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Simplified chromatography model and inverse of split delta shocks

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A B S T R A C T

A split delta shock is a representation of the Dirac delta function. It is made to provide a way of using it in nonlinear PDEs. We define a notion of a split delta shock inverse and use it for solving Riemann initial data problem for a special chromatography model. The obtained solution is unique in distributional sense.

1. Introduction

Split delta shocks are introduced in order to solve some systems of conservation laws without classical solutions (see [1]). The main idea is to split a physical domain $\Omega \subset \mathbb{R}\times\mathbb{R}_+$ into pieces. In the interior of each such piece, one has a classical solution to the system while a boundary could support a signed delta measure. After performing all necessary operations we join these pieces back and use the distributional derivatives in the original system. Such solution is called the split delta shock. The procedure works well if the system is linear in one of the variables. Here, we expand the above procedure for systems that involves division by a split delta shock and use it in calculations. Some models with fluxes of that kind are also given in [2,3] and [4], for example. Particularly, we are able to easily solve Riemann problem for a simplified model of chromatography

$$u_t + \left(\frac{u}{1-u+v}\right)_x = 0,\ v_t + \left(\frac{v}{1-u+v}\right)_x = 0 \tag{1}$$

using the split delta inverse. Let us note that the full chromatography system is given by

$$\left(\left(1+\frac{A}{1-u+v}\right)u\right)_t + u_x = 0,\ \left(\left(1+\frac{B}{1-u+v}\right)v\right)_t + v_x = 0.$$

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Physical domain for solutions is defined by $1-u+v>0$, or $v-u>-1$ and $A<B$. In [5,6] and [7] one can find all relevant things about that system. Let us note that the real model has determined values for $(x,0)$, $x>0$ and for $(0,t)$, $t>0$ instead of the standard initial data, as we have assumed above. One can also look in [8] about the model but with $A=B=1$.

2. The definition of split delta shocks

Let $\Omega_i \neq \emptyset$, $i=1,\dots,n$ be a finite family of disjoint open sets with piecewise smooth boundary curves Γ_i, $i=1,\dots,m$: $\Omega_i\cap\Omega_j=\emptyset$, $\bigcup_{i=1}^n \overline{\Omega}_i=\overline{R^2_+}$ where $\overline{\Omega}_i$ denotes the closure of Ω_i. Denote by $\mathcal{C}(\overline{\Omega}_i)$ the space of bounded and continuous real-valued functions on $\overline{\Omega}_i$, equipped with the L^∞-norm. Let $\mathcal{M}(\overline{\Omega}_i)$, be the space of measures on $\overline{\Omega}_i$.

Define

$$\mathcal{C}_\Gamma=\prod_{i=1}^n \mathcal{C}(\overline{\Omega}_i),\quad \mathcal{M}_\Gamma=\prod_{i=1}^n \mathcal{M}(\overline{\Omega}_i).$$

The multiplication of $G=(G_1,\dots,G_n)\in\mathcal{C}_\Gamma$ and $D=(D_1,\dots,D_n)\in\mathcal{M}_\Gamma$ is defined to be an element $D\cdot G=(D_1G_1,\dots,D_nG_n)\in\mathcal{M}_\Gamma$, where each component is defined as the usual product of a continuous function and a measure.

Every measure on $\overline{\Omega}_i$ can be identified with a measure defined on $\overline{\mathbb{R}^2_+}$ with support in $\overline{\Omega}_i$. Thus one can define the mapping m in the following way

$$m:\mathcal{M}_\Gamma\to\mathcal{M}(\overline{\mathbb{R}^2_+}),\ m(D)=D_1+D_2+\cdots+D_n.$$

A typical example is obtained when $\overline{\mathbb{R}^2_+}$ is divided into two regions Ω_1, Ω_2 by a piecewise smooth curve $x=\gamma(t)$. The delta function $\delta(x-\gamma(t))\in\mathcal{M}(\overline{\mathbb{R}^2_+})$ along the line $x=\gamma(t)$ can be split in a non unique way into a left-hand side $D^-\in\mathcal{M}(\overline{\Omega}_1)$ and the right-hand component $D^+\in\mathcal{M}(\overline{\Omega}_2)$ such that

