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On Finite-Difference Approximations and Entropy Conditions for Shocks*

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with Appendix by B. KEYFITZ

This paper is dedicated to Robert D. Richtmyer in recognition of his many important contributions to the numerical solutions of partial differential equations and of his great influence on scientific computing.

Abstract

Weak solutions of hyperbolic conservation laws are not uniquely determined by their initial values; an entropy condition is needed to pick out the physically relevant solution. The question arises whether finite-difference approximations converge to this particular solution. It is shown in this paper that in the case of a single conservation law, monotone schemes, when convergent, always converge to the physically relevant solution. Numerical examples show that this is not always the case with non-monotone schemes, such as the Lax-Wendroff scheme.

1. Introduction

In this paper we consider solutions $u(x, t)$, $t \geqq 0$, of the single conservation law

$$u_t + f(u)_x = 0 \tag{1.1a}$$

subject to the initial data

$$u(x, 0) = \phi(x)\,, \qquad -\infty < x < \infty\,, \tag{1.1b}$$

where $\phi(x)$ is a given function. Equation (1.1a) can be written in the form

$$u_t + a(u)u_x = 0\,, \qquad a(u) = \frac{df}{du}\,, \tag{1.2a}$$

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which asserts that u is constant along the characteristic curves $x = x(t)$, where

$$\frac{dx}{dt} = a(u)\,. \tag{1.2b}$$

The constancy of u along the characteristics combined with (1.2b) implies that the characteristics are straight lines. Their slope, however, depends upon the solution and therefore they may intersect, and where they do, no continuous solution can exist. To get existence in the large, i.e., for all time, we admit weak solutions which satisfy an integral version of (1.1),

$$\int_0^\infty \int_{-\infty}^\infty [w_t u + w_x f(u)]\, dx\, dt + \int_{-\infty}^\infty w(x, 0)\phi(x)\, dx = 0 \tag{1.3}$$

for every smooth test function $w(x, t)$ of compact support.

If u is a piecewise continuous weak solution, then it follows from (1.3) (see [10]) that across the line of discontinuity the Rankine-Hugoniot relation

$$f(u_R) - f(u_L) = S(u_R - u_L) \tag{1.4}$$

holds, where S is the speed of propagation of the discontinuity, and u_L and u_R are the states on the left and on the right of the discontinuity, respectively.

The class of all weak solutions is too wide in the sense that there is no uniqueness for the initial value problem, and an additional principle is needed for determining a physically relevant solution. Usually this principle identifies the physically relevant solution as a limit of solutions with some dissipation, namely

$$u_t + f(u)_x = \varepsilon[\beta(u)u_x]_x\,, \qquad \beta(u) > 0,\ \varepsilon \downarrow 0\,. \tag{1.5}$$

Oleinik [15] has shown that discontinuities of such admissible solutions can be characterized by the following condition:

$$\frac{f(u) - f(u_L)}{u - u_L} \geqq S \geqq \frac{f(u) - f(u_R)}{u - u_R} \tag{1.6}$$

for all u between u_L and u_R; this is called the *entropy condition*, or Condition E. Oleinik has shown, see [15], that weak solutions satisfying Condition E are uniquely determined by their initial data. Another elegant proof is given in [7].

Let $v(x, t)$ be a finite difference approximation to (1.1)

$$v_j^{n+1} = (L \cdot v^n)_j, \qquad v_j^n = v(j\,\Delta x, n\,\Delta t), \tag{1.7}$$

Δt and Δx are the time and space increments. Equation (1.7) is said to be in *conservation form* if it can be written in the following way:

$$v_j^{n+1} = v_j^n - \lambda(h_{j+1/2} - h_{j-1/2}), \tag{1.8a}$$

where

$$h_{j+1/2} = h(v_{j-k+1}, v_{j-k+2}, \cdots, v_{j+k}), \qquad h_{j-1/2} = h(v_{j-k}, v_{j-k+1}, \cdots, v_{j+k-1}),$$

and $\lambda = \Delta t/\Delta x$. In order for (1.8a) to be consistent with (1.1), h must be related to f as follows:

$$h(w, w, \cdots, w) = f(w). \tag{1.8b}$$

Lax and Wendroff [13] proved the following theorem: Let $v(x, t)$ be a solution of a finite difference scheme in conservation form. If $v(x, t)$ converges boundedly almost everywhere to some function $u(x, t)$ as Δx and Δt tend to zero, then $u(x, t)$ is a weak solution of (1.1).

Thus we know that if a finite difference scheme in conservation form is convergent, then it converges to a weak solution. *Is this limit the unique physically relevant solution*, i.e., do all its discontinuities satisfy the entropy condition (1.6)? The answer to this question will be discussed in the following sections. It will be shown in Section 2 that solutions of so-called monotone finite-difference schemes do satisfy the entropy condition. In Section 3 we shall present several examples to demonstrate that this is not always the case for non-monotone schemes.

2. Monotone Finite-Difference Schemes

A finite-difference scheme

$$v_j^{n+1} = H(v_{j-k}^n, v_{j-k+1}^n, \cdots, v_{j+k}^n) \tag{2.1}$$

is said to be *monotone* if H is a monotone increasing function of each of its arguments.

THEOREM. *Let*

$$\begin{aligned} v_j^{n+1} &= H_f(v_{j-k}^n, v_{j-k+1}^n, \cdots, v_{j+k}^n) \\ &= v_j^n - \lambda[h_f(v_{j-k+1}^n, \cdots, v_{j+k}^n) - h_f(v_{j-k}^n, \cdots, v_{j+k-1}^n)] \end{aligned} \tag{2.2a}$$

be a finite-difference approximation to (1.1) *in conservation form, i.e.,*

$$h_f(w, w, \cdots, w) = f(w) \tag{2.2b}$$

which is monotone:

$$\frac{\partial H_f}{\partial w_i}(w_{-k}, \cdots, w_{+k}) \geqq 0 \quad \textit{for} \quad \textit{all} \quad -k \leqq i \leqq k\,. \tag{2.2c}$$

Assume that, as Δt *and* Δx *tend to zero,* $\lambda = \Delta t/\Delta x = \text{const.}$, v_j^n *converges boundedly almost everywhere to some function* $u(x, t)$. *Then according to the theorem of Lax and Wendroff quoted earlier,* $u(x, t)$ *is a weak solution of* (1.1).

Assertion. The entropy condition (1.6) is satisfied for all discontinuities of u.

Proof: Our proof mimics one given by Hopf [6] and Krushkov [9] who have shown that if u is the limit of solutions of the parabolic equation (1.5), then u satisfies the inequality

$$U(u)_t + F(u)_x \leqq 0\,, \tag{2.3}$$

where

$$U(u) = \begin{cases} 0 & \text{for} \quad u < z\,, \\ u - z & \text{for} \quad u \geqq z\,, \end{cases} \qquad F(u) = \begin{cases} 0 & \text{for} \quad u < z\,, \\ f(u) - f(z) & \text{for} \quad u \geqq z\,, \end{cases} \tag{2.4}$$

and z is an arbitrary number. At a point of discontinuity, (2.3) implies

$$S[U(u_{\mathrm{L}}) - U(u_{\mathrm{R}})] - [F(u_{\mathrm{L}}) - F(u_{\mathrm{R}})] \leqq 0\,. \tag{2.5}$$

Inequality (2.5) is equivalent to Oleinik's Condition E given by (1.6). Our proof of the theorem consists in showing that likewise the limits of solutions of (2.2) satisfy inequality (2.3) with U and F given by (2.4).

