TOWARDS THE ULTIMATE CONSERVATIVE DIFFERENCE SCHEME
I. THE QUEST OF MONOTONICITY

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1. THE PROBLEM

The one-dimensional equations of ideal compressible flow are preferably written in conservation form:

$$\frac{\partial w}{\partial t} + \frac{\partial f(w)}{\partial x} = 0. \tag{1}$$

Many interesting flows, notably those containing shocks, can be computed with conservative, dissipative difference schemes based on Eq. (1). In order to analyze or design such schemes it is most practical to start from the single convection equation

$$\frac{\partial w}{\partial t} + a\,\frac{\partial w}{\partial x} = 0. \tag{2}$$

How to make a scheme for Eq. (2) useful to integrate Eq. (1) is explained by Van Leer [4]. The best-known conservative schemes, those of Lax, Godunov and Lax-Wendroff, are based on the cluster of nodal points C1 defined in Fig. 1.

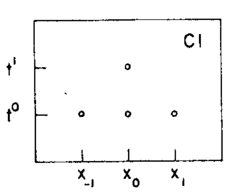

Figure 1. The cluster C1

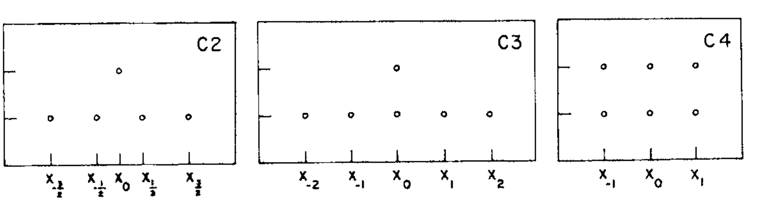

Figure 2. Some clusters suitable for conservative monotonic schemes

Eq. (2) transforms an initially monotonic distribution such that it remains monotonic at later times; in fact, the original distribution is just shifted over a distance a×t. A difference scheme for Eq. (2) can not deliver this exact solution, except for integer values of $\sigma = a\Delta t/\Delta x$, but it may at least be required to produce <u>monotonic</u> results for all stable values of σ. This requirement is called the monotonicity condition; schemes satisfying it will colloquially be called monotonic schemes.

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* This work was done while I was on leave of absence at the University of California, Berkeley, as a Miller Fellow.

Godunov [1] tested for monotonicity among the linear schemes for Eq. (2) defined on the cluster C1. These can be written as

$$w^0 = w_0 - \frac{\sigma}{2}(w_1 - w_{-1}) + \frac{q}{2}(w_1 - 2w_0 + w_{-1}); \tag{3}$$

the notation is clarified in Table 1.

TABLE 1

Notation used in the grid

symbol	definition
x_0	abcissa of central nodal point in cluster C1
$x_{\pm 1}$	$x_0 \pm \Delta x$
t^0	initial time level
t^1	advanced time level = $t^0 + \Delta t$
w_0, $w_{\pm 1}$	initial values of w in x_0, $x_{\pm 1}$
w^0	value of w in x_0 at advanced time level
$\Delta_{\frac{1}{2}}$	$w_1 - w_0$
$\Delta_{-\frac{1}{2}}$	$w_0 - w_{-1}$

Any function $q(\sigma)$ defines a scheme; for stability it is required that

$$\sigma^2 \leq q \leq 1, \tag{4}$$

and for monotonicity:

$$|\sigma| \leq q \leq 1. \tag{5}$$

The lower limit in (4) yields the second-order scheme of Lax-Wendroff; any other choice of q results in first-order accuracy. The scheme of Lax, corresponding to the upper limit in (4), is the least accurate of all. Godunov's scheme, corresponding to the lower limit in (5), is the best first-order scheme: it has the smallest q that still guarantees monotonicity. One might also say that this scheme maintains the optimum balance between dissipative and dispersive errors. The dissipation is just strong enough to damp shorter waves before they get to much out of step and show up as oscillations on top of the larger features.

Godunov proved there are no linear second-or-higher-order schemes for Eq. (2) that always preserve monotonicity. Such schemes can only handle very smooth initial values, in which higher derivatives are of minor importance. Whoever wants to pursue unconditional monotonicity must take refuge in nonlinear techniques. In the following, regard a and q as functions of w, their values varying from point to point.

Lax and Wendroff [3] showed how their scheme can be made more dissipative, without affecting its order of accuracy, by increasing $q_{\pm\frac{1}{2}}$ by an amount $\sim \frac{1}{2}|\Delta_{\pm\frac{1}{2}}a|/|a|_{\pm\frac{1}{2}}$. This helps damping numerical oscillations as well as nonlinear instabilities, which often go hand in hand. However, the extra dissipation is not necessarily most effective in places where it is most needed. In consequence, monotonicity is not generally achieved. Harten and Zwas [2] use the expression $|\Delta_{\pm\frac{1}{2}}a|/\max_x|\Delta a|$, which gives stronger but still rather arbitrary damping.

