Mimetic Properties of Difference Operators: Product and Chain Rules as for Functions of Bounded Variation and Entropy Stability of Second Derivatives

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For discretisations of hyperbolic conservation laws, mimicking properties of operators or solutions at the continuous (differential equation) level discretely has resulted in several successful methods. While well-posedness for nonlinear systems in several space dimensions is an open problem, mimetic properties such as summation-by-parts as discrete analogue of integration-by-parts allow a direct transfer of some results and their proofs, e.g. stability for linear systems.

In this article, similarities of chain and product rules for functions of bounded variation and difference approximations are discussed. Especially, such an analogue holds for second order operators and is not possible for higher order approximations. Furthermore, entropy dissipation by second derivatives with varying coefficients is investigated, showing again the far stronger mimetic properties of second order approximations compared to higher order ones.

1 Introduction

Ever since the widespread application of computers in numerical mathematics and even before, finite difference methods have been successfully applied to approximate solutions of differential equations. An important task is the development and investigation of stable and well-behaved numerical methods. While some general purpose methods can give satisfying results under certain circumstances, schemes that have been developed specifically for the target equation can be advantageous, e.g. if some properties of operators or solutions at the continuous level are mimicked discretely. This has been the goal of, e.g., geometric numerical integration methods for ordinary differential equations, cf. [16, 17].

In this regard, a well-developed theory of the problem at the continuous (differential equation) level is very important since it can be used as a guideline for the development of (semi-) discretisations. For linear systems of hyperbolic conservation laws, energy estimates play a fundamental role in the analysis of well-posedness [15]. An important technique is integration-by-parts. Thus, summation-by-parts (SBP) as a discrete analogue has been very successful, since manipulations at the continuous level can be mimicked discretely, yielding stability and
conservation results, cf. [2, 3, 20, 38]. Further references and results can be found in the review articles [9, 40].

For scalar conservation laws, functions of locally bounded variation play an important role as solution space. In his seminal work [43], Vol’pert investigated functions of locally bounded variation and developed a notion of products of possibly discontinuous functions and derivatives of functions of bounded variation as measures. Moreover, he developed a corresponding chain and product rule.

The investigation of semidiscretisations satisfying a single entropy inequality has received much interest, cf. [10, 11, 13, 14, 23, 29, 31, 32, 37, 41, 42, 46]. For some conservation laws such as Burgers’ equations, conservative corrections to the product rule can be used to obtain $L^2$ dissipative schemes, cf. [12, 34, 35]. Therefore, it is interesting whether the chain and product rules for functions of bounded variation have discrete analogues.

Furthermore, the investigation of numerical dissipation operators has received much interest, cf. [26, 33, 39, 45]. Such operators can be motivated by the vanishing viscosity approach to conservation laws, cf. [1]. For general entropies, the investigation of dissipation induced by such terms relies on the chain rule, cf. [22, Proof of Theorem I.3.4]. Thus, a natural question is to investigate the entropy dissipation of difference approximations.

This article is structured as follows. At first, functions of bounded variation are briefly reviewed in section 2, focusing on the chain and product rules. Next, corresponding difference operators are investigated in section 3. It is proven that there are analogous product and chain rules for classical second order periodic and SBP operators (Lemma 3.1 and Lemma 3.2). Furthermore, it is proven that such analogues do not exist for higher order difference approximations of the first derivative (Theorem 3.6 and Theorem 3.8). Thereafter, dissipation operators approximating second derivatives with possibly varying coefficients are investigated in section 4. It is proven that second order difference operators are dissipative for every convex entropy (Theorem 4.1). Moreover, a counterexample shows that such a result is impossible for classical operators with higher order of accuracy (Example 4.2). Finally, a summary and discussion is given in section 5.

2 Functions of Bounded Variation

Functions of locally bounded variation, i.e. those locally integrable functions whose distributional first derivatives are Radon measures, play an important role in analysis, for example in the theory of scalar conservation laws as described in the seminal work of Vol’pert [43]. Further results about conservation laws and references can be found in the monograph [5], e.g. Theorem 6.2.6 and chapter XI. Some general results about functions of bounded variation can be found in [8, 44].

