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COMMENT

A finite difference scheme with a Leibniz rule

Y Bouguenaya and D B Fairlie

Department of Mathematical Sciences, University of Durham, South Road, Durham DH1 3LE, UK

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Abstract. In a finite difference scheme for numerical approximation the usual notion of product is replaced by a convolution to circumvent the failure of the product rule for differentiation. The solution displays a complementarity: the more localised is the product the more extended is the approximation to the derivative and vice versa.

One of the problems of constructing discrete approximations to non-linear equations is the lack of a discrete analogue of the Leibniz rule for differentiation of a product—the familiar distributive law

$$\frac{\mathrm{d}}{\mathrm{d}x}(fg) = \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)g + f\frac{\mathrm{d}g}{\mathrm{d}x} \tag{1}$$

fails for any finite difference approximation to the derivative (Drell *et al* 1976). In this comment we explore a loophole in this conclusion and restore a version of the Leibniz rule by modifying the definition of a product of two functions defined on a discrete set. In fact, what we find is a kind of complementarity: the more the product is localised, the more extended is the definition of derivative and vice versa. The problem is easy to set up, but not straightforward to solve.

Suppose two functions f and g are defined on the integers with periodic boundary conditions:

$$f_i = f_{N+i}, \qquad g_i = g_{N+i} \qquad \{i = 0, \ldots, N-1\}. \tag{2}$$

Then we define the derivative at i as a linear combination

$$(Df)_i = \sum_j d_{ij} f_j \tag{3}$$

and the product by

$$(fg)_i = \sum_{j,k} c_{ijk} f_j g_k. \tag{4}$$

The coefficients d_{ij} and c_{ijk} satisfy further natural requirements. If f is a constant then its derivative must vanish, i.e.

$$\sum_j d_{ij} = 0. \tag{5}$$

Also if $f = c$ is constant

$$(fg)_i = cg_i$$

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giving

$$\sum_j c_{ijk} = \delta_{ik} \tag{6}$$

and c_{ijk} is symmetric in j and k as f and g are on the same footing, i.e.

$$c_{ijk} = c_{ikj}. \tag{7}$$

The final requirement we shall impose is associativity:

$$(h(fg)) = ((hf), g) \tag{8}$$

which translates into

$$\sum_s c_{ijs} c_{skl} = \sum_s c_{ils} c_{skj}. \tag{9}$$

Then the Leibniz rule is

$$\sum_l d_{il} c_{ljk} = \sum_l c_{ilk} d_{lj} + \sum_l c_{ijl} d_{lk}. \tag{10}$$

The normal definition of product requires that

$$c_{ijk} = \sum_r \delta_{ir} \delta_{jr} \delta_{kr} \tag{11}$$

which vanishes unless i, j, k are all equal. With this choice there is no solution for d. Further constraints arise from translation invariance:

$$d_{i+1,j+1} = d_{ij} \tag{12}$$

where $i + N = i$ is replaced by i and there are similar constraints upon the c coefficients. The set of relations (5) and (10) are non-linear and the only obvious approach is to first satisfy (6), the only equations which are inhomogeneous, together with (7). It turns out that it is easier to first find a particular solution, and then to generalise this later.

Consider the ansatz

$$c_{ijk} = \delta_{ij} P_k + \delta_{ik} P_j - P_j P_k \qquad \text{(all } i\text{)} \tag{13}$$

with

$$\sum_{k=0}^{N-1} P_k = 1. \tag{14}$$

This clearly satisfies (6) and (7) and can easily be verified to satisfy the associativity relationship (9). The equation (10) is satisfied provided only that

$$\sum_k P_k d_{kl} = 0. \tag{15}$$

This condition requires that d_{kl} is a matrix of rank $N-1$, and together with (5) implies that the general solution for d_{il} is

$$d_{il} = a_{il} - \sum_k \frac{P_i P_k}{P^2} a_{kl} - \sum_k a_{ik} P_l + \sum_k \sum_r (P_k a_{kr}) \frac{P_i P_l}{P^2} \tag{16}$$

where a_{il} is an arbitrary $N \times N$ matrix.

In particular, with the choice $\boldsymbol{P}=1/N(1,1,1,\ldots,1)$, the usual two-point choice for d_{il}, namely

$$d_{il}=\delta_{il}-\delta_{il+1} \tag{17}$$

satisfies (14) and (15) and gives for a product

$$(fg)=f\frac{1}{N}\sum_k g_k+g\frac{1}{N}\sum_k f_k-\frac{1}{N^2}\Big(\sum_k f_k\Big)\Big(\sum_l g_l\Big) \tag{18}$$

$$=f\langle g\rangle+g\langle f\rangle-\langle f\rangle\langle g\rangle \tag{19}$$

where $\langle f\rangle$ denotes an average over sites. Equations (17) and (19) clearly satisfy translation invariance requirements. This definition of product is highly non-local: in order to modify it we require a more general ansatz than (13). Consider a second vector q_k, similarly normalised so that its components sum to unity, and the ansatz

$$c_{ijk}=\delta_{ij}P_k+\delta_{ik}P_j-P_jP_k+(q_j-P_j)(q_k-P_k)\frac{P^2q_i-(q\cdot P)P_i}{(P^2q^2-(q\cdot P)^2)}$$

