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A formalism for the differentiation of conservation laws

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Abstract In this paper we present a synthetic method to differentiate with respect to a parameter partial differential equations in divergence form with shocks. We show that the usual derivatives contain the differentiated interface conditions if interpreted by the theory of distributions. We apply the method to three problems: the Burgers equation, the shallow water equations and Euler equations for fluids. ***To cite this article: C. Bardos, O. Pironneau, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 839–845.***

Un formalisme pour la dérivation des lois de conservations

Résumé On présente une méthode synthétique pour calculer les équations vérifiées par la dérivée par rapport à un paramètre de la solution v d'un système sous forme $\nabla \cdot v = 0$. On montre, pour les équations de Burgers, Euler et Saint-Venant que la dérivée au sens usuel, mais interpretée au sens des distributions, contient les conditions de saut, c'est à dire les dérivées des conditions de transmission aux chocs. On retrouve ainsi les résultats de Godlewski–Raviart et al. que l'on étend aux équations d'Euler. ***Pour citer cet article : C. Bardos, O. Pironneau, C. R. Acad. Sci. Paris, Ser. I 335 (2002) 839–845.***

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En général les études de sensibilité par rapport aux données d'un système d'equations aux dérivées partielles passent par leurs dérivations par rapports aux paramètres du système. Ainsi pour l'équation de Burgers, on aimerait pouvoir écrire que

$$\partial_t u + \partial_x \frac{u^2}{2} = 0, \quad \text{implique} \quad \partial_t u' + \partial_x (uu') = 0, \tag{1}$$

où u' est la dérivée de u par rapport a un paramètre a de la condition initiale. Le problème vient de ce qui si u est discontinue, u' sera une distribution et uu' n'aura pas de sens.

Ce problème a été identifié par Godlewski et al. dans un article précurseur [7] et aussi par Hafez (cf. [2,13] et Giles [4]) pour le problème du contrôle des systèmes avec chocs.

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Pourtant les implémentations numériques de (1) donnent des résultats corrects [11,2]. Nous montrons ici que c'est probablement parce que (1) est bien exact au sens des distributions et que toute discrétisation sous forme faible devrait donc être valide.

Nous proposons ici une méthode de dérivation des équations sous forme divergencielle avec solution discontinue (Propositions 2.1, 2.2). Ensuite nous appliquons le résultat aux équations de Burgers, Saint-Venant et Euler car elles sont sous forme divergencielle dans les variables temps-espace. Nous retrouvons par cette méthode les résultats de Godlewski–Raviart [6,5] et nous montrons aussi que les formes dérivées contiennent les conditions d'interfaces nécéssaires à l'unicité des solutions.

The plan of the paper is as follows:

First we recall that a "simple" differentiation of the partial differential equation and of its interface conditions lead to the result. However, such results would be difficult to justify in complex situations.

In the next section we show that the derivatives in the sense of distributions of a function v which has a line/surface discontinuity of normal n and its divergence can be computed when $v \cdot n = 0$.

Finally in the third part we apply the result to 3 problems: the Burgers' equation, the shallow water equations and the Euler equations for fluids. We recover the results of [7] and [1] and show, among other results, that the differentiated equations contain the jump conditions necessary for the well posedness of the differentiated problem.

1. Standard sensitivity analysis for Burgers' equation

Burgers' equation (1a) in $Q := \mathbb{R} \times (0, +\infty)$ may have discontinuous solutions (shocks) depending on the initial condition $u(x,0) = u^0(x,a)\ \forall x \in \mathbb{R}$. With compatible (entropy) discontinuous initial data at, say $x = 0$, the solution has a discontinuity at $x = x(t,a)$, which propagates at velocity

$$\dot{x} := \partial_t x = \bar{u} := \frac{1}{2}\big(u^+\big(x(t,a),t,a\big) + u^-\big(x(t,a),t,a\big)\big). \tag{2}$$

