chapter 2 of [5] for the specific declination of the method for 1D scalar conservation laws. The analytical solution of (11) is:

$$u_a^c(x, t) = u_a^+(x, t)H(x - x_s(t)) + u_a^-(x, t)H(x_s(t) - x), \quad (12)$$

where u_a^\pm are the same as in (10), since they are defined in the regular zones.

4 First order estimate of the variance of the shock position

In this section we provide a first order estimate of the variance of the position of the shock $x_s(t)$. In this context, the parameter of interest a is a random variable, whose expected value μ_a and variance σ_a^2 are known, and $x_s = x_s(t; a)$ is a function of this random variable. One can write a first order Taylor expansion of x_s with respect to a , centred in μ_a , obtaining:

$$x_s(t; a) = x_s(t; \mu_a) + (a - \mu_a) \partial_a x_s(t; \mu_a) + o((a - \mu_a)^2). \quad (13)$$

Then computing the average, one has:

$$\mathbb{E}[x_s(t; a)] \simeq x_s(t; \mu_a) + \mathbb{E}[a - \mu_a] \partial_a x_s(t; \mu_a) = x_s(t; \mu_a),$$

and for the variance:

$$\begin{aligned} \text{var}[x_s(t; a)] &\simeq \mathbb{E}[(x_s(t; a) - x_s(t; \mu_a))^2] \\ &= \mathbb{E}[(a - \mu_a)^2] (\partial_a x_s(t; \mu_a))^2 = (\sigma_a \partial_a x_s(t; \mu_a))^2. \end{aligned}$$

Therefore, in order to estimate the variance of the position of the shock, we need to compute $\partial_a x_s(t)$. This can be obtained from u , u_a , and u_a^c as follows:

$$\partial_a x_s(t) = \int_{\mathbb{R}} \frac{u_a(x, t) - u_a^c(x, t)}{u^- - u^+} dx. \quad (14)$$

The identity (14) can easily be verified by subtracting (12) from (10) and using the definition of a Dirac delta function.

5 Numerical strategy

The aim of this section is to present the numerical strategy to compute (14), which can then be used to estimate the variance of the shock position.

From now on, we will consider the equations on an interval (x_0, x_N) , which is divided into N cells, all of the same length Δx . The subscript i indicates the i -th cell, while $i \pm \frac{1}{2}$ refers to the interfaces. Concerning the time discretisation, we will use a variable time step Δt , chosen such that the CFL-condition is respected. The superscript n indicates the n -th time step.

Systems (1) and (8) are classical hyperbolic conservation laws, for which classical schemes can be used. However, for (11), a good discretisation of the source term is crucial.

The method chosen for the state equation is the approximate Riemann solver of Roe: the reason of this choice is that it provides the exact solution in the case of an isolated shock. For the sake of simplicity we consider the case $f'(u) > 0$. The scheme in the internal cells (i.e. $i \neq 0$) is the following:

$$u_i^{n+1} = u_i^n + \frac{\Delta t}{\Delta x} (f(u_{i-1}^n) - f(u_i^n)), \quad (15)$$

while for the first cell we impose $u_0^n = g(x_0) \forall n$.

For the sensitivity equation (8), i.e. the one without the source term, the same scheme used for the state can be applied:

$$u_{a,i}^{n+1} = u_{a,i}^n + \frac{\Delta t}{\Delta x} (f_a(u_{i-1}^n, u_{a,i-1}^n) - f_a(u_i^n, u_{a,i}^n)).$$

We remark that this scheme provides a sensitivity with spikes.

We here propose a second scheme, which comes from a quite natural discretisation of the source term:

$$u_{a,i}^{n+1} = u_{a,i}^n + \frac{\Delta t}{\Delta x} (f_a(u_{i-1}^n, u_{a,i-1}^n) - f_a(u_i^n, u_{a,i}^n)) + v_{a,i}^n (u_i^n - u_{i-1}^n) \delta_i^n, \quad (16)$$

where $\delta_i^n = 1$ if there is a shock in the i -th cell at the n -th time step, $\delta_i^n = 0$ otherwise. One of the main difficulties of this problem is to find an efficient shock detector. If one considers a Riemann problem, the simplest definition of a shock detector that works is:

$$\delta_i^n = \begin{cases} 0 & \text{if } u_{i-1}^n = u_i^n, \\ 1 & \text{otherwise.} \end{cases} \quad (17)$$

This of course does not work if the initial data is not a piecewise constant function. An option is the following shock detector based on the second derivative. Let D be the maximum of the second derivative of the initial data and let k be a constant to be tuned. Then

$$\delta_i^n = \begin{cases} 0 & \text{if } \frac{|u_{i-1}^n - 2u_i^n + u_{i+1}^n|}{\Delta x^2} > kD, \\ 1 & \text{otherwise.} \end{cases} \quad (18)$$

The shock detector is used to compute the source term for the corrected sensitivity system, but also to compute the jump of the state that appears in (14), which is computed as follows:

$$(u^+ - u^-)(t^n) = u_{k_1}^n - u_{k_2}^n,$$

where k_1 is such that $\delta_{k_1-1}^n = 1$ and $\delta_{k_1}^n = 0$, and k_2 is such that $\delta_{k_2}^n = 0$ and $\delta_{k_2+1}^n = 1$.

6 Numerical results

In this section, we show some numerical results for different test cases: we consider three different initial conditions for the state. For every test case, the interval $(0, 1)$ is discretised using $N = 1000$ cells.

