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CONDITIONS FOR THE CONSTRUCTION OF MULTI-POINT TOTAL VARIATION DIMINISHING DIFFERENCE SCHEMES

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Conditions are derived for the construction of total variation diminishing difference schemes with multi-point support. These conditions, which are proved for explicit, implicit, and semi-discrete schemes, correspond in a general sense to the introduction of upwind biasing.

1. Introduction

It is natural that the rapid evolution of increasing powerful computers should inspire attempts to solve previously intractable problems by numerical calculation. One might imagine that within a fairly short time, advances in processing speed and memory capacity ought to reduce the simulation of physical systems governed by partial differential equations to a matter of routine. The numerical computation of solutions of nonlinear conservation laws has proved, in fact, to be perhaps unexpectedly difficult. Discontinuities are likely to appear in the solution, and schemes which are accurate in smooth regions tend to produce spurious oscillations in the neighbourhood of the discontinuities. These oscillations can be eliminated by the use of strongly dissipative first order accurate schemes, but these schemes severely degrade the accuracy and usually produce excessively smeared discontinuities.

The scalar nonlinear conservation law in one space dimension

$$\partial u/\partial t + \partial f(u)/\partial x = 0 \tag{1}$$

provides a model which already contains the phenomena of shockwave formation and expansion fans. Thus it can be used to provide insight into the likely behavior of numerical approximations to more complex physical systems, while it is still simple enough to be fairly easily amenable to analysis. A rather complete mathematical theory of solutions to (1) is by now available [1–3].

Equation (1) describes wave propagation at a speed

$$a(u) = \partial f/\partial u.$$

The solution is constant along the characteristic lines

$$\partial x/\partial t = a(u)$$

provided that they do not interact to form a shock wave. Tracing the solution backward along the characteristics, it can be seen that the total variation

$$\mathrm{TV}(u) = \int_{-\infty}^{\infty} \left| \frac{\partial u}{\partial x} \right| \mathrm{d}x$$

is constant prior to the formation of a shockwave, while it may decrease when the shockwave is

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formed. Corresponding to this property it may be observed that no new local extrema may be created, and that the value of a local minimum is nondecreasing while the value of a local maximum is nonincreasing. It follows that an initially monotone profile continues to be monotone.

It seems desirable that these properties should be preserved by a numerical approximation to (1). This will guarantee the exclusion of spurious oscillations in the numerical solution. Harten [4] has recently introduced the concept of total variation diminishing (TVD) difference schemes, which have the property that the discrete total variation

$$\mathrm{TV}(v) = \sum_{k=-\infty}^{\infty} |v_k - v_{k-1}|$$

of the solution vector v cannot increase. Harten also devised procedures for constructing both explicit and implicit TVD schemes [4,5].

The purpose of this paper is to state and prove conditions for the construction of multi-point TVD schemes. Conditions are derived for explicit, implicit, and also semi-discrete operators to be TVD. The conditions are both necessary and sufficient in the case of the explicit and semi-discrete schemes. The reasoning is a modification and extension of the reasoning used by Lax [5, Appendix]. The results were first presented in a lecture at ICASE in March 1984. The present paper is an amplification and revision of a Princeton University report issued under the same title in April 1984 [6]. In the intervening period Osher and Chakravarthy have given another proof that conditions (3.12) are sufficient for an explicit scheme to be TVD [7].

2. Conditions for reduction of the l_1 norm

One-dimensional difference operators act on doubly infinite sequences

$$u = \{u_k\}, \quad -\infty < k < \infty. \tag{2.1}$$

The l_1 norm of such a vector u is defined as

$$|u|_1 = \sum_{-\infty}^{\infty} |u_k|. \tag{2.2}$$

The space of all vectors u with finite l_1 norm is denoted by l_1.