Let v_j^n be a solution of the finite-difference scheme (2.2); we shall show that

$$V_j^n = U(v_j^n)\,,$$

where U is defined by (2.4), satisfies an inequality of the form

$$\frac{V_j^{n+1} - V_j^n}{\Delta t} + \frac{h_F(v_{j-k+1}^n, \cdots, v_{j+k}^n) - h_F(v_{j-k}^n, \cdots, v_{j+k-1}^n)}{\Delta x} \leqq 0, \tag{2.6}$$

h_F being given by

$$h_F(w_{-k+1}, \cdots, w_k) \tag{2.7}$$
$$= \sum_{j=-k+1}^{k} \dot{U}(w_j)(w_j - z) \int_0^1 \frac{\partial h_f}{\partial w_j}(w_{-k+1}(\theta), \cdots, w_k(\theta))\, d\theta .$$

Here $w_j(\theta)$, $-k+1 \leqq j \leqq k$, denotes the straight line connecting z with w_j, i.e., $w_j(\theta) = z + \theta(w_j - z)$ and

$$\dot{U}(u) = \frac{d}{du} U(u) = \begin{cases} 0 & \text{for} \quad u < z , \\ 1 & \text{for} \quad u > z . \end{cases} \tag{2.8}$$

Notice that h_F as defined by (2.7) is continuous and is consistent with $F(u)$ given by (2.4); i.e.,

$$\begin{aligned} h_F(u, u, \cdots, u) &= \dot{U}(u) \int_0^1 \sum_{j=-k+1}^{k} \frac{\partial h_f}{\partial w_j}(u(\theta), \cdots, u(\theta))(u - z)\, d\theta \\ &= \dot{U}(u) \int_0^1 \frac{d}{d\theta} h_f(u(\theta), \cdots, u(\theta))\, d\theta \\ &= \dot{U}(u)[h_f(u, \cdots, u) - h_f(z, \cdots, z)] \\ &= \dot{U}(u)[f(u) - f(z)] = F(u) . \end{aligned}$$

Therefore it follows from (2.6), as in the Lax-Wendroff theorem quoted earlier, that if $v_j^n \to u$ boundedly a.e., then the limit u satisfies the inequality (2.3). Thus, a verification of (2.6) will complete the proof of our theorem.

Again we introduce the parametrization

$$v_{j+i}(\theta) = z + \theta(v_{j+i}^n - z) , \qquad -k \leqq i \leqq k ,$$

and define

$$v(\theta) = H_f(v_{j-k}(\theta), \cdots, v_{j+k}(\theta)) , \tag{2.9a}$$

where H_f is defined by (2.2a). It follows from (2.2b) and (2.2a) that

$$v(0) = z , \qquad v(1) = v_j^{n+1} . \tag{2.9b}$$

Next we express V_j^{n+1} by

$$U(v_j^{n+1}) = U(v_j^{n+1}) - U(z) = \int_0^1 \frac{d}{d\theta} U(v(\theta))\, d\theta$$

$$= \int_0^1 U(v(\theta)) \sum_{i=-k}^{k} \frac{\partial H_f}{\partial w_i}(v_{j-k}(\theta), \cdots, v_{j+k}(\theta))(v_{j+1}^n - z)\, d\theta .$$

Similarly we see, using (2.7), that

$$-U(v_j^n) + \lambda[h_F(v_{j-k+1}^n, \cdots, v_{j+k}^n) - h_F(v_{j-k}^n, \cdots, v_{j+k-1}^n)]$$

$$= -\int_0^1 U(v_j(\theta))(v_j - z)\, d\theta + \lambda \int_0^1 \sum_{i=-k+1}^{k} \left[\frac{\partial h_f}{\partial w_i}(v_{j-k+1}(\theta), \cdots, v_{j+k}(\theta))\right.$$

$$\left. - \frac{\partial h_f}{\partial w_{i-1}}(v_{j-k}(\theta), \cdots, v_{j+k-1}(\theta))\right] \dot{U}(v_{i+j}(\theta))(v_{j+1}^n - z)\, d\theta$$

$$= -\int_0^1 \sum_{i=-k}^{k} \dot{U}(v_{j+1}(\theta)) \frac{\partial H_f}{\partial w_i}(v_{j-k}(\theta), \cdots, v_{j+k}(\theta))(v_{j+i}^n - z)\, d\theta .$$

Multiplying (2.6) by Δt and using the above two expressions, we obtain

$$U(v_j^{n+1}) - U(v_j^n) + \lambda[h_F(v_{j-k+1}^n, \cdots, v_{j+k}^n) - h_F(v_{j-k}^n, \cdots, v_{j+k-1}^n)]$$

$$= \sum_{i=-k}^{k} (v_{j+i}^n - z) \int_0^1 \frac{\partial H_f}{\partial w_i}(v_{j-k}(\theta), \cdots, v_{j+k}(\theta))[\dot{U}(v(\theta)) - \dot{U}(v_{j+i}(\theta))]\, d\theta . \tag{2.10}$$

By our assumption, $\partial H_f(w_{-k}, \cdots, w_k)/\partial w_i \geqq 0$ for all $-k \leqq i \leqq k$. We claim that

$$[\dot{U}(v(\theta)) - \dot{U}(v_{j+i}(\theta))](v_{j+i}^n - z) \geqq 0 . \tag{2.11}$$

For, if $v_{j+1}^n - z < 0$, by (2.8), $\dot{U}(v_{j+i}(\theta)) \equiv 0$ and $\dot{U}(v(\theta)) \geqq 0$ for all $0 \leqq \theta \leqq 1$; if, on the other hand, $v_{j+i}^n - z > 0$, then again, by (2.8), $\dot{U}(v_{j+i}(\theta)) \equiv 1$ and $\dot{U}(v(\theta)) \leqq 1$ for all $0 \leqq \theta \leqq 1$. This proves (2.11). Thus all the terms in the sum on the right-hand side of (2.10) are nonpositive and so (2.6) holds; this completes the proof of the theorem.

A different proof of this theorem, using the characterization of solutions of (1.1) which satisfy the entropy condition as an L_1-contractive semigroup, is given by Barbara Keyfitz in an appendix.

We remark that the convergence of solutions of monotone schemes to the physically relevant solutions can be explained by the very close relation between monotonicity and the presence of viscosity terms. To see this, we compute the truncation error of scheme (2.1). First we prove several identities. Let

$$\bar{u}=(u_{-k},\cdots,u_{k-1}) \quad \text{and} \quad T\bar{u}=(u_{-k+1},\cdots,u_k),$$

where $u_j=u(x+j\,\Delta x, t)$. It follows from (2.2a) and (2.2b) that

$$H(u,\cdots,u)=u, \tag{2.12a}$$

where the subscript f is omitted. By differentiation of the consistency relation (2.2b) we get

$$\sum_{j=-k}^{k-1} h_j(u,u,\cdots,u)=a(u), \tag{2.12b}$$

where a subscript j denotes partial differentiation with respect to the j-th components and $h_j\equiv 0$ for $j\geqq k$ or $j\leqq -k-1$. Differentiating (2.2a) we get

$$H_l=\delta_{0,l}-\lambda[h_{l-1}(T\bar{u})-h_l(\bar{u})], \qquad -k\leqq l\leqq k, \tag{2.13a}$$

$$H_{l,m}=-\lambda[h_{l-1,m-1}(T\bar{u})-h_{l,m}(\bar{u})], \qquad -k\leqq m\leqq k. \tag{2.13b}$$

It follows from (2.12) and (2.13) that

$$\sum_{l=-k}^{k} H_l(u,u,\cdots,u)=\sum \delta_{0,l}=1, \tag{2.14}$$

$$\begin{aligned}\sum_{l=-k}^{k} lH_l(u,\cdots,u)&=-\lambda\sum(h_{l-1}-h_l)l\\ &=-\lambda\sum[(l+1)-l]h_l=-\lambda a(u),\end{aligned} \tag{2.15}$$

$$\sum_{l,m=-k}^{k}(l-m)^2H_{l,m}(u,\cdots,u)=-\lambda\sum_{l,m}(l-m)^2[h_{l,m}-h_{l-1,m-1}]=0. \tag{2.16}$$

Using the Taylor series and (2.12a) we get

$$
\begin{aligned}
H(u_{-k}, u_{-k+1}, \cdots, u_k) &= H(u_0, u_0, \cdots, u_0) \\
&\quad + \sum_{j=-k}^{k} H_j(u_0, \cdots, u_0)(u_j - u_0) \\
&\quad + \frac{1}{2} \sum_{l,m} H_{l,m}(u_0, \cdots, u_0)(u_l - u_0)(u_m - u_0) + O((\Delta x)^3) \\
&= u_0 + \Delta x - u_x \sum_j jH_j + (\tfrac{1}{2}\Delta x)^2 u_{xx} \sum j^2 H_j \\
&\quad + (\tfrac{1}{2}\Delta x)^2 u_x^2 \sum_{l,m} lmH_{l,m} + O((\Delta x)^3) \\
&= u_0 + \Delta x u_x \sum jH_j + (\tfrac{1}{2}\Delta x)^2 [\sum j^2 H_j u_x]_x \\
&\quad + (\tfrac{1}{2}\Delta x)^2 u_x^2 \sum_{l,m} H_{l,m}(lm - l^2) + O((\Delta x)^3) .
\end{aligned}
$$