In the present paper I shall show that unconditional monotonicity involves the use of the ratio $\Delta_{+\frac{1}{2}}a/\Delta_{-\frac{1}{2}}a$ in the dissipation coefficient. Unfortunately, a scheme based on C1 that includes this expression can never be conservative; see Van Leer [4, Sec. 2.2]. To me, this represents the first valid reason to step up to a larger number of points in the basic cluster. Suitable five- and six-point clusters are shown in Fig. 2. Having no results ready for these more elaborate clusters, I shall occupy myself with the Lax-Wendroff scheme in the further sections of this paper.

2. A NONLINEAR DEVICE

Regard (2) again as a linear equation. To fix our thoughts, let a be positive. I shall start from the Lax-Wendroff scheme, raising q above the value σ^2 as the initial values of w lack smoothness. In this way a nonlinear but monotonic scheme is obtained for a linear equation. For the sake of clarity, the derivation of this scheme given below follows a geometrical rather than an algebraic line of reasoning.

Fig. 3 shows the full range of circumstances under which the ordinary Lax-Wendroff scheme may produce non-monotonic results; the limiting cases of just monotonic behaviour are included. The smoothness of initial-value triplets (w_{-1}, w_0, w_1) is most conveniently characterized by the ratio

$$\zeta = \frac{2\Delta_{-\frac{1}{2}}w}{\Delta_{\frac{1}{2}}w - \Delta_{-\frac{1}{2}}w}. \tag{6}$$

In the sequence of Fig. 3 this expression runs from -1 to +1.

In each graph a parabola is drawn (thin curve marked LW) through the points $(x = -\Delta x,\ w = w_{-1})$, $(x = 0,\ w = w_0)$ and $(x = \Delta x,\ w = w_1)$. The new value w^0, as computed with the Lax-Wendroff scheme, can be found on this parabola at $x = -\sigma\Delta x$, somewhere in the left mesh. An explanation of this quadratic interpolation routine can be found in Van Leer [4, Sec. 3.5]. For $-1 < \zeta < 1$ the parabola LW undershoots the dotted line LL which indicates the Lower of the Levels $w = w_{-1}$ and $w = w_0$. For

$\zeta = \pm 1$, LW does not undershoot: it is just tangent to LL. For $|\zeta| > 1$, not illustrated here, there is no more danger of undershooting.

In most circumstances where the Lax-Wendroff scheme predicts a new value lower than any of the initial values, there is no reason at all to believe that such lower values really occur in the exact solution. Thus the undershooting value does not represent a gain in accuracy but merely shows the low compliance of the interpolation curve LW. If monotonicity is to be achieved, LW must be replaced in the danger zone $|\zeta| < 1$ by a different curve.

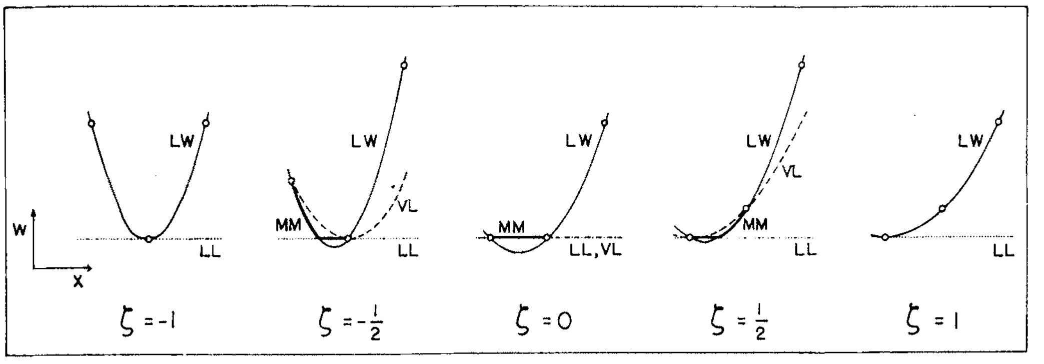

Figure 3. The danger zone of ζ. The choice of concave initial values $(\Delta_{\frac{1}{2}}w - \Delta_{-\frac{1}{2}}w > 0)$ is arbitrary; a similar sequence exists for convex data

The curve closest to LW that still preserves monotonicity is obtained by cutting LW short with LL, whenever LW dips under LL. The result is the heavy curve MM (for Marginal Monotonicity) with the kink; it is indicated only in the left mesh. Using MM in a scheme, however, is halting between two opinions: if the curve LW is not trusted, why retain even a part of it? With the application to nonlinear equations in mind, it is better anyway to choose a curve lying safely above MM, preferably one without a kink. For $\zeta = \pm 1$, the curve must coincide with LW in order to achieve a smooth transition between the "emergency" scheme and the ordinary Lax-Wendroff scheme. The simplest possible replacement curve is a parabola that runs through w_{-1} and w_0 but is not forced through w_1; instead, it is chosen tangent to the line LL. This parabola is the broken curve VL in Fig. 3; for $\zeta = 0$, VL degenerates into LL itself.