A difference operator maps l_1 into l_1 and is of the form

$$A(u)_k = \sum_j a_j u_{k-j}. \tag{2.3}$$

The coefficients a_j depend on k, either explicitly or through dependence on u. In either case we write

$$a_j = a_j(k).$$

Theorem A. *The operator A defined by* (2.3) *satisfies*

$$|A(u)|_1 \leqslant |u|_1 \tag{2.4}$$

for all u in l_1 if and only if

$$\sum_j |a_j(h+j)| \leqslant 1 \tag{2.5}$$

for all h.

An operator A satisfying (2.4) is a *contraction*.

Proof. The signum function is defined for every real u by

$$\text{signum } u = \begin{cases} 1 & \text{for} \quad u > 0, \\ 0 & \text{for} \quad u = 0, \\ -1 & \text{for} \quad u < 0. \end{cases} \tag{2.6}$$

Now set

$$s_k = \text{signum } A(u)_k; \tag{2.6*}$$

then, by definition (2.2) of the l_1 norm and definition (2.6) of signum we have

$$\begin{aligned} |A(u)|_1 &= \sum_k |A(u)_k| = \sum_k s_k A(u)_k \\ &= \sum_k s_k \sum_j a_j(k) u_{k-j} = \sum_{h,j} a_j(h+j) s_{h+j} u_h = \sum_h w_h u_h \leqslant \sum_h |w_h| \; |u_h|, \end{aligned} \tag{2.7}$$

where

$$w_h = \sum_j a_j(h+j) s_{h+j}. \tag{2.7'}$$

Since s_k takes on the values ± 1 or 0, it follows from (2.7) that

$$|w_h| \leqslant \sum_j |a_j(h+j)|.$$

It follows therefore from assumption (2.5) that

$$|w_h| \leqslant 1$$

for all h. Setting this into (2.7) we deduce that (2.4) holds for all u in l_1.

To show the necessity of (2.5) suppose on the contrary that it fails for some $h = h_0$. Set $u^{(0)}$ equal to

$$u_l^{(0)} = \begin{cases} 1 & \text{for } l = h_0, \\ 0 & \text{for } l \neq h_0. \end{cases} \tag{2.8}$$

For this $u^{(0)}$ it follows from (2.3) that

$$A(u^{(0)})_k = a_{k-h_0}(k)$$

and so

$$\begin{aligned} |A(u^{(0)})|_1 &= \sum_k |A(u^{(0)})_k| = \sum_k |a_{k-h_0}(k)| \\ &= \sum_j |a_j(h_0+j)| > 1 \end{aligned} \tag{2.9}$$

since h_0 was so chosen that (2.5) is violated. On the other hand, it is obvious from (2.8) that

$$|u^{(0)}|_1 = 1.$$

This combined with (2.9) shows that (2.4) fails for $u^{(0)}$. □

For use in implicit schemes the following result is needed.

Theorem B. *Define the operator B by*

$$B(u)_k = \sum_j b_j(k) u_{k-j}. \tag{2.10}$$

B satisfies

$$|B(u)|_1 \geqslant |u|_1 \tag{2.11}$$

for all u in l_1 if

$$b_0(h) - \sum_{j\neq 0} |b_j(h+j)| \geqslant 1. \tag{2.12}$$

An operator B satisfying (2.11) is called an *expansion*.

Proof. We define

$$s_k = \text{signum } u_k. \tag{2.13}$$

Since $|s_k| \leqslant 1$,

$$|B(u)|_1 = \sum_k |B(u)_k| \geqslant \sum_k s_k B(u)_k. \tag{2.14}$$

Analogously to (2.7), (2.7′) we have

$$\sum_k s_k B(u)_k = \sum_h w_h u_h \tag{2.15}$$

where

$$w_h = \sum_j b_j(h+j) s_{h+j}. \tag{2.15′}$$

It follows readily from (2.12) that if $u_h \neq 0$,

$$|w_h| \geqslant 1.$$

Using (2.13) we get

$$\text{signum } w_h = \text{signum } u_h.$$

These two imply that

$$\sum_h w_h u_h \geqslant |u|_1. \tag{2.16}$$

Combining (2.14), (2.15), and (2.16) we get (2.11). □

We remark that (2.12) is far from being necessary for B to be expansive. For example, take the right shift operator T, with

$$b_j = \begin{cases} 1 & \text{for } j = 1, \\ 0 & \text{for } j \neq 1. \end{cases}$$

Clearly, T is an isometry:

$$(Tu)_1 = |u|_1,$$

but condition (2.12) is utterly violated.