From (2.15), $\Delta x \cdot u_x \sum jH_j = \Delta x u_x[-\lambda a(u)] = -\Delta t f(u)_x$. Using the symmetry $H_{l,m} = H_{m,l}$ and (2.16) we get

$$
\sum_{l,m} H_{l,m}(lm - l^2) = -\frac{1}{2} \sum H_{l,m}(l - m)^2 = 0 .
$$

Thus the Taylor series expansion of the numerical scheme is

$$
\begin{aligned}
&H(u(x - k\,\Delta x, t), \cdots, u(x + k\,\Delta x, t)) = u(x, t) - \Delta t f(u)_x \\
&\qquad + (\tfrac{1}{2}\Delta x)^2 \left\{ \sum_{j=-k}^{k} j^2 H_j(u(x, t), \cdots, u(x, t)) u_x(x, t) \right\}_x + O((\Delta x)^3) .
\end{aligned} \tag{2.17}
$$

If u is a smooth solution of (1.1), then

$$
\begin{aligned}
u(x, t + \Delta t) &= u(x, t) + \Delta t u_t + (\tfrac{1}{2}\Delta t)^2 u_{tt} + O((\Delta t)^3) \\
&= u(x, t) - \Delta t f(u)_x + (\tfrac{1}{2}\Delta t)^2 [a^2(u) u_x]_x + O((\Delta t)^3) .
\end{aligned} \tag{2.18}
$$

Consequently, the truncation error is

$$
\begin{aligned}
&u(x, t + \Delta t) - H(u(x - k\,\Delta x, t), \cdots, u(x + k\,\Delta x, t)) \\
&\qquad = -(\Delta t)^2 [\beta(u, \lambda) u_x]_x + O((\Delta t)^3) ,
\end{aligned} \tag{2.19a}
$$

where

$$\beta(u, \lambda)=\frac{1}{2\lambda^2}\sum_{j=-k}^{k} j^2 H_j(u, \cdots, u)-\tfrac{1}{2}a^2(u)\,. \tag{2.19b}$$

We claim that, except in a trivial case, $\beta(u, \lambda)\geqq 0$ and $\beta(u, \lambda)\not\equiv 0$; this shows that *monotone finite-difference schemes in conservation form are of first-order accuracy*. This result is well known in the linear case, see [2] and [11].

Proof: Using the monotonicity assumption $H_j\geqq 0$, we can write

$$\sum jH_j=\sum j\sqrt{H_j}\sqrt{H_j}\,;$$

by using Schwarz's inequality, we get, from (2.14) and (2.15),

$$\begin{aligned}\lambda^2 a^2(u)&=\Big(\sum jH_j\Big)^2=\Big(\sum j\sqrt{H_j}\sqrt{H_j}\Big)^2\\ &\leqq \sum j^2H_j\cdot\sum H_j=\sum j^2H_j\,.\end{aligned} \tag{2.20}$$

It follows from (2.20) and (2.19b) that $\beta(u, \lambda)\geqq 0$. This inequality becomes an identity if and only if $H_j(u, \cdots, u)\equiv 0$ for all j except one, i.e., the finite-difference operator is a pure translation—this is the trivial case mentioned above.

Suppose that w is a smooth solution of the parabolic equation

$$w_t+f(w)_x=\Delta t[\beta(w, \lambda)w_x]_x\,, \tag{2.21}$$

where $\beta(w, \lambda)\geqq 0$ is given by (2.19b); then, in the same way as (2.19) was derived from (2.17) and (1.1), we deduce that

$$w(x, t+\Delta t)-H(w(x-k\,\Delta x, t), \cdots, w(x+k\,\Delta x, t))=O((\Delta t)^3)\,. \tag{2.22}$$

This implies by standard arguments that $v(x, t)$ given by (2.1), which is a first-order accurate approximation to smooth solutions of the conservation law (1.1), is a second-order accurate approximation to smooth solutions of the parabolic equation (2.21).

Although the preceding statement was derived by assuming smoothness of the solutions, a similar statement can be made for solutions of the linear equation

$$u_t+cu_x=0\,, \qquad c=\text{const.}\,, \tag{2.23}$$

with *discontinuous* initial data. It is shown in [3] that if $u(x, t)$ is the solution of (2.23), $v(x, t)$ the solution of (2.1), and $w(x, t)$ the solution of (2.21), then

$$\|v(x,t)-u(x,t)\| \leqq \text{const.}\,(\Delta t)^{1/4}\,, \tag{2.24}$$

$$\|v(x,t)-w(x,t)\| \leqq \text{const.}\,(\Delta t)^{3/4}\,, \tag{2.25}$$

where $\| \ \|$ is the L_2-norm. Thus even for linear discontinuities, the numerical solution approximates the solution of the parabolic equation (2.21) better than it approximates the solution of the original conservation law.

The numerical solution $v(x, t)$, and the solution $w(x, t)$ of the parabolic equation (2.21) are both approximations to *shock* solutions of the conservation law (1.1). Both approximations share many properties like maximum principle, L_1-contractiveness (see Appendix) and most importantly, existence of monotone steady progressing profiles (see [3] and reference [A2]). A numerical study in [3] revealed exceptional agreement between numerical and viscous profiles. This shows that solutions of the monotone scheme in conservation form (2.1) appear to approximate solutions of the parabolic equation (2.21) better than they approximate solutions of the original conservation law, continuous as well as discontinuous. Since the physically relevant solution was defined as the limit of solutions of the parabolic equation, this may explain why solutions of monotone schemes in conservation form converge to the physically relevant solutions.

3. Non-Monotone Finite-Difference Schemes

In this section we consider schemes of type (2.1) which are *not* monotone, i.e., for which the function H defined in (2.1) is not a monotone function of all its arguments. As we remarked at the end of the last section, difference schemes which have order of accuracy higher than 1 are not monotone. In this section we shall give examples of non-monotone difference schemes in conservation form whose solutions converge to weak solutions which are not physically relevant, i.e., which violate the entropy Condition E.

We consider numerical solutions to the following initial value problem:

$$u_t + f(u)_x = 0\,, \qquad f(u) = u - \alpha u^2(u-1)^2, \tag{3.1a}$$

$$u(x,0) = u_0(x) = \begin{cases} 1 & \text{for} \quad x \leqq 0.5\,, \\ 0 & \text{for} \quad x > 0.5\,. \end{cases} \tag{3.1b}$$

Here α is a positive parameter. Figure 1 shows a plot of $f(u)$ for $\alpha = 3\sqrt{3}$; note that f is not convex or concave. In fact, $f(u)$ is not convex or concave for all $\alpha > 0$.

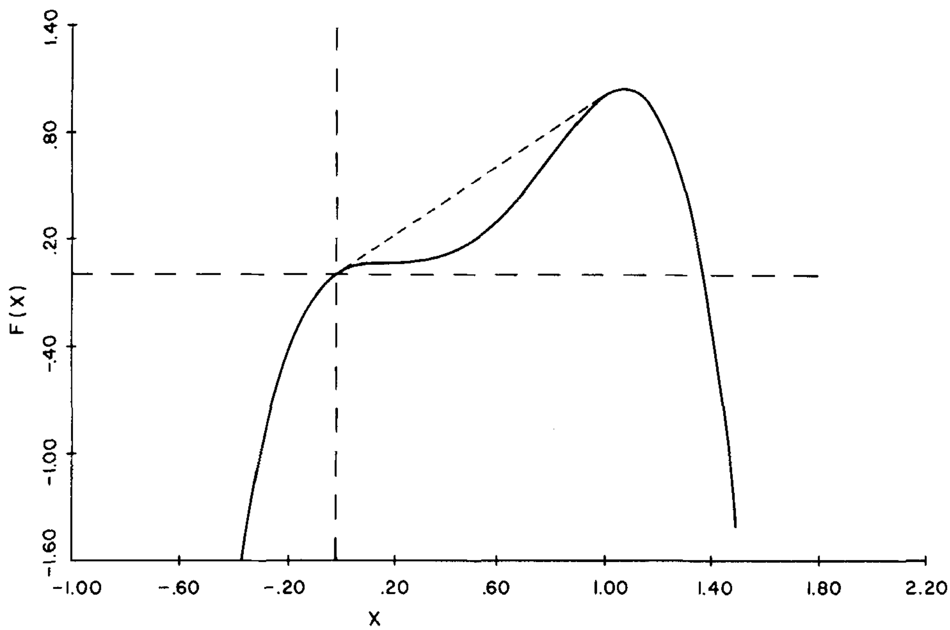

FIGURE 1

The function

$$u(x, t) = u_0(x - t) \tag{3.2}$$

solves the initial value problem and satisfies the Rankine-Hugoniot condition across the discontinuity. It follows from the geometrical interpretation of the entropy condition, see [7], that (3.2) satisfies the entropy condition. Therefore by the uniqueness theorem it is the only solution.