Here we assume that the initial data is function of a parameter a and we wish to find an equation for u'_a, the derivative of u with respect to a. We also assume that the shock is a unique curve $x(t,a)$ defined at $t = 0$ by the discontinuity of u^0 at 0. A simple pointwise differentiation of (1a) and of (2) gives the following result:

PROPOSITION 1.1. – *Burgers' equation differentiated with respect to a parameter, a, in the initial data is*

$$\partial_t u'_a + \partial_x (u u'_a) = 0 \quad \text{in } \Omega \setminus S, \qquad \dot{x}' = \bar{u}'_a + x' \partial_x \bar{u} \quad \text{on } S, \tag{3}$$

where x' is the derivative with respect to a of the shock position $x(t)$, $\bar{u}' = (u'^+ + u'^-)/2$ and $\partial_x \bar{u}$ is the half sum of the left x of the right x derivative of u on the shock curve.

The fact that the original solution $u(x,a)$ satisfies the entropy condition has for consequence that u'_a and (in most cases) x' are solutions of a well posed problem [15], because the characteristics left and right of the shock never cross the shock, so it is not necessary to complement (3a) with a jump condition.

2. Derivatives in the sense of distributions

We proceed now to re-derive and reinterpret these results in the light of distribution theory.

2.1. Preliminaries

Let Ω be an open bounded set of $\mathbb{R}^d$ and A an interval of $\mathbb{R}$. Consider a vector valued function from Ω to $\mathbb{R}^d$ function of a parameter $a \in A$:

$$(x,a) \in \Omega \times A \to v(x,a) \in \mathbb{R}^d. \tag{4}$$

Let $S(a)$ is a smooth surface which cuts Ω into two parts Ω^+, Ω^-. Assume that the restrictions of v, $v^\pm$ to $\Omega^\pm$ are continuously differentiable. We denote by C^1_S the space of such functions.

Assume also that v is differentiable with respect to a everywhere except on $S(a)$ and denote by v'_a this pointwise derivative.

We introduce the following notations:

- $x = x(s,a)$, $s \in I_S \subset \mathbb{R}^{d-1}$, a parametrization of $S(a)$, x' its partial derivative with respect to a.
- $Q = \Omega \times A$, $\Sigma = \{(x,a) : x \in S(a),\ a \in A\}$, $Q^\pm = \{(x,a) : x \in \Omega^\pm(a),\ a \in A\}$.
- n, n_Σ: the normals to $S(a)$ and Σ pointing inside Ω^+ and Q^+.
- $[v] := v^+ - v^-$ is the jump of v across $S(a)$.

PROPOSITION 2.1. – *Let v be a function in C^1_S. The derivative of v with respect to a, in the sense of distribution, v', is*

$$v' = v'_a - [v]x' \cdot n\delta_S, \tag{5}$$

where v'_a is the pointwise derivative of v with respect to a and δ_S is the Dirac function on S defined by $\int_\Omega w\delta_S = \int_S w\ \forall w \in \mathcal{D}(\Omega)$.

Proof. – For clarity we demonstrates the proof for $d = 3$ only. By definition of derivatives in the sense of distributions,

$$\forall w \in \mathcal{D}(Q): \quad \int_Q v'w = -\int_Q vw'. \tag{6}$$

Let us make use of the fact that $v^\pm := v|_{\Omega^\pm}$ are smooth:

$$\int_Q vw' = \int_{Q^-} v^- w' + \int_{Q^+} v^+ w' = -\int_{Q^-} (v^-)'w - \int_{Q^+} (v^+)'w + \int_\Sigma (v^+ - v^-) n_{\Sigma d+1} w, \tag{7}$$

where $n_{\Sigma d+1}$ is the last component of the normal to Σ. If Σ has for equation $\sigma(x,a) = 0$, then a normal is $(\partial_x\sigma, \partial_a\sigma)^{\mathrm{T}}$. Now if $x = x(s,a)$ is an parametric representation of $S(a)$ then $\sigma(x(s,a),a) = 0$ for all a so $(\partial_x\sigma)x' + \partial_a\sigma = 0$. This shows that the normal to σ is also $(n, -x' \cdot n)$ because $\partial_x\sigma$ is n, a normal to S. The scaling factor to make this vector of norm one is cancelled by the ratio of area elements between S and Σ.