Theorem A has a continuous analogue:

Theorem C. *Let $u(t)$ be a differentiable function of t real whose values lie in l_1, and which satisfies a differential equation of the form*

$$\mathrm{d}u/\mathrm{d}t = C(u), \tag{2.17}$$

where C is a difference operator, i.e., an operator of the form

$$C(u)_k = \sum_j c_j u_{k-j}. \tag{2.18}$$

The coefficients c_j may depend on k and t either directly or through a dependence on u. Then $|u(t)|_1$ is a nonincreasing function of t if and only if for all h and all t

$$c_0(h) + \sum_{j \neq 0} |c_j(h+j)| \leqslant 0. \tag{2.19}$$

Proof. Define $s_k(t)$ by

$$s_k(t) = \text{signum } u_k(t). \tag{2.20}$$

Then

$$|u(t)|_1 = \sum_k s_k(t) u_k(t). \tag{2.21}$$

Since each s_k is piecewise constant,

$$\frac{\mathrm{d}}{\mathrm{d}t} |u(t)|_1 = \sum_k s_k(t) \frac{\mathrm{d}u_k}{\mathrm{d}t}. \tag{2.22}$$

According to (2.17),

$$\frac{\mathrm{d}u_k}{\mathrm{d}t} = \sum_j c_j(k) u_{k-j}. \tag{2.23}$$

Setting this into the right in (2.22) we get, after relabelling the index of summation,

$$\frac{\mathrm{d}}{\mathrm{d}t} |u(t)|_1 = \sum_k s_k \sum_j c_j(k) u_{k-j} = \sum_h w_h u_h \tag{2.24}$$

where

$$w_h = \sum_j c_j(h+j) s_{h+j}. \tag{2.25}$$

Suppose $u_h \neq 0$; then by (2.20), $s_h \neq 0$. Multiply (2.25) by s_h; using assumption (2.19) we get

$$s_h w_h = c_0(h) + \sum_{j \neq 0} c_j(h+j) s_h s_{h+j} \leqslant 0.$$

Since by definition, s_h and u_h have the same sign, it follows that for all h

$$u_h w_h \leqslant 0;$$

this relation clearly holds also when $u_h = 0$. Setting this into (2.24) we obtain

$$\mathrm{d}|u(t)|_1/\mathrm{d}t \leqslant 0;$$

this proves that $|u(t)|_1$ decreases as t increases.

Next we indicate why condition (2.19) is necessary. Suppose it is violated at t_0, h_0. Let $u(t)$ be that solution of (2.17) whose value at t_0 equals

$$u_k(t_0) = \delta_{k,h_0} = \begin{cases} 1 & \text{for } k = h_0, \\ 0 & \text{for } k \neq h_0. \end{cases}$$

Using (2.23) we get

$$u_k(t_0+\epsilon)=\delta_{k,h_0}+\epsilon\sum_j c_j(k)\delta_{k-j,h_0}+O(\epsilon^2).$$

Summing with respect to k gives

$$\sum_k u_k(t_0+\epsilon)=1+\epsilon\sum_j c_j(h_0+j)+O(\epsilon^2).$$

Since condition (2.19) is violated at t_0, h_0 we conclude that for ϵ small enough positive,

$$\sum_k |u_k(t_0+\epsilon)|=1+\epsilon c_0(h_0)+\epsilon\sum_{j\neq 0}|c_j(h_0+j)|+O(\epsilon^2)>1.$$

Thus

$$|u(t_0+\epsilon)|_1>1$$

while

$$|u(t_0)|_1=1.$$

This shows that $|u(t)|_1$ is not a decreasing function of t, completing the proof of Theorem C. □

3. Construction of total variation diminishing schemes

Theorems A, B, and C may be used to find conditions on the coefficients of a difference operator which guarantee that the total variation of a solution does not increase for

(E) explicit schemes,
(I) implicit schemes,
(S) semi-discrete schemes.