First we consider the solution of (3.1) by the Lax-Wendroff scheme (LW):

$$\begin{aligned} v_j^{n+1} &= v_j^n - \tfrac{1}{2}\lambda(f_{j+1}^n - f_{j-1}^n) \\ &\quad + \tfrac{1}{2}\lambda^2[a_{j+1/2}^n(f_{j+1}^n - f_j^n) - a_{j-1/2}^n(f_j^n - f_{j-1}^n)]\,, \end{aligned} \tag{3.3a}$$

$f_k^n = f(v_k^n)$, $a_{k+1/2}^n = a(\frac{1}{2}(v_k^n + v_{k+1}^n))$; $\lambda = \Delta t/\Delta x$ is chosen at the beginning of each time-step by

$$\lambda \max_j |a(v_j^n)| = 0.9\,. \tag{3.3b}$$

Figures 2a, 2b and 2c show v_j^n of the LW scheme for $n = 5$, 15, 150; the dashed line in these figures is the correct solution (3.2).

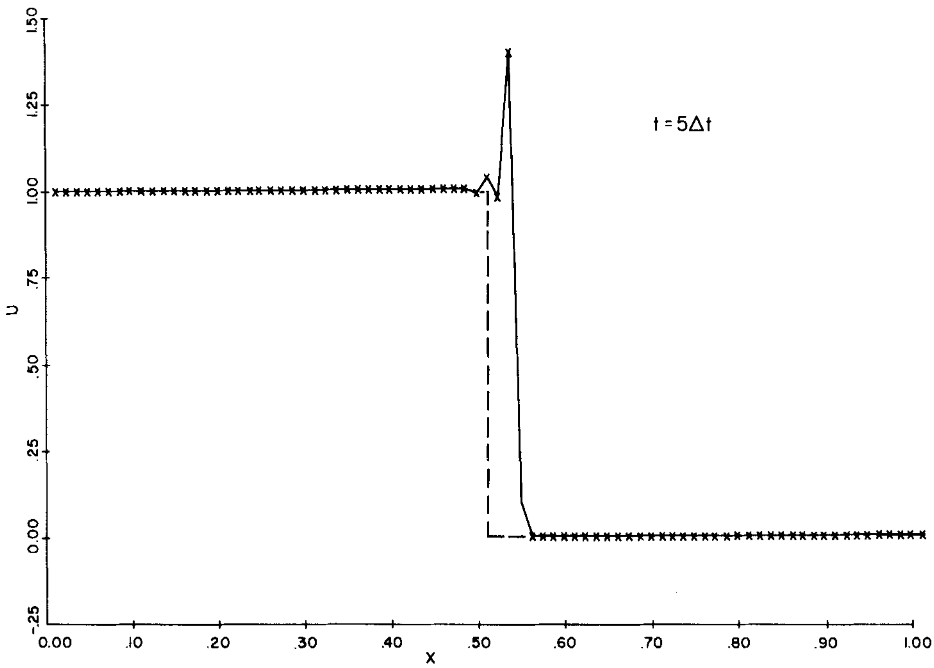

FIGURE 2a

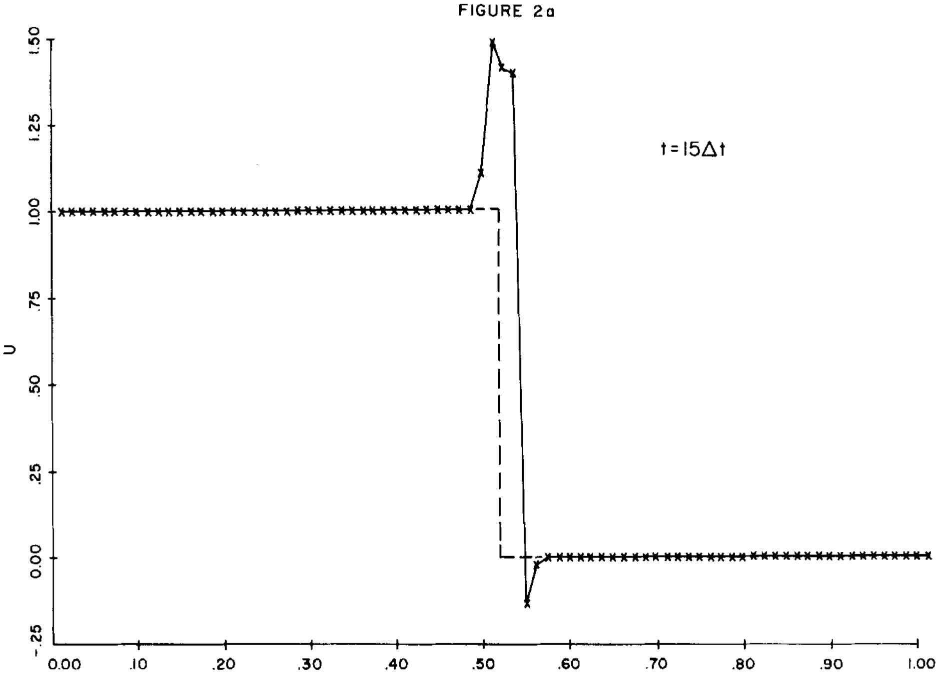

FIGURE 2b

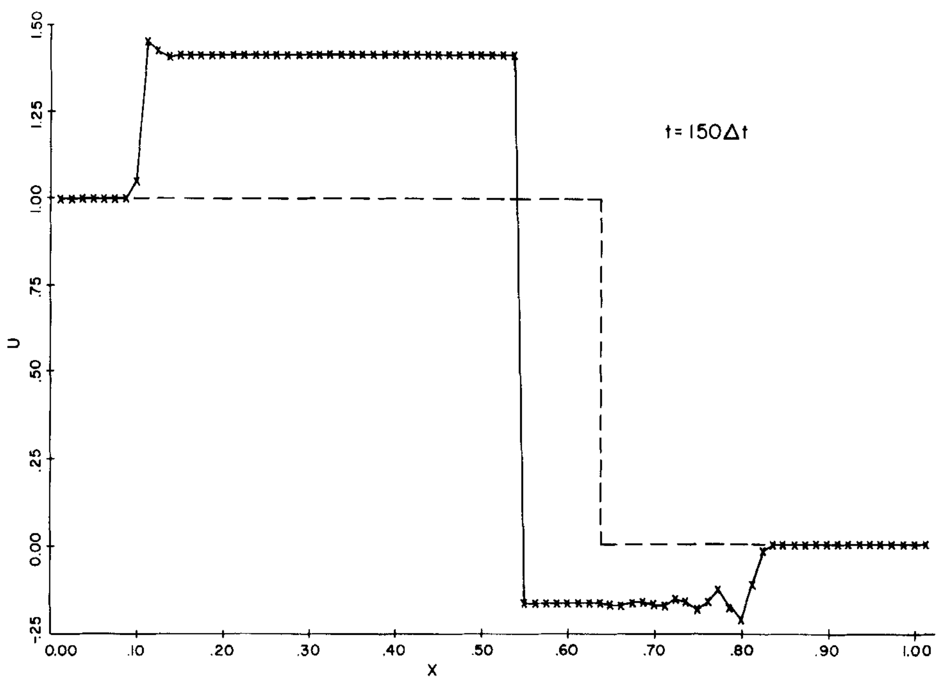

FIGURE 2c

The numerical evidence presented in these figures indicates that the solution of (3.2) by the LW scheme converges as $n \to \infty$ to

$$
(3.4) \qquad u(x,t) = \begin{cases} u_L = 1 & \text{for} \quad -\infty < x < 0.5 - 3.3t, \\ u_0 = 1.41 & \text{for} \quad 0.5 - 3.3t < x < 0.5, \\ u_U = -0.17 & \text{for} \quad 0.5 < x < 0.5 + 2.2t, \\ u_R = 0 & \text{for} \quad 0.5 + 2.2t < x < +\infty. \end{cases}
$$

The Rankine-Hugoniot conditions (1.4) at the three discontinuities are satisfied within the accuracy of the calculation, i.e., $u(x, t)$ given by (3.4) is a weak solution of (3.1). This is as it has to be according to the theorem of Lax and Wendroff quoted earlier. On the other hand, observe that whereas the entropy condition is satisfied for the discontinuity between u_L and u_0 as well as for the discontinuity between u_U and u_R, it is violated at the discontinuity between u_0 and u_U. This is again as it has to be; for, according to the uniqueness theorem, there is only one solution of (3.1) which satisfies the entropy condition, and that solution is given by (3.2).