For functions of locally bounded variation, a product of a possibly discontinuous function and a measure occurs in both the chain rule and the product rule. If the function is integrable with respect to the measure, this product is well-defined as a measure, cf. [43]. In one space dimension, a function of bounded variation is continuous almost everywhere and the limits from the left and the right exist everywhere. If $u \in BV_{loc}([a, b]; \mathbb{R}^m)$ and $f : \mathbb{R}^m \to \mathbb{R}$ is (for simplicity) continuous, then Vol’pert [43] defined the averaged composition of $f$ and $u$ via

$$\bar{f}(u)(x) := \int_0^1 f(u_- + s(u_+ - u_-)) \, ds,$$

where $u_\pm = \lim_{\varepsilon \downarrow 0} u(x \pm \varepsilon)$ are the unique limits of $u$ from the left and right hand side, respectively. With this definition, the following chain and product rules have been obtained in [43, Section 13].

**Theorem 2.1.** If $u \in BV([a, b]; \mathbb{R}^m)$ and $f \in C^1(\mathbb{R}^m; \mathbb{R})$, the averaged composition $\bar{f}(u)$ is locally integrable with respect to the measure $\partial_x u_k$ for $k \in \{1, \ldots, m\}$, $f(u) \in BV_{loc}$, and

$$\partial_x f(u) = \frac{m}{k=1} \partial_{u_k} f(u) \partial_x u_k.$$
Especially, for \( u, v \in \text{BV}[a, b] \),
\[
\partial_x(uv) = \tilde{u}\partial_x v + \tilde{v}\partial_x u. \tag{3}
\]

The product rule is also proven in the monograph [44, Section 6.4]. A generalisation of the corresponding definition of a possibly nonconservative product \( f(u)\partial_x v \) has been developed and investigated by Dal Maso, LeFloch, and Murat [6]. See also [24, 36] for further studies.

If \( u, v \in \text{BV}[a, b] \) are jump functions,
\[
u(x) = \begin{cases} u_-, & x < 0, \\ u_+, & x > 0, \end{cases} \quad v(x) = \begin{cases} v_-, & x < 0, \\ v_+, & x > 0, \end{cases}
\]
the product rule (3) yields
\[
(\partial_x(uv))(\{0\}) = u_+v_+ - u_-v_-
= \frac{u_+ + u_-}{2}(v_+ - v_-) + \frac{v_+ + v_-}{2}(u_+ - u_-)
= (\tilde{u}\partial_x v)(\{0\}) + (\tilde{v}\partial_x u)(\{0\}),
\]
where the measures on both sides of (3) have been applied to the set \{0\} containing only the jump point. Similarly, for \( f \in \mathcal{C}^1 \), the chain rule (2) becomes
\[
(\partial_x f(u))(\{0\}) = f(u_+) - f(u_-) = \int_0^1 f'(u_+ + s(u_+ - u_-)) \, ds = (\tilde{f}(u)\partial_x u)(\{0\}). \tag{6}
\]

Interpreting the difference \( u_+ - u_- \) as a discrete derivative, these are discrete product and chain rules using averages instead of the usual point values occurring in the continuous analogues for differentiable functions. Thus, it is interesting whether this can be generalised.

### 3 Difference Operators

Consider a general discrete derivative/difference operator \( D \), acting on grid functions \( u = (u_i)_i = (u(x_i))_i \) defined on a possibly non-uniform grid with nodes \( x_i \in \mathbb{R} \) and \( h := \min(x_{i+1} - x_i) > 0 \). Note that this includes both classical finite difference operators and spectral collocation operators such as nodal discontinuous Galerkin ones.

In practice, the grid function is represented by the vector of its point values and the discrete derivative operator by a matrix with entries \( D_{ij} \). General nonlinear operations such as composition or multiplication are conducted pointwise, i.e. if \( u \) and \( v \) are two grid functions, their product \( uv \) is the grid function with components \( (uv)_i = u_i v_i \).

#### 3.1 Classical Second Order Derivative Operators

The classical second order finite difference operator on a uniform grid is given by
\[
(Du)_i = \frac{u_{i+1} - u_{i-1}}{2h} \approx u'(x_i). \tag{7}
\]
The corresponding summation-by-parts (SBP) operator uses this stencil in the interior and — if the nodes \( x_0, \ldots, x_N \) are used — the boundary closures
\[D(u)_0 = \frac{u_1 - u_0}{h} \approx u'(x_0), \quad (Du)_N = \frac{u_N - u_{N-1}}{h} \approx u'(x_N). \tag{8}\]