The total variation of a vector u is

$$\mathrm{TV}(u)=\sum_k |u_k-u_{k-1}|.$$

Using the right shift operator T

$$T(u)_k=u_{k-1}$$

we can express $\mathrm{TV}(u)$ as

$$\mathrm{TV}(u)=|(I-T)u|_1. \tag{3.1}$$

We turn now to explicit $(2J+1)$ point schemes

$$u^{n+1}=D(u^n) \tag{3.2}$$

where

$$D(u)_k=\sum_{-J}^{J} d_j(k)u_{k-j}. \tag{3.3}$$

We assume that the difference operator D preserves constants. In view of (3.3), this is the case if

$$\sum_j d_j(k)=1 \tag{3.4}$$

for all k. Schemes (3.3) satisfying this condition can be written in the form

$$D(u)_k = u_k + \sum_{-J \leqslant j < J} e_j(k)(u_{k-j} - u_{k-j-1}) \tag{3.5}$$

or in operator notation

$$D = I + E(I - T), \tag{3.6}$$

where

$$E = \sum e_j T^j. \tag{3.6$'$}$$

We want to find conditions which guarantee that D is TVD, i.e., satisfies for all u

$$\mathrm{TV}(Du) \leqslant \mathrm{TV}(u). \tag{3.7}$$

Using (3.1) this is the same as

$$|(I - T)Du|_1 \leqslant |(I - T)u|_1. \tag{3.7$'$}$$

Using formula (3.6) we can write

$$(I - T)D = (I + (I - T)E)(I - T) = A(I - T), \tag{3.8}$$

where

$$A = I + (I - T)E. \tag{3.8$'$}$$

We now set (3.8) into (3.7′); denoting

$$(I - T)u = u^*$$

we obtain the equivalent inequality

$$|Au^*|_1 \leqslant |u^*|_1. \tag{3.9}$$

This is certainly the case if A is an l_1 contraction, for which we have derived in Section 2 the criterion (2.5):

$$\sum_j |a_j(h + j)| \leqslant 1 \tag{3.10}$$

where

$$(Au)_k = \sum_j a_j(k) u_{k-j}. \tag{3.10$'$}$$

It follows from (3.8′) that the coefficients a_j of A can be expressed in terms of the coefficients e_j of E as

$$a_0(k) = 1 + e_0(k) - e_{-1}(k - 1) \tag{3.11}$$

and

$$a_j(k) = e_j(k) - e_{j-1}(k - 1), \quad j \neq 0. \tag{3.11$'$}$$

It follows from these relations that

$$\sum_j a_j(h + j) = 1;$$

but then (3.10) can hold if and only if for all j and k

$$a_j(k) \geqslant 0.$$

Using (3.11), (3.11′) we can express this condition as follows:

$$\begin{aligned} &e_{-1}(k-1) \geqslant e_{-2}(k-2) \geqslant \cdots \geqslant e_{-J}(k-J) \geqslant 0, \\ &-e_0(k) \geqslant -e_1(k+1) \geqslant \cdots \geqslant -e_{J-1}(k+J-1) \geqslant 0, \\ &1 + e_0(k) - e_{-1}(k-1) \geqslant 0. \end{aligned} \tag{3.12}$$

Thus we have proved the following theorem.