It seems that both the non-monotonicity of the finite-difference scheme and the non-convexity of the flux function are responsible for this non-physical behavior of the solution (3.4). The non-monotonicity of the finite-difference scheme causes the development of an overshoot u_0 (see Figure 2a) and an undershoot u_U (see Figure 2b). The non-convexity of the flux function allows $a(u_0) < a(u_L)$ and $a(u_U) > a(u_R)$. These inequalities explain the backward propagating shock (u_L, u_0) and the forward propagating shock (u_U, u_R) in (3.4).

We remark that numerical experiments with the LW scheme and a flux function $f(u)$,

$$f(u) = \begin{cases} u - \alpha u^2(u-1)^2 & \text{for} \quad 0 \leqq u \leqq 1\,, \\ u & \text{for} \quad u \geqq 1 \quad \text{or} \quad u \leqq 0\,, \end{cases}$$

which is identical to (3.1a) in [0, 1], but is linear otherwise, did not exhibit nonphysical solutions, although the overshoot was as large as in the case of (3.1).

Computer experiments with the second-order accurate 2-step Richtmyer scheme (cf. [17]), as well as with the third- and fourth-order accurate generalizations of the LW scheme (cf. [19]), produced results similar in nature to the one described in Figure 2.

We present now an example which shows that the LW scheme (3.3a) can produce a solution of the conservation law (1.1a) which violates the entropy condition even when f is convex.

We shall consider a function f for which

$$f(-1) = f(1)\,. \tag{3.5}$$

It can be verified immediately that for such f

$$v_j = \begin{cases} -1 & \text{for} \quad j \leqq 0\,, \\ 1 & \text{for} \quad j > 0\,, \end{cases} \tag{3.6}$$

is a steady solution of (3.3a). That is, if the initial value v_j^0 is taken to be v_j as given by (3.6), $v_j^1 = v_j^2 = \cdots = v_j^n$ are all equal to v_j. The limit of these approximate solutions is, clearly,

$$u(x, t) = \begin{cases} -1 & \text{for} \quad x < 0\,, \\ 1 & \text{for} \quad x > 0\,. \end{cases} \tag{3.7}$$

This is a weak solution of the conservation law (1.1a) when (3.5) holds. On the other hand, the solution (3.5) will violate the entropy condition when $f'(1)$

is positive; for then the characteristic directions on both sides of the discontinuity point away from the discontinuity and this is well known to be contrary to the entropy condition.

We turn to investigating the stability of the solution (3.6). Our analysis, partly theoretical and partly numerical, suggests very persuasively that even when the entropy condition is violated, (3.6) is semistable in the sense that if we take initial values close to (3.6), the solution ground out by the LW scheme tends to a weak solution which still has a discontinuity at the origin violating the entropy condition.

We start by linearizing the LW scheme (3.3a) around the solution (3.6). We write

$$
\begin{aligned}
v_j^{(n)} &= v_j + \varepsilon w_j , \\
v_j^{(n+1)} &= v_j + \varepsilon W_j + o(\varepsilon) .
\end{aligned} \tag{3.8}
$$

Substitute (3.8) into (3.3a) and differentiate with respect to ε; we get

$$
\begin{aligned}
W_j = {} & \tfrac{1}{2}\lambda a_{j-1}(1+\lambda a_{j-1/2})w_{j-1} \\
& + (1-\tfrac{1}{2}\lambda^2(a_{j-1/2}+a_{j+1/2})a_j)w_j - \lambda a_{j+1}(1-\lambda a_{j+1/2})w_{j+1} .
\end{aligned} \tag{3.9}
$$

We abbreviate $\lambda f'(1)$ by b. For the sake of simplicity we assume that $\lambda f'(-1) = -b$; this will be so whenever f is an even function.

It follows from (3.6) and the definition of $a_{j+1/2}$ in (3.3a) that

$$
\lambda a_j = \begin{cases} -b & \text{for } j \leqq 0 , \\ b & \text{for } j > 0 , \end{cases} \qquad \lambda a_{j+1/2} = \begin{cases} -b & \text{for } j < 0 , \\ 0 & \text{for } j = 0 , \\ b & \text{for } j > 0 . \end{cases} \tag{3.10}
$$

Substituting this into (3.9) we get

$$
W_j = (-\tfrac{1}{2}b + \tfrac{1}{2}b^2)w_{j-1} + (1-b^2)w_j + (\tfrac{1}{2}b+\tfrac{1}{2}b^2)w_{j+1}
$$

for $j < 0$,

$$
\begin{aligned}
W_0 &= (-\tfrac{1}{2}b + \tfrac{1}{2}b^2)w_{-1} + (1-\tfrac{1}{2}b^2)w_0 - \tfrac{1}{2}bw_1 , \\
W_1 &= -\tfrac{1}{2}bw_0 + (1-\tfrac{1}{2}b^2)w_1 + (-\tfrac{1}{2}b+\tfrac{1}{2}b^2)w_2 ,
\end{aligned} \tag{3.11}
$$

and

$$
W_j = (\tfrac{1}{2}b + \tfrac{1}{2}b^2)w_{j-1} + (1-b^2)w_j + (-\tfrac{1}{2}b+\tfrac{1}{2}b^2)w_{j+1}
$$

for $j > 1$.

We simplify the operator (3.11) by introducing

$$\begin{aligned} p_j &= w_j + w_{1-j}\,, & q_j &= w_j - w_{1-j}\,, \\ P_j &= W_j + W_{1-j}\,, & Q_j &= W_j - W_{1-j}\,, \end{aligned} \tag{3.12}$$

$j = 1, 2, \cdots$. In the first equation of (3.11) replace j by $1-j$ and add it to, respectively subtract it from, the last equation in (3.11). We get

$$\begin{aligned} P_j &= (\tfrac{1}{2}b + \tfrac{1}{2}b^2)p_{j-1} + (1 - b^2)p_j + (-\tfrac{1}{2}b + \tfrac{1}{2}b^2)p_{j+1}\,, \\ Q_j &= (\tfrac{1}{2}b + \tfrac{1}{2}b^2)q_{j-1} + (1 - b^2)q_j + (-\tfrac{1}{2}b + \tfrac{1}{2}b^2)q_{j+1}\,. \end{aligned} \tag{3.13$_j$}$$

Adding and subtracting the second equation from the third in (3.11) we get

$$\begin{aligned} P_1 &= (1 - \tfrac{1}{2}b^2 - \tfrac{1}{2}b)p_1 + (-\tfrac{1}{2}b + \tfrac{1}{2}b^2)p_2\,, \\ Q_1 &= (1 - \tfrac{1}{2}b^2 + \tfrac{1}{2}b)q_1 + (-\tfrac{1}{2}b + \tfrac{1}{2}b_2)q_2\,. \end{aligned} \tag{3.14}$$

Now (3.14) can be rewritten as $(3.13)_j$ with $j = 1$, provided that we define

$$\begin{aligned} p_0 &= \frac{b-1}{b+1}\,p_1\,, \\ q_0 &= q_1\,. \end{aligned} \tag{3.15}$$

We use (3.15) as boundary conditions for equation (3.13).

In equations (3.13), (3.14) and (3.15) the p's are completely decoupled from the q's. We denote by $T_p(b)$ the operator relating the p to P, by $T_q(b)$ the operator relating q to Q.

Equations (3.13) with the boundary conditions (3.15) are simple scalar examples of difference equations for mixed initial-boundary value problems. A stability theory for such equations has been developed by Kreiss; another approach to this theory is due to S. Osher. The idea of using the Kreiss theory for shock problems occurs in [20].