PROPOSITION 2.2. – *Let v be tangent to $S(a)$. Denote by $\nabla_S\cdot$ the surface divergence on S. Then*

$$\nabla \cdot (v\delta_S) = \delta_S \nabla_S \cdot v. \tag{8}$$

Proof. –

$$\int_\Omega v\delta_S \cdot \nabla w = \int_S v \cdot \nabla w = \sum_{i=1}^{d-1} \int_S v \cdot s^i \partial_{s^i} w = -\sum_{i=1}^{d-1} \int_S \partial_{s^i} v \cdot s^i w. \tag{9}$$

Consequently, from (5), we have the following property.

COROLLARY 2.3. – *If $[v \cdot n] = 0$ and the pointwise derivative in a, v'_a has a trace left and right of S,*

$$\nabla \cdot v' = \nabla \cdot v'_a + [v'_a \cdot n]\delta_S - \delta_S \nabla_S \cdot \big([v]x' \cdot n\big). \tag{10}$$

Remark 1. – Notice that v'_a being discontinuous across S, its divergence contains also a Dirac mass and $\nabla \cdot v'_a + [v'_a \cdot n]\delta_S$ is $\nabla \cdot v'_a$ in the distribution sense.

2.1.1. *Symbolic notation*

Let f, g be C^1_S functions, differentiable with respect to a in $\Omega^\pm$. Let $\bar f = f^\pm$ in $\Omega^\pm$ and $\bar f = \frac{1}{2}(f^+ + f^-)$ on $S(a)$ and similarly for g. Then

$$(fg)' = f'\bar g + \bar f g'. \tag{11}$$

Justification. – Derivatives of fg, f and g may have Dirac masses on $S(a)$, but by the identity $[fg] = \bar f[g] + [f]\bar g$, we have equality of the Dirac masses (see Proposition 2.1). Within $\Omega^\pm$ Eq. (11) is obviously true.

Remark 2. – Such definition is of course symbolic because it makes no sense to define a function on a set of measure zero, but it allows us to go further in a symbolic calculus of derivatives for products. Furthermore note that we do not provide a rule to compute $(g\bar h)'$ for instance, except in the case of Corollary 2.3, which makes it difficult to apply the above formula recursively to compute triple products such as $(fgh)'$. As is well known products of distributions are dangerous objects.

Remark 3. – In [5] it is observed that the Volpert product is the natural symbolic notation in such studies. If $A(W)$ is the Jacobian matrix of $F(W)$ then Volpert's notation is that $A(W)W'$ should be understood at the shock as a Dirac mass of weight $[F(W)]$. Here it is the same idea, at the shock the derivative is replaced by the jump, i.e., $(fg)'$ becomes $[fg]$. In the case of conservation laws (29) both approaches give the same result.

2.2. Sensitivity analysis for Burgers' equation (II)

Let $v = (v_1, v_2)^{\mathrm T}$, $v_1 = u$, $v_2 = u^2/2$. Calling $x_1 = t$, $x_2 = x$, we see that (1a) is $\nabla\cdot v = 0$.
The normal to the shock $S = (t, x(t))$, is $n = (-\dot x, 1)^{\mathrm T}/\sqrt{1+\dot x^2}$; Proposition 2.1 says that

$$u' = u'_a - [u]\frac{x'}{\sqrt{1+\dot x^2}}\delta_S, \qquad \left(\frac{u^2}{2}\right)' = uu'_a - \left[\frac{u^2}{2}\right]\frac{x'}{\sqrt{1+\dot x^2}}\delta_S. \tag{12}$$