Theorem E. *The explicit scheme* (3.3) *is TVD if conditions* (3.12) *are satisfied for all k, where e_j are the coefficients appearing in formula* (3.5) *for D.*

We turn next to implicit schemes:

$$F(u^{n+1}) = u^n. \tag{3.13}$$

We take F to be a $2J+1$ term difference operator that preserves constants. Such an F can be written in the form

$$F = I + G(I - T) \tag{3.14}$$

where

$$G(u)_k = \sum_{-J \leqslant j < J} g_j(k) u_{k-j}. \tag{3.14′}$$

We want to find conditions under which scheme (3.13) is TVD, i.e., for all u

$$\mathrm{TV}(Fu) \geqslant \mathrm{TV}(u). \tag{3.15}$$

Using formula (3.1), this is the same as

$$|(I-T)Fu|_1 \geqslant |(I-T)u|_1. \tag{3.15′}$$

Using formula (3.14) we can write

$$(I-T)F = (I + (I-T)G)(I-T) = B(I-T) \tag{3.16}$$

where

$$B = I + (I-T)G. \tag{3.16′}$$

We set (3.16) into (3.15′); denoting

$$(I-T)u = u^*$$

we obtain the equivalent inequality

$$|Bu^*|_1 \geqslant |u^*|_1. \tag{3.17}$$

This is the case if B is an expansion. In Theorem B we have derived criterion (2.12) that guarantees that an operator B is an expansion:

$$b_0(h) \geqslant \sum_{j \neq 0} |b_j(h+j)| + 1. \tag{3.18}$$

It follows from (3.16′) that the coefficients b_j of B can be expressed in terms of the coefficients g_j of G as

$$b_0(k) = 1 + g_0(k) - g_{-1}(k-1)$$

and

$$b_j(k) = g_j(k) - g_{j-1}(k-1), \quad j \neq 0.$$

Adding up these relations we deduce that

$$b_0(k) = 1 - \sum_{j \neq 0} b_j(k+j);$$

but then (3.18) can hold if and only if for all k and for $j \neq 0$

$$b_j(k) \leqslant 0.$$

Using (3.19), these conditions can be restated as

$$g_0(k) \geqslant g_1(k+1) \geqslant \cdots \geqslant g_{J-1}(k+J-1) \geqslant 0 \tag{3.20}$$

and

$$-g_{-1}(k-1) \geqslant -g_{-2}(k-2) \geqslant \cdots \geqslant -g_{-J}(k-J) \geqslant 0. \tag{3.20$'$}$$

Thus we have proved the following theorem.

Theorem I. *The implicit scheme* (3.13) *is TVD if conditions* (3.20), (3.20′) *are satisfied, where* g_j *are the coefficients of the operator G related by formula* (3.14), (3.14′) *to the operator F appearing in* (3.13).

We remark that we can combine, as Harten does, Theorems I and E to study implicit-explicit schemes of the form

$$F(u^{n+1}) = D(u^n). \tag{3.21}$$

Such a scheme is TVD if F satisfies the conditions of Theorem I, and D the conditions of Theorem E.

Finally we turn to semi-discrete schemes:

$$\mathrm{d}u/\mathrm{d}t = Hu, \tag{3.22}$$

with H some $2J+1$ point difference operator. We assume that $u \equiv$ const. is a solution of (3.22); this is the case if H annihilates all constant vectors. In this case H can be written in the form

$$H(u)_k = \sum_{-J \leqslant j < J} m_j(k)(u_{k-j} - u_{k-j-1}), \tag{3.23}$$

or in operator form

$$H = M(I-T). \tag{3.23$'$}$$

We want to find conditions on H which guarantee that $\mathrm{TV}(u)$ is a decreasing function of t for all solutions u of (3.22). By formula (3.1), this is the same as

$$|(I-T)u(t)|_1$$

being a decreasing function of t. So we multiply (3.22) by $(I-T)$; using (3.23′) we get