Kreiss' theory says that a difference scheme is strongly stable, in the sense that the l_2 norm of its solutions remains uniformly bounded for all time, if there are *no unstable modes, genuine* or *generalized.* It is not hard to show the following:

For $b > 0$, the operator $T_p(b)$ has no unstable eigenvector, and $T_q(b)$ has the unstable eigenvector

$$\begin{aligned} q_j &= 1\,, \qquad j = 1, 2, \cdots, \\ T_q(b)q &= q\,. \end{aligned} \tag{3.16}$$

For $b<0$, the operator $T_q(b)$ has no unstable eigenvector but the operator $T_p(b)$ has the unstable eigenvector

$$T_p(b)p(b)=p(b)\,,\qquad p_j=\left(\frac{b+1}{b-1}\right)^j,\qquad j=1,2,\cdots, \tag{3.17}$$

The reason is that in the case $b<0$ there is a one parameter family of stationary shock profiles which are exponentially small at $\pm\infty$. Their derivative with respect to the parameter is the eigenvector (3.17).

It follows from Kreiss' theorem that $T_p(b)$ is *strongly stable* for $b>0$ and $T_q(b)$ is *strongly stable* for $b<0$. We surmise that $T_q(b)$ is *weakly unstable* for $b>0$, $T_p(b)$ *is weakly unstable* for $b<0$ in the following sense:

$$\begin{aligned} \|T_q^n(b)\| &\simeq \text{const.}\,\sqrt{n}\,, && b>0\,,\\ \|T_p^n(b)\| &\simeq \text{const.}\,\sqrt{n}\,, && b<0\,. \end{aligned} \tag{3.18}$$

We deduce easily from (3.13), (3.14) that

$$T_q^*(b)=T_p(-b)\,, \tag{3.19}$$

where * denotes the adjoint with respect to the l_2 norm. It follows from (3.19) that

$$\|T_p^n(-b)\|=\|T_q^n(b)\|\,; \tag{3.20}$$

so it suffices to prove only one of the two statements in (3.18). To study $T_q(b)$, $b>0$, we compare $T_q^n(b)$ to the solution operator of the differential operator which it approximates. Then (3.13) is an approximation to

$$q_t+bq_x=0\,, \tag{3.21a}$$

and (3.15) is an approximation to

$$q_x=0 \qquad \text{at} \qquad x=0\,. \tag{3.21b}$$

The solution of (3.21) whose initial value is $\phi(x)$ is, for $b>0$, given by the formula

$$q(x,t)=\begin{cases}\phi(0) & \text{for} \quad x<bt\,,\\ \phi(x-bt) & \text{for} \quad x\geqq bt\,.\end{cases} \tag{3.22}$$

Table 1* of $T_q^n(b)\phi$, $b=(0.9)$, defined by (3.13)

j	ϕ	$T_q^5(0.9)\phi$	$T_q^{10}(0.9)\phi$	$T_q^{15}(0.9)\phi$	$T_q^{20}(0.9)\phi$
0		1.053	1.053	1.053	1.053
1	1.0	1.053	1.053	1.053	1.053
2	0.0	1.052	1.053	1.053	1.053
3	0.0	1.064	1.053	1.053	1.053
4	0.0	1.094	1.053	1.053	1.053
5	0.0	0.965	1.051	1.053	1.053
6	0.0	0.457	1.050	1.053	1.053
7	0.0	0.0	1.074	1.053	1.053
8	0.0	0.0	1.117	1.052	1.053
9	0.0	0.0	1.038	1.049	1.053
10	0.0	0.0	0.673	1.047	1.053
11	0.0	0.0	0.209	1.073	1.053
12	0.0	0.0	0.0	1.125	1.053
13	0.0	0.0	0.0	1.096	1.048
14	0.0	0.0	0.0	0.838	1.044
15	0.0	0.0	0.0	0.413	1.066
16	0.0	0.0	0.0	0.095	1.123
17	0.0	0.0	0.0	0.0	1.134

* Observe that, by (3.25), $l(\phi)=\dfrac{2}{0.9-1}\cdot\dfrac{0.9-1}{0.9+1}=1.053.$

By analogy with (3.22) we expect[1] the solution of the initial value problem for the difference scheme (3.13), (3.15) to be of the form

$$q_j^n \simeq l(\phi) \qquad \text{for} \qquad j \leqq bn, \tag{3.23}$$

where $l(\phi)$ is some linear functional of the initial data. Numerical calculations bear out this contention, see Table 1.

The linear functional $l(\phi)$ is easily determined. With p given by (3.17) but b replaced by $-b$ and using (3.19) we have, for $b>0$,

$$(T_q^n(b)\phi, p(-b)) = (\phi, T_p^n(-b)p(-b)) = (\phi, p(-b))\,. \tag{3.24}$$

It follows from (3.23) that, as $n\to\infty$, the left side of (3.24) tends to

$$l(\phi)\sum p_j(b) = l(\phi)\frac{(b-1)/(b+1)}{1-(b-1)/(b+1)} = l(\phi)\tfrac{1}{2}(b-1)\,.$$

So from (3.24) we get

$$l(\phi) = \frac{2}{b-1}(\phi, p) = \frac{2}{b-1}\sum \phi_j\left(\frac{b-1}{b+1}\right)^j . \tag{3.25}$$

[1] We thank Stanley Osher for suggesting this approach.

Table 2 of $T_p^n(b)\phi$, $b=(-0.9)$, defined by (3.13)

$n \backslash j$	1	2	3	4	5	6
0*	1.0	1.0	1.0	1.0	1.0	1.0
5	5.68	0.81	1.01	1.0	1.0	1.0
10	10.42	0.56	1.02	1.0	1.0	1.0
15	15.16	0.31	1.03	1.0	1.0	1.0
20	19.89	0.06	1.05	1.0	1.0	1.0
25	24.63	−0.19	1.06	1.0	1.0	1.0
30	29.37	−0.44	1.07	1.0	1.0	1.0
35	34.10	−0.69	1.09	1.0	1.0	1.0
40	38.84	−0.94	1.10	1.0	1.0	1.0

$$* \; \phi_j = \begin{cases} 1 & \text{for} \quad 1 \leqq j \leqq 49\,, \\ 0 & \text{for} \quad j \geqq 50\,. \end{cases}$$

This relation was borne out by numerical calculations, see Table 1. It would follow from (3.23) that, for $b>0$, $\|T_q^n(b)\| \geqq \text{const.}\sqrt{n}$. We surmise that $T_q(b)$ is stable on the subspace of data ϕ which are orthogonal to p.

By (3.20) the same inequality follows for $T_p^n(-b)$, completing the proof of (3.18). It is interesting to note that the instability of $T_p(-b)$ is more violent than the instability of $T_q(b)$; in the former case, instability is manifested by the first component of $T_p^n(-b)$ tending to ∞, see Table 2. Recall that $T_p(-b)$, $b>0$, corresponds to a shock which satisfies the entropy condition whereas $T_q(b)$, $b>0$, corresponds to a discontinuity that violates the entropy condition. It is amusing that the former should be more unstable than the latter, in the linearized analysis.

A number of numerical experiments carried out in the case $f(u)=u^2/2$ show that in the full nonlinear theory there is no instability at all of the discontinuity which satisfies the entropy condition, see Figures 3a and 3b. When the values (3, 6) are perturbed, iterations of the LW operator (3.3a) tend rapidly, as n tends from ∞, to one of a one-parameter family of steady profiles connecting -1 to 1. For discontinuities which violate the entropy condition, there is a mild instability. Finite perturbation causes a pair of rarefaction waves to issue from the point of discontinuity, without however completely dissolving the discontinuity into single rarefaction waves. See Figures 4a, 4b and 4c.