1. The first test case is a Riemann problem, so that the analytical solution is known:

$$g_1(x) = u_L H(x_c - x) + u_R H(x - x_c), \quad (19)$$

with $u_L = 1$, $u_R = 0.1$, $x_c = 0.5$. For this problem, we consider two different uncertain parameters: the left value u_L , which gives a Riemann problem for the sensitivity as well, since $g_{1,u_L} = H(x_c - x)$; and the initial position of the discontinuity, which gives $g_{1,x_c}(x) = (u_L - u_R)\delta(x_c - x)$ as initial condition for the sensitivity.

2. A problem with a piecewise linear initial condition:

$$g_2(x) = \begin{cases} u_L & x < x_L, \\ \frac{u_R - u_L}{x_R - x_L}x + \frac{u_L x_R - u_R x_L}{x_R - x_L} & x_L \leq x \leq x_R, \\ u_R & x > x_R, \end{cases} \quad (20)$$

with $u_L = 2$, $u_R = 0.1$, $x_L = 0.25$, $x_R = 0.75$. The uncertain parameter for this case is u_L , which gives

$$g_{2,u_L}(x) = \begin{cases} 1 & x < x_L, \\ x \frac{1}{x_L - x_R} + \frac{x_R}{x_R - x_L} & x_L \leq x \leq x_R, \\ 0 & x > x_R. \end{cases} \quad (21)$$

The interest of this case is that we are able to compute the analytical solution as for the Riemann problem, but the breaking time t_s is strictly positive.

3. Finally, a problem with the following continuous initial condition:

$$g_3(x) = \begin{cases} A \sin^2\left(\frac{\pi}{L}(x - x_c) + \frac{\pi}{2}\right) & \text{if } -1 < 2\frac{x - x_c}{L} < 1 \\ 0 & \text{otherwise,} \end{cases} \quad (22)$$

where $A = 1$, $L = 0.6$, $x_c = 0.5$. The uncertain parameters considered here are L , which gives

$$g_{3,L}(x) = \begin{cases} A \frac{\pi}{L^2}(x - x_c) \sin\left(\frac{2\pi}{L}(x - x_c)\right) & \text{if } -1 < 2\frac{x - x_c}{L} < 1 \\ 0 & \text{otherwise,} \end{cases} \quad (23)$$

and A , which gives

$$g_{3,A}(x) = \begin{cases} \sin^2\left(\frac{\pi}{L}(x - x_c) + \frac{\pi}{2}\right) & \text{if } -1 < 2\frac{x-x_c}{L} < 1 \\ 0 & \text{otherwise.} \end{cases} \quad (24)$$

For each test case, the uncertain parameter has a variance of 5% of its average (i.e. $\sigma_a^2 = 0.05\mu_a$). In Figure 1 we plot the confidence intervals for the position of the shock, which are computed as follows :

$$CI := \left[\mathbb{E}[x_s] - \sqrt{\frac{\text{var}[x_s]}{\alpha}}, \mathbb{E}[x_s] + \sqrt{\frac{\text{var}[x_s]}{\alpha}} \right] \quad (25)$$

where α is the level of the confidence interval and we chose $\alpha = 0.95$. The form (25) is a straightforward consequence of the Chebyshev inequality [6], for more details see for instance [7]. For the test cases for which an analytical solution is

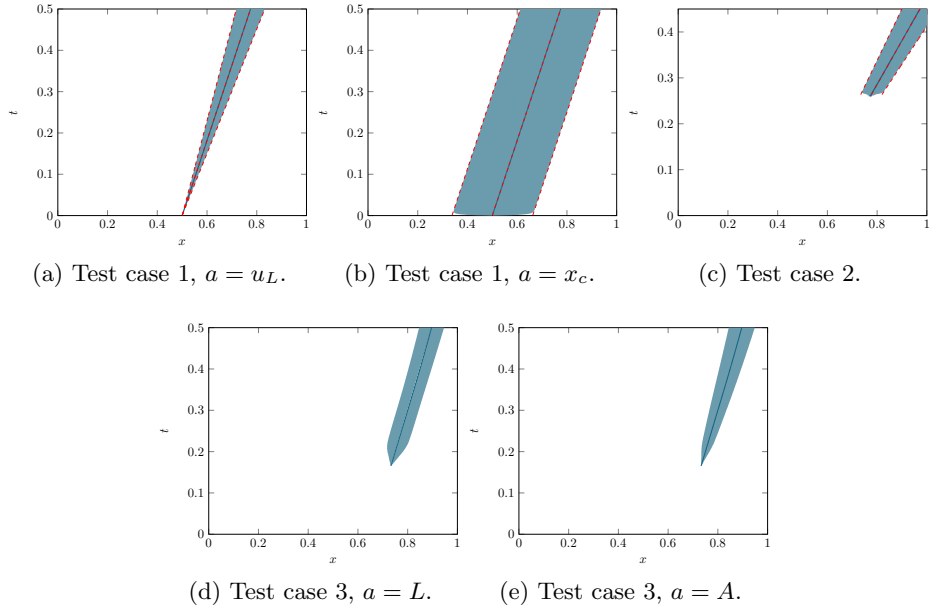


Fig. 1: Confidence intervals for the position of the shock. In blue, the numerical solution. In red, the analytical solution when available.

available, we observe perfect concordance with the numerical results. We remark that one drawback of this method is the inability to estimate the variance of the breaking time.

7 Conclusion and perspectives

In this work, we use two different definitions of the sensitivity to provide a first order estimate of the variance of the position of discontinuities, present in hyperbolic conservation laws. This can then be used to compute confidence intervals for the position of the shock. This method can be easily extended to system of conservation laws, provided that anti-diffusive numerical schemes (such as, for instance, the Glimm method) are used to solve both the state and the sensitivity. The extension to higher space dimension is more challenging, mainly due to the fact that anti-diffusive numerical schemes are needed in order to correctly solve the sensitivity. Numerical schemes based on neural network, such as [8], or shock tracking techniques [9] could be used for this.

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