Similarly, denoting by $d_t f$ the time derivative of $f(x(t), t)$, Corollary 2.3 says that

$$\begin{aligned} 0 = \nabla\cdot v' &= \nabla\cdot v'_a + [v']\cdot n\delta_S - \nabla_S\cdot\big([v]x'\cdot n_\Sigma\big)\delta_S \\ &= \partial_t u'_a + \partial_x(uu'_a) - [u'_a]\dot x + [uu'_a] - d_t\left(x'\frac{[u] + [\frac{u^2}{2}]\dot x}{1+\dot x^2}\right)\delta_S, \end{aligned} \tag{13}$$

where ∂_t and ∂_x are classical derivatives and $s = (1, \dot x)^{\mathrm T}/\sqrt{1+\dot x^2}$. Recall that $\dot x = \bar u$ and that $[uu'_a] = \bar u[u'_a] + \bar u'_a[u]$ and therefore $[u] + [u^2/2]\dot x = [u](1+\dot x^2)$ we have:

PROPOSITION 2.4. – *Burgers' equation differentiated in the sense of distribution is*

$$\begin{aligned} &\partial_t u'_a + \partial_x(uu'_a) = 0 \quad \text{in } \Omega\setminus S, \\ &-[u]\bar u'_a + d_t\big([u]x'\big) = 0 \quad \text{on } S \text{ with } \bar u'_a = \big((u^+_a)' + (u^-_a)'\big)/2. \end{aligned} \tag{14}$$

and (14b) *is the derivative of the Rankine–Hugoniot conditions with respect to the parameter in the initial data.*

Proof. – Recall the identities

$$\partial_x\big(\bar u[u]\big) = \bar u\partial_x[u] + [u]\partial_x\bar u = \partial_x\left[\frac{u^2}{2}\right] = -\partial_t[u] = -d_t[u] + \bar u\partial_x[u]. \tag{15}$$

Multiplied by $[u]$, (3) gives

$$[u]\dot x' = [u]\bar u'_a + [u]x'\partial_x\bar u = [u]\bar u'_a - x'd_t[u] \Rightarrow d_t\big([u]x'\big) = [u]\bar u'_a \tag{16}$$

which is (3b).

PROPOSITION 2.5. – *The equation $\partial_t u' + \partial_x(\bar{u}u') = 0$ read in the sense of Distribution theory contains* (3b). *With the initial condition $u'(x,0) = (u^0)'$ it has a unique solution in* $\mathrm{H}^{-1}(Q)$.

Proof. – As explained above,

$$\partial_t u' + \partial_x(uu') = 0 \quad \text{is} \quad \nabla\cdot\begin{pmatrix} u' \\ uu' \end{pmatrix} = 0 \quad \text{and also} \quad \nabla\cdot\begin{pmatrix} u \\ u^2/2 \end{pmatrix}' = 0. \tag{17}$$

Now by Proposition 2

$$0 = \nabla\cdot\begin{pmatrix} u \\ u^2/2 \end{pmatrix}' = \nabla\cdot\begin{pmatrix} u' \\ uu' \end{pmatrix} + \big([u']\dot{x} - [uu'] - d_t\big([u]x'\big)\big)\delta_S \tag{18}$$

which is also

$$0 = \partial_t u' + \partial_x(uu') - \big([u]\bar{u}' + d_t\big([u]x'\big)\big)\delta_S. \tag{19}$$

So we must have (3a) in $\Omega\backslash S$ and by density this shows that (3b) holds on S.

Remark 4. – Uniform BV estimates for nonlinear hyperbolic systems in one space variable with convenient hypotheses show that for any continuous test function with compact support φ,

$$\lim_{\delta a\to 0}\int_Q \frac{u(x,t,a+\delta a) - u(x,t,a)}{\delta a}\varphi = \int_Q u'\varphi. \tag{20}$$