4. Conclusions

Our study shows that solutions of certain difference approximations to conservation laws fail to converge to the physically relevant solutions. On the other hand, we have shown that a limit of solutions of monotone difference

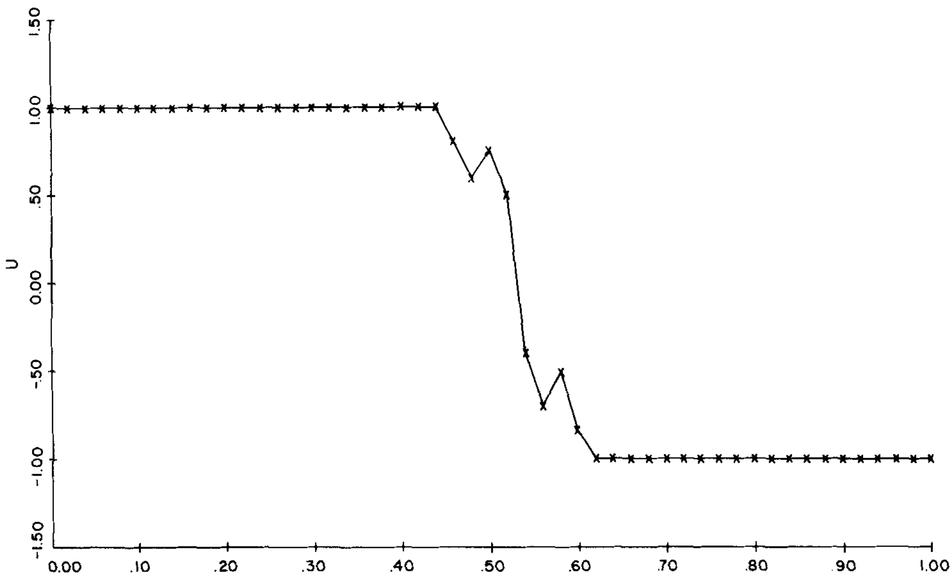

FIGURE 3a. Initial value

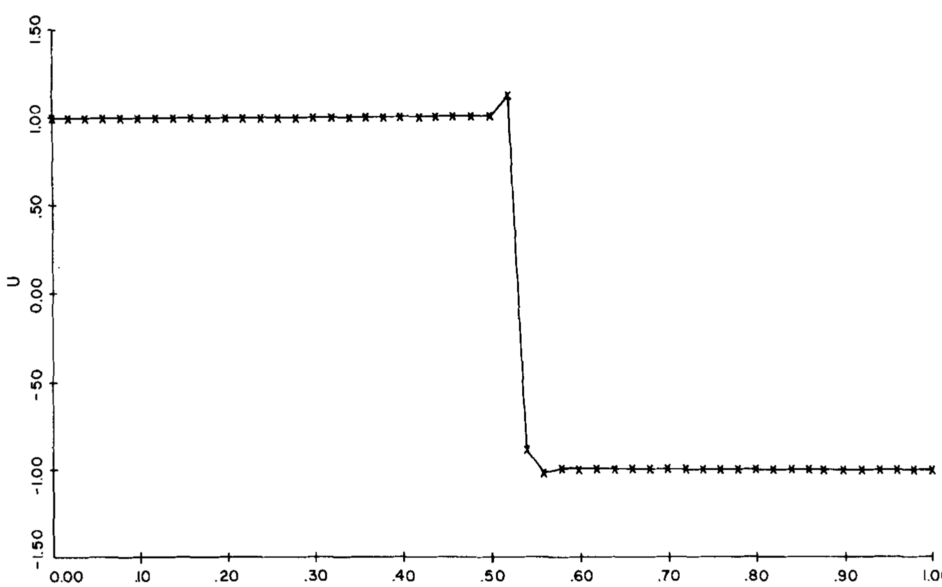

FIGURE 3b. Steady state

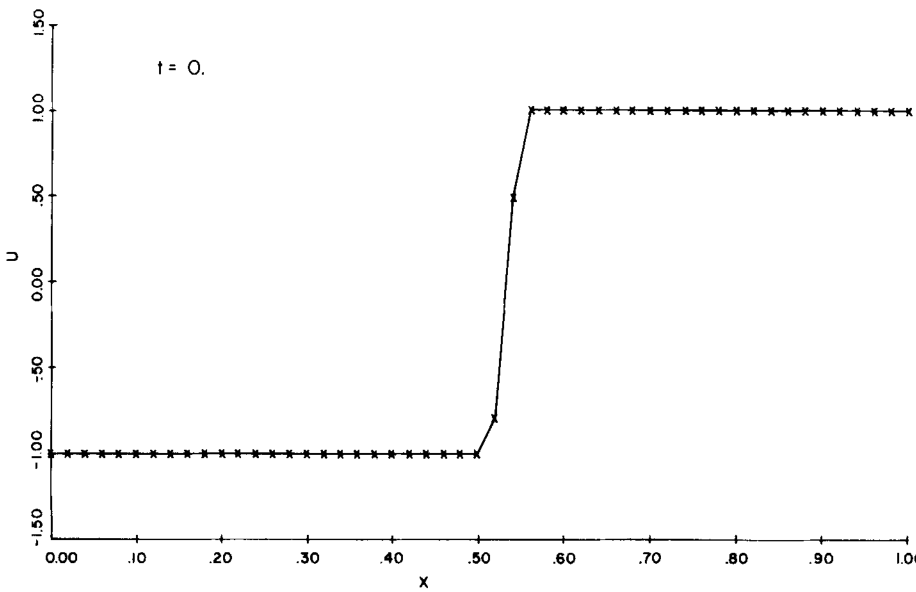

FIGURE 4a

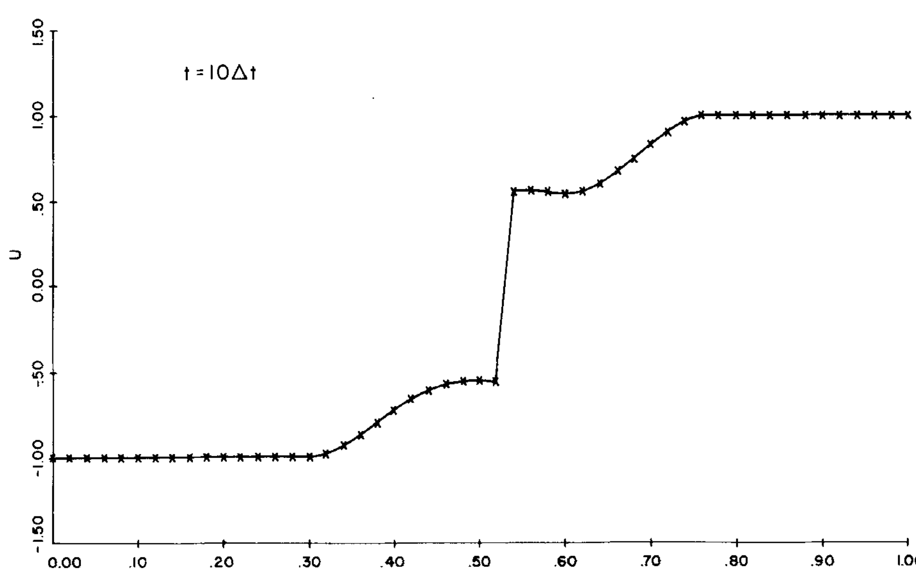

FIGURE 4b

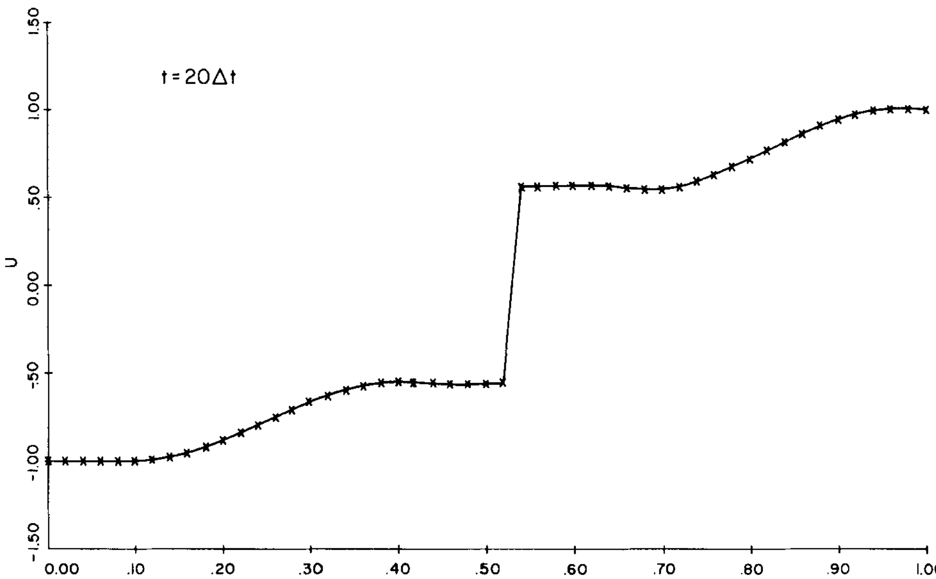

FIGURE 4c

schemes is always the physically relevant solution. This quality, as well as their extreme stability, makes monotone schemes attractive at first. On the other hand, monotone schemes are necessarily of first-order accuracy and this severely limits their accuracy and resolving power. In two- or three-dimensional problems, where mesh sizes are necessarily crude, first-order schemes are practically useless. Indeed, the practical schemes today combine high-order accuracy in smooth regions with a sufficient amount of dissipation in shock regions. Dissipation is provided either by some version of artificial viscosity, introduced 25 years ago by von Neumann and Richtmyer, see [18], [13], [1], [4], [14], or by some form of hybridization as in the method of Harten and Zwas [5]. The role of artificial viscosity as an entropy-producing mechanism was clearly recognized by von Neumann and Richtmyer, although it is also a device for reducing overshooting, and excessive oscillation, for stabilizing calculations. These two roles of artificial viscosity are related.