$$\delta(x-\gamma(t))=m(\alpha_0(t)D^-+\alpha_1(t)D^+)$$

with $\alpha_0(t)+\alpha_1(t)=1$. The solution concept which allows to incorporate such two sided delta functions as well as shock wave is modeled along the lines of the classical weak solution concept and proceeds as follows:
Step 1: Perform all nonlinear operations of functions in the space $\mathcal{C}_\Gamma$.
Step 2: Perform multiplications with measures in the space $\mathcal{M}_\Gamma$.
Step 3: Map the space $\mathcal{M}_\Gamma$ into $\mathcal{M}(\overline{\mathbb{R}^2_+})$ by means of the map m and embed it into the space of distributions.
Step 4: Perform the differentiation in the sense of distributions and require that the equation is satisfied in this sense.

Let us define an inverse of a split delta function now.

Definition 1. Suppose that

$$u=\begin{cases}u_0, & x\le ct\\ u_1, & x\ge ct\end{cases}+\alpha_0(t)\delta^-(x-ct)+\alpha_1(t)\delta^+(x-ct). \tag{2}$$

We define $\frac{1}{u}\in\mathcal{C}_\Gamma$, $\Gamma=\{(x,t):\ x=ct\}$, to be a function satisfying $\frac{1}{u}u=1$ in the $\mathcal{M}_\Gamma$ sense.

Using the above definition one gets the condition for the inverse

$$\begin{aligned}&\frac{1}{u}\cdot\left(\begin{cases}u_0, & x\le ct\\ u_1, & x\ge ct\end{cases}+\alpha_0(t)\delta^-(x-ct)+\alpha_1(t)\delta^+(x-ct)\right)\\ =&1+\frac{\alpha_0(t)}{u_0}\delta^-(x-ct)+\frac{\alpha_1(t)}{u_1}\delta^+(x-ct)\overset{m}{\mapsto}1+\Big(\frac{\alpha_0(t)}{u_0}+\frac{\alpha_1(t)}{u_1}\Big)\delta(x-ct).\end{aligned}$$

Thus, the condition for u in (2) to have an inverse is

$$\alpha_0(t)/u_0+\alpha_1(t)/u_1=0. \tag{3}$$

3. Systems given in a general form

Let us consider the following Riemann problem

$$\begin{aligned} u_t + \Big(\frac{a_0+a_1u}{v} + \frac{b_0+b_1v}{u}\Big)_x = 0,\ u(x,0) = \begin{cases} u_0, & x<0 \\ u_1, & x>0 \end{cases} \\ v_t + \Big(\frac{\bar a_0+\bar a_1u}{v} + \frac{\bar b_0+\bar b_1v}{u}\Big)_x = 0,\ v(x,0) = \begin{cases} v_0, & x<0 \\ v_1, & x>0. \end{cases} \end{aligned} \tag{4}$$

We assume that $(u,v) \in \Omega$, where $\Omega \subset \mathbb{R}^2$ is a physical domain, i.e. a set of all possible values for (u,v). Let us look for a solution in the form of two component split delta shock

$$u(x,t) = \underbrace{\begin{cases} u_0, & x \le ct \\ u_1, & x \ge ct \end{cases}}_{=:\hat u} + (\alpha_0\delta^- + \alpha_1\delta^+)t,\ v(x,t) = \underbrace{\begin{cases} v_0, & x \le ct \\ v_1, & x \ge ct \end{cases}}_{=:\hat v} + (\beta_0\delta^- + \beta_1\delta^+)t, \tag{5}$$

In the sequel, notation $[u]$ is used for a jump in $\hat u$. The values $(\alpha_0+\alpha_1)t$ and $(\beta_0+\beta_1)t$ are called strength of a split delta shock. For a given point (u_0,v_0) in a physical domain Ω for (4), a set of all (u_1,v_1) in the domain such that there exists a split delta shock connecting these states is called split delta locus denoted by $L((u_0,v_0))$.

Theorem 1. *There is a split delta shock solution to (4) if there exists c such that u_i, v_i, $i = 0,1$ satisfy*

$$\begin{aligned} a_1[u/v]\kappa_1/[u] + b_1[v/u]\kappa_2/[v] &= c\kappa_1 \\ \bar a_1[u/v]\kappa_1/[u] + \bar b_1[v/u]\kappa_2/[v] &= c\kappa_2,\ v_1 \ne v_0,\ u_1 \ne u_0. \end{aligned} \tag{6}$$

Here

$$\kappa_1 := c[u] - \Big[\frac{a_0+a_1u}{v} + \frac{b_0+b_1v}{u}\Big],\ \kappa_2 := c[v] - \Big[\frac{\bar a_0+\bar a_1u}{v} + \frac{\bar b_0+\bar b_1v}{u}\Big],$$

are so called Rankine–Hugoniot deficits for the first and second equations.