The emergency scheme corresponding to the interpolation curve VL can be written as

$$\begin{aligned} w^0 - w_0 &= -\sigma^2 \Delta_{-\frac{1}{2}} w, && -1 < \zeta < 0; \\ w^0 - w_0 &= -\sigma(2 - \sigma)\Delta_{-\frac{1}{2}} w, && 0 \leqq \zeta < 1. \end{aligned} \tag{7}$$

It is easily verified that this scheme can be obtained from the Lax-Wendroff scheme by adding to q the term

$$\sigma(1 - \sigma)(1 - |\zeta|), \qquad |\zeta| < 1. \tag{8}$$

Note that this expression is positive definite, hence damping is indeed increased.

3. A NUMERICAL EXAMPLE

Now assume that a depends linearly on w, such as in the quadratic conservation law

$$\frac{\partial w}{\partial t} + \frac{\partial(\frac{1}{2}w^2)}{\partial x} = 0, \tag{9}$$

where a = w. I redefine ζ as

$$\zeta = \frac{2\Delta_{-\frac{1}{2}}a}{\Delta_{\frac{1}{2}}a - \Delta_{-\frac{1}{2}}a}, \tag{10}$$

which for Eq. (9) gives the same result as definition (6). For the numerical experiment reported below I added the non-conservative ζ-term (8) to the conservative Lax-Wendroff scheme for Eq. (9). In (8) I substituted for σ the local value σ_0. With the resulting scheme a rarefaction wave[1] was followed which at t = 0 was defined by the values

$$\begin{aligned} w_m &= \tfrac{1}{3}, & m &\leqq 25; \\ w_m &= \tfrac{2}{3}, & m &= 26; \\ w_m &= 1, & m &\geqq 27. \end{aligned} \tag{11}$$

The results after 24 time-steps, with $\sigma = \frac{1}{2}$, are shown in Fig. 4 together with the results for the unmodified Lax-Wendroff scheme and with the exact solution. Both schemes show a starting error in the position of the wave of about $-0.3\Delta x$. At the head of the wave, the schemes give almost identical results; at the foot, the monotonic scheme is clearly superior. The representation of the foot can be made even more acute by basing the scheme on a curve that fits MM more tightly than VL does. Furthermore, it is worth considering a reduction of the value of q for $-3 < \zeta < -1$, when the parabola LW undershoots LL in the right mesh and should not yet be taken to seriously. With the scheme thus modified, the head of the rarefaction wave will turn out sharper too.

[1] I did not make the obvious shock wave computation, as the non-conservative scheme would have produced meaningless results.

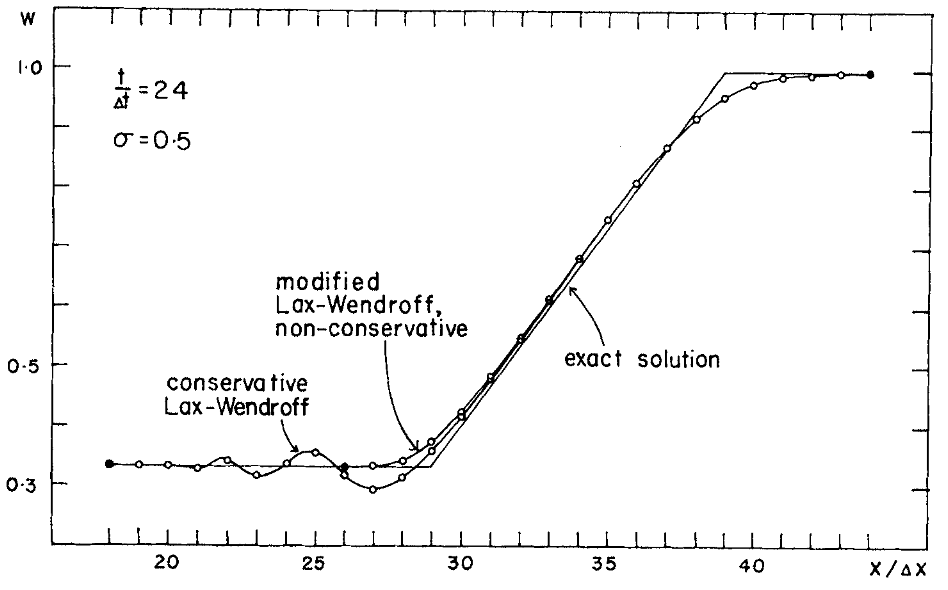

Figure 4. Numerical representation of a rarefaction wave. Beyond the black dots, the numerical results differ less than 0.0001 from the exact solution

The above results clearly demonstrate the usefulness of the smoothness monitor (10) in constructing a monotonic scheme for a single nonlinear conservation law. The main point is now to design a monotonic scheme that is also conservative. The final step is applying it to a nonlinear system of conservation laws, in particular, the equations of ideal compressible flow.

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