It would be extremely desirable to extend the result of Section 2 from monotone schemes to all schemes which have a certain amount of viscosity in regions of rapid transition and show that limits of such schemes satisfy the entropy condition.

It would also be extremely important to extend these results to systems. A notion of entropy for systems is discussed in [12]; it is shown there that limits of solutions of the Lax-Friedrichs scheme satisfy an entropy condition, provided that $\Delta t/\Delta x$ is less than a fraction of the Courant-Friedrichs-Lewy limit.

Another important problem is to study the effect of shocks on the overall accuracy of schemes which are of higher order in smooth regions.

Appendix

by

Barbara Keyfitz

It was shown in [7] that piecewise smooth solutions of a single conservation equation satisfying Condition E form an L_1-contractive semigroup. To be precise, if $u(x, t)$ and $w(x, t)$ are two solutions of (1.1a), and $u(x, 0)-w(x, 0) \in L_1$, and if u and w both satisfy Condition E, then

$$\|u(\cdot, t_2)-w(\cdot, t_2)\| \leqq \|u(\cdot, t_1)-w(\cdot, t_1)\| \tag{A.1}$$

for all $t_2 \geqq t_1 \geqq 0$; here $\| \ \|$ denotes the L_1-norm in the space variable. The converse of this proposition is also true, in the following sharp form: if (A.1) is satisfied for a particular weak solution u and all smooth solutions w, then u satisfies Condition E.

To test whether a given weak solution $u(x, t)$ satisfies Condition E, it is thus sufficient to show that $\|u(\cdot, t)-w(\cdot, t)\|$ is a non-increasing function of t for all *smooth* solutions w. For proofs, see [7], and [A1] in which Krushkov extended this result to general weak solutions.

In this appendix we give an alternate proof of the theorem of Section 2 by showing that if u is a limit of solutions of a monotone difference scheme, then (A.1) is indeed satisfied for all smooth solutions w. This is based on the observation by Gray Jennings [A2] that solutions of a monotone difference scheme satisfy a finite-difference analogue of L_1-contractiveness: if v_j^n and z_j^n are two solutions of (2.2) defined at grid points (jx, nt), and $v_j^0 - z_j^0$ is l_1-summable, then

$$|v^m - z^m| \leqq |v^n - z^n| \qquad \text{for} \qquad m \geqq n \geqq 0\,, \tag{A.2}$$

where $| \ |$ denotes the l_1-norm over the spatial grid. For the sake of completeness we present a proof.

Clearly it suffices to show that (A.2) holds for $m = n+1$. Introducing the notation $\bar{v}_j^n = (v_{j-k}^n, \cdots, v_{j+k}^n)$, a $(2k+1)$-dimensional string of points from $\{v_j^n\}$, and letting $s_j^n = \operatorname{sgn}(v_j^n - z_j^n)$, we can write

$$\|v^{n+1} - z^{n+1}\|_1 = \sum_j s_j^{n+1}(v_j^{n+1} - z_j^{n+1}) = \sum_j s_j^{n+1}(H(\bar{v}_j^n) - H(\bar{z}_j^n))\,.$$

Now, dropping the superscripts,

$$H(\bar{v}_j) - H(\bar{z}_j) = H((1-\theta)\bar{z}_j + \theta\bar{v}_j)|_0^1 = \int_0^1 \frac{d}{d\theta} H \, d\theta .$$

Let $\bar{\xi}_j(\theta) = (1-\theta)\bar{z}_j + \theta\bar{v}_j$, a $(2k+1)$-dimensional string from $\{(1-\theta)v_j + \theta z_j\}$; then

$$\|v^{n+1} - z^{n+1}\|_1 = \sum_j s_j^{n+1} \int_0^1 \sum_{l=1}^{2k+1} (v_{j-k+l-1} - z_{j-k+l-1}) \frac{\partial H}{\partial u_l} (\bar{\xi}_j(\theta)) \, d\theta .$$

Rearranging terms, we obtain

$$\sum_m (v_m - z_m) \int_0^1 \sum_{l=1}^{2k+1} s_{m+k-l+1}^{n+1} \frac{\partial H}{\partial u_l} (\bar{\xi}_{m+k-l+1}(\theta)) \, d\theta ,$$

and since $\partial H/\partial u_l \geqq 0$ for $l = 1, \cdots, 2k+1$, we may drop the terms s_j^{n+1} and write

$$\|v^{n+1} - z^{n+1}\|_1 \leqq \sum_m |v_m^n - z_m^n| \left\{ \int_0^1 \sum_{l=1}^{2k+1} \frac{\partial H}{\partial u_l} (\bar{\xi}_{m+k-l+1}(\theta)) \, d\theta \right\} .$$

However,

$$H(u_1, \cdots, u_{2k+1}) = u_{k+1} - \lambda\{h(u_2, \cdots, u_{2k+1}) - h(u_1, \cdots, u_{2k})\}$$

and so

$$\frac{\partial H}{\partial u_1} = \lambda \frac{\partial h}{\partial u_1} (u_1, \cdots, u_{2k}) ,$$

$$\frac{\partial H}{\partial u_{2k+1}} = -\lambda \frac{\partial h}{\partial u_{2k}} (u_2, \cdots, u_{2k+1}) ,$$

$$\frac{\partial H}{\partial u_{k+1}} = 1 - \lambda \frac{\partial h}{\partial u_k} (u_2, \cdots, u_{2k+1}) + \lambda \frac{\partial h}{\partial u_{k+1}} (u_1, \cdots, u_{2k}) ,$$

and

$$\frac{\partial H}{\partial u_i} = -\lambda \frac{\partial h}{\partial u_{i-1}} (u_2, \cdots, u_{2k+1}) + \lambda \frac{\partial h}{\partial u_i} (u_1, \cdots, u_{2k})$$

otherwise .

Hence, for each fixed value of θ, dropping the θ-dependence of ξ,

$$\sum_{l=1}^{2k+1} \frac{\partial H}{\partial u_l}(\xi_{m-l+1}, \xi_{m-l+2}, \cdots, \xi_{m+2k-l+1})$$

$$= \lambda \frac{\partial h}{\partial u_1}(\xi_m, \xi_{m+1} \cdots) + \sum_{l=2}^{2k} \left\{ -\lambda \frac{\partial h}{\partial u_{l-1}}(\xi_{m-l+2}, \cdots) + \lambda \frac{\partial h}{\partial u_l}(\xi_{m-l+1}, \cdots) \right\} + 1 \quad \text{(for the } k+1 \text{ term)}$$

$$- \lambda \frac{\partial h}{\partial u_{2k}}(\xi_{m-2k+1}, \cdots) = 1 .$$

Thus

$$\|v^{n+1} - z^{n+1}\|_1 \leqq \sum_m |v_m^n - z_m^n| \int_0^1 1 \, d\theta = \|v^n - z^n\|_1 ,$$

proving (A.1).

To complete the argument, let $u(x, t)$ be the strong limit of solutions v_j^n of (2.2) as $\Delta x, \Delta t \to 0$ with λ fixed. Let $w(x, t)$ be any smooth solution of (1.1a) with $u(x, 0) - w(x, 0) \in L_1$. Now w can be approximated by a solution z_j^n of (2.2) which converges strongly to w as $\Delta x \to 0$ with λ fixed, as a consequence of a result of Strang [A3], which shows that for positive methods (including monotone schemes) convergence to smooth solutions is guaranteed.

In (A.2) let $\Delta x \to 0$ with λ fixed, and $m, n \to \infty$ so that $m \Delta t = t_2$, $n \Delta t = t_1$. Since v_j^n and z_j^n converge strongly and hence in norm,

$$\Delta x \|v^n - z^n\| \to \|u(\cdot, t) - w(\cdot, t)\| ,$$

whence (A.1) follows.

We remark that monotonicity is necessary for (A.2) to hold: a difference scheme approximating (1.1a) which is consistent and conservative and satisfies (A.2) is monotone.

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