2.2.1. *Numerical consequences*

Finite volume methods are based on the weak form of the Burgers equation and a finite difference approximation of the time derivative. From the above we learn that a space–time approximation such as used by Johnson [3] would be preferable because it would be potentially capable of handling the singularities of u'. A formulation based on

$$\int_Q (u'\partial_t w + uu'\partial_x w) = 0 \tag{21}$$

would contain the differentiated Rankine–Hugoniot condition. Still, u' has a Dirac singularity on $S(a)$ and special numerical care must be applied to handle it, such as explicitly writing the Dirac masses hidden in (21)

$$\int_Q (u'\partial_t w + uu'\partial_x w) - \int_0^T [u]x'\frac{\mathrm{d}w}{\mathrm{d}t}\big(x(t),t\big) = 0. \tag{22}$$

This is an immediate consequence of Proposition 2.1. More generally:

COROLLARY 2.6. – *Let u, v be C^1_S functions of $(x,t)\in Q := \Omega\times(0,T)$; let u', v' be their derivative with respect to a in the sense of distribution. Assume that, in the sense of distribution,*

$$\partial_t u + \partial_x v = 0, \quad \partial_t u' + \partial_x v' = 0. \quad \textit{Then} \quad \int_Q (u'_a\partial_t w + v'_a\partial_x w) - \int_0^T [u]x'\frac{\mathrm{d}w}{\mathrm{d}t}\big(x(t),t\big) = 0. \tag{23}$$

Proof. – By definition $\int_Q (u'\partial_t w + v'\partial_x w) = 0$, therefore, by Proposition 2.1

$$\int_Q (u'_a\partial_t w + v'_a\partial_x w) - \int_\Sigma [u]\big(\partial_t w + [v]\partial_x w\big)x'\cdot n = 0. \tag{24}$$

Now by (23a) $[v] = [u]\dot{x}$ and $x'\cdot n\,\mathrm{d}\sigma = x'\,\mathrm{d}t$.

2.3. The shallow water equations

In $\mathbb{R}^d$, $d = 1$, 2 or 3, consider

$$\partial_t \rho + \nabla \cdot (\rho u) = 0, \qquad \partial_t (\rho u) + \nabla \cdot (\rho u \otimes u) + \nabla\big(p(\rho)\big) = 0, \tag{25}$$

with $p(\rho) = \rho$. With appropriate initial and boundary conditions, the water height ρ and its velocity u are uniquely defined, at least when $d = 1$ (see Lions [12]). Across S the Rankine–Hugoniot conditions are

$$[\rho]\dot{x} + [\rho u] \cdot n = 0, \qquad [\rho u]\dot{x} + [\rho u \otimes u \cdot n] + [\rho]n = 0. \tag{26}$$

Accordingly a pointwise differentiation of (25), (26) should yield a complete set of equations to define u', ρ', x', but the system is complex. Let us apply the symbolic calculus introduced above, at least to the one dimensional case $d = 1$. In the variable (t, x), Eq. (25a) is a divergence of $V = (\rho, v)^{\mathrm{T}}$ and so the same result can be obtained in the sense of Distribution theory by Corollary 2.3. However in order to differentiate the products we need to write the equations as:

$$\partial_t \rho + \partial_x v = 0, \quad \partial_t v + \partial_x (vu) + \partial_x \rho = 0, \quad v = \rho u. \tag{27}$$

Then the derivative of the quadratic terms being $(vu)' = v'\bar{u} + \bar{v}u'$, $v' = \rho'\bar{u} + \bar{\rho}u'$, we obtain

$$\partial_t \rho' + \partial_x v' = 0, \qquad \partial_t v' + \partial_x \big(\rho'\bar{u}^2 + (\bar{\rho}\bar{u} + \overline{\rho u})u' + \rho'\big) = 0. \tag{28}$$