Proof. Condition (3) implies

$$\alpha_0/u_0 + \alpha_1/u_1 = 0,\ \beta_0/v_0 + \beta_1/v_1 = 0. \tag{7}$$

Using the procedure for split delta shock calculations, from the first equation in (4) one gets

$$\begin{aligned} &- c[u]\delta + \Big[\frac{a_0+a_1u}{v} + \frac{b_0+b_1v}{u}\Big]\delta + (\alpha_0+\alpha_1)\delta \\ &- ct(\alpha_0+\alpha_1)\delta' + \Big(\frac{a_1}{v_0}\alpha_0 + \frac{a_1}{v_1}\alpha_1 + \frac{b_1}{u_0}\beta_0 + \frac{b_1}{u_1}\beta_1\Big)t\delta' = 0, \end{aligned}$$

where the support of δ and δ' is the line $x = ct$.

The above equality is true if

$$\alpha_0+\alpha_1 = \kappa_1 = c[u] - \Big[\frac{a_0+a_1u}{v} + \frac{b_0+b_1v}{u}\Big] \tag{8}$$

$$c(\alpha_0+\alpha_1) = \frac{a_1}{v_0}\alpha_0 + \frac{a_1}{v_1}\alpha_1 + \frac{b_1}{u_0}\beta_0 + \frac{b_1}{u_1}\beta_1. \tag{9}$$

With the same arguments, one gets

$$\beta_0+\beta_1 = \kappa_2 = c[v] - \Big[\frac{\bar a_0+\bar a_1u}{v} + \frac{\bar b_0+\bar b_1v}{u}\Big] \tag{10}$$

$$c(\beta_0+\beta_1) = \frac{\bar a_1}{v_0}\alpha_0 + \frac{\bar a_1}{v_1}\alpha_1 + \frac{\bar b_1}{u_0}\beta_0 + \frac{\bar b_1}{u_1}\beta_1, \tag{11}$$

from the second equation in (4).

If $u_0 \neq u_1$ and $v_0 \neq v_1$ then the variables $\alpha_0, \alpha_1, \beta_0, \beta_1$ are uniquely determined by

$$\begin{array}{ll} \alpha_0 + \alpha_1 = \kappa_1 & \beta_0 + \beta_1 = \kappa_2 \\ \alpha_0/u_0 + \alpha_1/u_1 = 0 & \beta_0/v_0 + \beta_1/v_1 = 0. \end{array} \tag{12}$$

Here, we have used (7), (8) and (10). All possible values for c and a relation between left- and right-hand initial data are determined by (8), (9), (10) and (11). Particularly, c can be determined by solving the following system of equations

$$a_1(\alpha_0/v_0 + \alpha_1/v_1) + b_1(\beta_0/u_0 + \beta_1/u_1) = c\kappa_1$$
$$\bar{a}_1(\alpha_0/v_0 + \alpha_1/v_1) + \bar{b}_1(\beta_0/u_0 + \beta_1/u_1) = c\kappa_2,$$

that reduces to a quadratic equation. After solving (12) and inserting a solution in the above system one gets system (6) as a condition. □

In general, we expect that one could get a value(s) for c and a locus $L((u_0, v_0))$ being a curve. Of course, there are a lot of specific situations. For a real model one has to check whether $(u_1, v_1) \in \Omega$ and an admissibility condition for split delta shocks, too. The most usual admissibility condition is that split delta shocks are required to be overcompressive, i.e. all characteristics should run into the shock curve. Another admissible solution is delta shock with a constant strength that propagates along characteristics. It is called a delta contact discontinuity (see [1] or [9]). That is possible for systems having a linearly degenerate field.