where

$$(q\cdot P)\text{ denotes }\sum_{l=0}^{N-1}q_lP_l. \tag{20}$$

This clearly satisfies (6) and (7) and after a little more calculation can be seen to fulfil associativity (9). Then equations (10) are satisfied provided that d_{ij}, in addition to satisfying (5) and (15), also satisfies

$$\sum_l q_l d_{lj}=\sum d_{il}(P^2q_l-(q\cdot P)P_l)=0. \tag{21}$$

This d_{ij} is now of rank $N-2$, and is not so localised as in the former case. Further linearly independent vectors r, s, t, etc, all similarly normalised may be added to introduce more parameters into the choice of d_{ij}: this is the complementarity referred to earlier. The structure of this family of solutions is already evident with only three vectors P, q and r. The solution

$$c_{ijk}=+\frac{1}{\Delta}\begin{vmatrix} P_i & q_i & r_i & -P_j\delta_{ik}-P_k\delta_{ij}+P_jP_k\ (\text{all } i)\\ P^2 & Pq & Pr & 0\\ qP & q^2 & qr & (P_j-q_j)(P_k-q_k)\\ rP & rq & r^2 & (P_j-r_j)(P_k-r_k)\end{vmatrix} \tag{22}$$

where

$$\Delta=\begin{vmatrix} P^2 & P\cdot q & P\cdot r\\ q\cdot P & q^2 & q\cdot r\\ r\cdot P & r\cdot q & r^2\end{vmatrix} \tag{23}$$

satisfies (6) and (7). Here Pq denotes

$$\sum_{l=0}^{N-1}P_lq_l.$$

To demonstrate that (22) satisfies associativity it is best to proceed by establishing the lemma

$$\sum_i V_i c_{ijk} = V_j V_k \tag{24}$$

(where V is P, q or r) by the use of simple determinantal properties. With the help of this lemma, and the simple identity

$$P_j P_k - v_j v_k = (P_j - v_j)P_k + (P_k - v_k)P_j - (P_j - v_j)(P_k - v_k) \tag{25}$$

the left-hand side of (9) may be calculated to give

$$\sum c_{ijs} c_{skl} = P_j c_{ikl} + P_k c_{ilj} + P_l c_{ijk}$$
$$+\frac{1}{\Delta}\begin{vmatrix} P_i & q_i & r_i & +P_jP_l\delta_{ik} + P_kP_l\delta_{ij} + P_kP_j\delta_{il} - P_jP_kP_l \text{ (all } i) \\ P^2 & Pq & Pr & 0 \\ qP & q^2 & qr & (P_j - q_j)(P_k - q_k)(P_l - q_l) \\ rP & rq & r^2 & (P_j - r_j)(P_k - r_k)(P_l - r_l) \end{vmatrix}. \tag{26}$$

This expression is clearly symmetric in j, k, l and hence is equal to the right-hand side. The final equation (10) imposes the condition that P, q, r are left null eigenvectors of d_{ij}, while the column vectors $(1, 1, 1, \ldots, 1)^{\mathrm{T}}$, $p_j v^2 - (pv)v_j$ are right null eigenvectors of d_{ij}, i.e. d is of rank $N-3$. Translation invariance is automatically implemented in (22) because the product formula involves scalar products of f and g with P, q, r, but remains an extra requirement on d. It is evident from (22) how to extend this solution to incorporate N independent vectors. As the number of parameters increases the product is effectively more and more localised until with N vectors the usual formula (11) is recovered. To see this it is sufficient to take (22) with $N=3$. Choosing $p_i = \delta_{i0}$, $q_i = \delta_{i1}$ and $r_i = \delta_{i2}$ the product formula becomes

$$\begin{aligned}(fg)_i &= f_0 g_i + f_i g_0 - f_0 g_0 \qquad \text{(all } i) \\ &\quad + \delta_{i1}(f_0 - f_1)(g_0 - g_1) + \delta_{i2}(f_0 - f_2)(g_0 - g_2) \\ &= f_i g_i \qquad \text{(by enumeration of cases).}\end{aligned} \tag{27}$$

A further generalisation of (22) which treats the vectors on a similar footing and which satisfies all the equations (5)-(10) may be constructed as follows. Define an $N \times L$ matrix $P_{i\alpha}$ ($i = 0, \ldots, N-1$; $\alpha = 0, \ldots, L-1$) whose columns are the vectors P, q, r, etc, and introduce an L component vector λ_α whose components sum to unity.

Then, C is defined as the determinant of the partitioned matrix

$$c_{ijk} = \frac{1}{\Delta}\begin{vmatrix} P_{i\beta} & \Sigma_\beta \lambda_\beta (P_{j\beta} P_{k\beta} - \delta_{ij} P_{k\beta} - \delta_{ik} P_{j\beta}) \\ \Sigma_l P_{l\alpha} P^{l\beta} & \Sigma_\beta \lambda_\beta (P_{j\alpha} - P_{j\beta})(P_{k\alpha} - P_{k\beta}) \end{vmatrix} \tag{28}$$

where

$$\Delta = \det \sum_l P_{l\alpha} P_{l\beta}.$$

What is remarkable about this expression is that although it is a linear combination of terms of the form (22) it still contrives to satisfy the non-linear equations (9), by virtue of the mechanism of equations (24) and (25). The side conditions upon d_{ij} which follow from (10) are simply that the columns of $P_{i\alpha}$ are both right and left null eigenvectors of d.

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Reference

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