2.3.1. *Interpretation*

As for the Burgers' equation, (28) contains the standard derivative of (25) and 3 jump conditions involving $[u]$, $[v]$, $[\rho]$, x'. System (25) is of the form

$$\partial_t W + \partial_x F(W) = 0 \tag{29}$$

with $W = (\rho, \rho u)^{\mathrm{T}}$, therefore the linearized equation and the differentiated equations have the same Jacobian matrix $A_{ij} = \partial_{W_i} F(W)_j$, $i, j = 1, 2$. The analysis of shocks is based on the computation of eigenvalues and eigenvectors of A. For One-Shocks for the shallow water system one Riemann invariant is computed from characteristics on the right side of the shock with a transmission condition for the left side one, while the other invariant is computed with left and right characteristics independently on both sides of the shock, without transmission condition across the shock. This means that the jump of this second invariant is fixed by (28) understood in the classical sense. So we have the 3 jump conditions issued from (27), in the distribution sense for $[u]$, $[v]$, $[\rho]$, x' but with one more equation due to the knowledge of the jump of the second Riemann invariant.

Remark 5. – If we had in the momentum equation ρ^γ instead of ρ, the same analysis applies. The momentum equation is the divergence of $(v, vu + \rho^\gamma)^{\mathrm{T}}$ so the terms which appears in the jump condition is $[v]\dot{x} + [vu + \rho^\gamma]$ and it is also the jump found from

$$\partial_t v' + \partial_x (u'\bar{v} + \bar{u}v' + a') = 0,$$

but we must find a such that $\bar{a}[\rho] = \rho^\gamma$. When $\gamma = 3/2$ (air) it can be done as follows:

$$b^2 = \rho, \ a = b\rho \Rightarrow 2\bar{b}b' = \rho', \ a' = \bar{b}\rho' + b'\bar{\rho} \Rightarrow a' = \overline{\sqrt{\rho}}\rho' + \bar{\rho}\frac{\rho'}{2\overline{\sqrt{\rho}}}. \tag{30}$$

3. Euler's equations

Perfect inviscid fluids are governed also by (25) but p is not a function of ρ and there is an additional equation for the conservation of energy:

$$\partial_t\theta+\partial_x\left(v\left(\frac{u^2}{2}+\theta\right)\right)=0\quad\text{with } \theta=\frac{\gamma}{\gamma-1}\frac{p}{\rho}. \tag{31}$$

To decompose all products into binary multiplications we multiply by ρ the second equation and set $w=u^2/2$. Differentiation leads to

$$\partial_t\theta'+\partial_x(v'\bar{w}+\bar{v}w'+\theta')=0,\qquad \frac{\gamma}{\gamma-1}p'=\bar{\theta}\rho'+\bar{\rho}\theta',\qquad w'=\bar{u}u'. \tag{32}$$

Therefore the result is

$$\begin{aligned}&\partial_t\rho'+\partial_x(\bar{\rho}u'+\bar{u}\rho')=0,\qquad \partial_t(\bar{\rho}u'+\bar{u}\rho')+\partial_x\big(\bar{u}^2\rho'+(\bar{\rho}\bar{u}+\overline{\rho u})u'+p'\big)=0,\\ &\frac{\gamma}{\gamma-1}\partial_t\left(\frac{p'}{\bar{\rho}}-\overline{\left(\frac{p}{\rho}\right)}\rho'\right)+\partial_x\left(\frac{\gamma}{\gamma-1}\left(\left(\frac{p'}{\bar{\rho}}-\overline{\left(\frac{p}{\rho}\right)}\rho'\right)\overline{\rho u}+\overline{\left(\frac{p}{\rho}\right)}(\bar{\rho}u'+\bar{u}\rho')\right)\right.\\ &\quad\left.+\left(\bar{u}\overline{\rho u}+\frac{\overline{u^2}\bar{\rho}}{2}\right)u'+\frac{\overline{u^2}\bar{u}}{2}\rho'\right)=0.\end{aligned}$$

4. Conclusion

We have seen that equations in divergence form can be differentiated even in the presence of shocks. The differentiated equation, taken in the sense of distribution, contains the transmission condition across the shock which fixes its motion. Therefore integration by parts of the differentiated equation is valid, an important information for numerical methods. Other equations will be analyzed also by this method in forthcoming publications, such as Darcy's law and the transonic equation [14,8]. In data assimilation, the problem arises also for meteorological fronts [10].

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