$$\frac{\mathrm{d}}{\mathrm{d}t}(I-T)u = (I-T)M(I-T)u = C(I-T)u \tag{3.24}$$

where

$$C = (I-T)M. \tag{3.25}$$

Denoting

$$(I-T)u = u^*$$

(3.24) becomes

$$du^*/dt = Cu^*.$$

According to Theorem C, $|u^*|_1$ is a decreasing function of t if condition (2.19) of Section 2 is satisfied,

$$c_0(k) + \sum_{j\neq 0} |c_j(k+j)| \leqslant 0. \tag{3.26}$$

Using (3.25) we can express the coefficients c_j in terms of those of M as follows:

$$c_j(k) = m_j(k) - m_{j-1}(k-1). \tag{3.27}$$

Thus

$$\sum_j c_j(k+j) = 0.$$

It follows from this that (3.26) can hold if and only if

$$c_j(k+j) \geqslant 0, \quad j \neq 0.$$

Using (3.27) we can restate this as

$$m_{-1}(k-1) \geqslant m_{-2}(k-2) \geqslant \cdots \geqslant m_{-J}(k-J) \geqslant 0 \tag{3.28}$$

and

$$-m_0(k) \geqslant -m_1(k+1) \geqslant \cdots \geqslant m_{J-1}(k+J-1) \geqslant 0. \tag{3.28'}$$

Thus we have proved the next theorem.

Theorem S. *The semi-discrete scheme* (3.22) *is TVD if conditions* (3.28) *and* (3.28′) *are satisfied, where the* m_j *are the coefficients of the operator* M *related by formula* (3.23′) *to the operator* H.

4. Conclusion

The conservation law (1) describes a right running wave when $a(u)$ is positive. Conditions (3.12) and (3.28) of Theorems E and S state that the explicit and semi-discrete schemes (E) and (S) are TVD if only if the coefficients of the differences $u_{k-j} - u_{k-j-1}$ have the same sign as $a(u)$ for $j \geqslant 0$, (points on the upwind side), and the opposite sign for $j < 0$ (points on the downwind side). If the differences are moved over to the right of equation (3.13), then condition (3.20) of Theorem I states that the implicit scheme (I) will be TVD if it satisfies a similar condition on the sign of its coefficients. In all three cases only the differences on the upwind side have the correct sign for consistency with (1), and can contribute to wave propagation in the correct direction. In this sense upwind biasing is a necessary feature of explicit TVD schemes, and it is also useful in the construction of implicit TVD schemes.

It is thus not surprising to find that most of the attempts to design schemes with the capability of capturing shockwaves and contact discontinuities, dating back to the early work of Courant, Isaacson and Rees [8], and Godunov [9], have introduced upwinding either directly or indirectly. Second order accurate upwind schemes have been devised by Van Leer [10], Harten [4,5], Roe [11], Osher and Chakravarthy [12], and Sweby [13]. These all use flux limiters to attain the TVD property.

Another approach to the construction of TVD schemes stems from the observation that central difference formulas for odd and even derivatives have odd and even distributions of signs, and they can be superposed and combined with flux limiters to satisfy conditions (3.12) or (3.28). Upwind biasing is then produced indirectly by cancellation of terms of opposite sign. One possible starting point for such a construction is a central difference scheme in which the numerical flux $\frac{1}{2}(f_{j+1}+f_j)$ is augmented by a third order dissipative flux. This scheme is the basis of a method which has been widely used to solve the Euler equations of compressible flow [14]. It can be converted into an attractively simple TVD scheme by the introduction of flux limiters in the dissipative terms [15]. The modified numerical flux retains a symmetric distribution of terms about the cell boundary $j+\frac{1}{2}$. The resulting symmetric scheme is one of the variants of a class of symmetric TVD schemes recently proposed by Yee [16]. Her derivation follows an entirely different line of reasoning, building on the work of Davis [17], and Roe [18]. In comparison with upwind TVD schemes, symmetric TVD schemes offer a significant reduction of computational complexity, while exhibiting comparable shock capturing capabilities.

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