4. Simplified chromatography model

Theorem 2. *There exists a unique solution to Riemann problem for (1) in the region where u, v and $1 - u + v$ are non-negative. The solution consists of elementary waves, vacuum states and split delta shocks. Uniqueness holds in the sense of distributions.*

Proof. System (1) has the eigenvalues $\lambda_a = \frac{1}{1-u+v}$ and $\lambda_b = \frac{1}{(1-u+v)^2}$ with the appropriate eigenvectors $r_a = (1,1)$ and $r_b = (1, v/u)$. The a–field is linearly degenerate, while b–field is genuinely nonlinear for $v \neq u$. Let us denote by I the region where $v \geq u$ and by II the one where $u > v > u - 1$. In I, $\lambda_1 = \lambda_b$, $r_1 = r_b$ and $\lambda_2 = \lambda_a$, $r_2 = r_a$. The opposite holds in II. Assume the initial data given in (4). If $(u_i, v_i) \in I$, $i = 0,1$. a solution is the following combination $S_1 + Cd_2$ or $R_1 + Cd_2$. In II it is a combination $Cd_1 + S_2$ or $Cd_1 + R_2$. If initial data values lie in different region, the situation is more complex. Then one could try with states when u or v equals zero ("vacuum in u or v").

Case 1. Suppose that $(u_0, v_0) \in I$ and $(u_1, v_1) \in II$. Then one could connect (u_0, v_0) with $(0,0)$ by S_1 with speed $c_0 = \frac{1}{(1-u_0+v_0)^2} \in (0,1)$. Then, one can connect the point $(0,0)$ with some $(u_s, 0)$ by a rarefaction wave in u while $v = 0$: u is a solution to the scalar equation $u_t + \left(\frac{1}{1-u}\right)_x = 0$, $\lambda(0,0) = 1 > c_0$ and $\lambda(u_s, 0) = \frac{1}{1-u_s} > 1$. The value u_s is chosen such that $(u_s, 0)$ could be connected by a contact discontinuity attached to the vacuum rarefaction wave — its speed equals $c_1 = \frac{1}{1-u_s} = \lambda(u_s, 0)$.

Case 2. Let $(u_0, v_0) \in II$ and $(u_1, v_1) \in I$. Then, there is no classical solution to the problem. One can try to connect (u_0, v_0) to $(0,0)$ by an S_2 with speed $c_0 = \frac{1}{1-u_0+v_0} > 1$. If we want to connect $(0,0)$ to some $(u_s, v_s) \in I$ (or $u_s = 0$), a speed would be $c_s = \frac{1}{1-u_s+v_s} < 1 < c_0$ that is impossible.

Let us try with a split delta shock solution of the form (5). One can use the definition for inverse since $1 - u + v$ is again split delta shock function. The inverse condition (3) is now

$$\frac{\beta_0 - \alpha_0}{1 - u_0 + v_0} + \frac{\beta_1 - \alpha_1}{1 - u_1 + v_1} = 0, \tag{13}$$

with $\alpha_0 + \alpha_1 \geq 0$, $\beta_0 + \beta_1 \geq 0$. Using a similar calculation as in the proof of Theorem 1 one could see that the following equations should be satisfied.

$$\alpha_0 + \alpha_1 = \kappa_1 := c[u] - \left[\frac{u}{1-u+v}\right]$$
$$c(\alpha_0 + \alpha_1) = \frac{\alpha_0}{1-u_0+v_0} + \frac{\alpha_1}{1-u_1+v_1}$$
$$\beta_0 + \beta_1 = \kappa_2 := c[v] - \left[\frac{v}{1-u+v}\right]$$
$$c(\beta_0 + \beta_1) = \frac{\beta_0}{1-u_0+v_0} + \frac{\beta_1}{1-u_1+v_1}.$$

One can find α_0 and α_1 from the first two, and β_0 and β_1 from the last two equations since $v_1 - v_0 - (u_1 - u_0) > 0$. Substitution of these values into (13) gives the condition $\kappa_1 = \kappa_2$. From that condition one can calculate a speed c,

$$c = \frac{1}{(1-u_0+v_0)(1-u_1+v_1)}.$$

The overcompressibility condition

$$\underbrace{\frac{1}{1-u_0+v_0}}_{=\lambda_1(u_0,v_0)} \geq \underbrace{\frac{1}{(1-u_0+v_0)(1-u_1+v_1)}}_{=c} \geq \underbrace{\frac{1}{(1-u_1+v_1)^2}}_{=\lambda_2(u_1,v_1)}$$

is satisfied since $u_0 > v_0$ and $u_1 < v_1$. That completes the proof. □

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