Analogously to the product rule (5) for a step function of bounded variation, considering scalar valued grid functions \( u \) and \( v \),
\[
(Duv)_i = \frac{u_{i+1}v_{i+1} - u_{i-1}v_{i-1}}{2h} = \frac{u_{i+1} + u_{i-1}}{2} \frac{v_{i+1} - v_{i-1}}{2h} + \frac{u_{i+1} - u_{i-1}}{2h} \frac{v_{i+1} + v_{i-1}}{2}
= (Au)_i(Dv)_i + (Du)_i(Av)_i, \tag{9}
\]
if the averaging operator $A$ is defined by
\[
(Au)_i = \frac{u_{i+1} + u_{i-1}}{2} \approx u(x_i). \tag{10}
\]
For the corresponding SBP operator, the terms at the left boundary are
\[
(Duv)_0 = \frac{u_1v_1 - u_0v_0}{h} = \frac{u_1 + u_0}{2}v_1 - \frac{u_1 - u_0}{2}v_0 + \frac{u_1 - u_0}{2}v_1 = (Au)_0(Dv)_0 + (Dv)_0(Au)_0, \tag{11}
\]
if the boundary closures of $A$ are given by
\[
(Au)_0 = \frac{u_1 + u_0}{h} \approx u(x_0), \quad (Au)_N = \frac{u_N + u_{N-1}}{h} \approx u(x_N). \tag{12}
\]
The terms at the right boundary are similar. This is summed up in

**Lemma 3.1.** The classical second order derivative operator $D$ (on a periodic grid or with boundary closures given above) fulfils the product rule
\[
D(uv) = (Au)(Dv) + (Du)(Av), \tag{13}
\]
where the averaging operator $A$ defined above is of the same order of accuracy as the derivative operator $D$, i.e. it fulfils $(Au)_i = u(x_i) + O(h^2)$ in the interior and $(Au)_{0,N} = u(x_{0,N}) + O(h)$ at the boundaries for a smooth function $u$.

Similarly, a general chain rule as discrete analogue of (6) is satisfied. Indeed, if $f$ is continuously differentiable and $u$ a possibly vector valued grid function,
\[
(Df(u))_i = \frac{f(u_{i+1}) - f(u_{i-1})}{2h} = \int_0^1 f'(u_i + s(u_{i+1} - u_{i-1})) \, ds \cdot \frac{u_{i+1} - u_{i-1}}{2h} = (A_{f'}u)_i(Du)_i \tag{14}
\]
for interior nodes, where the possibly nonlinear averaging operator $A_{f'}$ has been introduced. At the boundary nodes, it is given by
\[
(A_{f'}u)_0 = \int_0^1 f'(u_0 + s(u_1 - u_0)) \, ds \approx f'(u(x_0)), \\
(A_{f'}u)_N = \int_0^1 f'(u_{N-1} + s(u_N - u_{N-1})) \, ds \approx f'(u(x_N)). \tag{15}
\]
This is summed up in

**Lemma 3.2.** The classical second order derivative operator $D$ (on a periodic grid or with boundary closures) satisfies the chain rule
\[
Df(u) = (A_{f'}u)(Du), \tag{16}
\]
where the averaging operator $A_{f'}$ defined above is of the same order of accuracy as the derivative operator $D$, i.e. it fulfils $(A_{f'}u)_i = f'(u(x_i)) + O(h^2)$ in the interior and $(A_{f'}u)_{0,N} = f'(u(x_{0,N})) + O(h^2)$ at the boundaries for smooth functions $u$ and $f$.

**Remark 3.3.** The averaging operator $A$ used for the product rule is a special case of the general averaging operator $A_{f'}$. Indeed, $A = A_{id}$, where $id$ is the identity mapping.

**Remark 3.4.** In general, $A_{f'}$ is neither a linear operator nor an averaging operator acting on $f'(u)$. Instead, it is a nonlinear operator using values of $u$ and averages $f'$ using intermediate values. It is linear if and only if $f'$ is linear, especially in the case $f' = id$, i.e. $A_{id} = A$ discussed in Remark 3.3.
3.2 Higher Order Derivative Operators

The product and chain rules for second order derivative operators cannot be generalised to higher order derivative operators. In order to prove this, the asymptotic expansion of the error of the derivative operator will be used.

**Lemma 3.5.** Assume that $D$ is a discrete derivative operator of order $p$, i.e. $(Du)_i = u'(x_i) + O(h^p)$ or, equivalently, $D$ is exact for polynomials of degree $\leq p$, with $p$ maximal. If $u$ is a smooth scalar-valued function,

$$ (Du)_i = u'(x_i) + u^{(p+1)}(x_i)C_i^D h^p + O(h^{p+1}), $$

where $C_i^D h^p = O(h^p)$ depends only on the grid and the derivative operator.

**Proof.** By Taylor expansion, using the exactness of $D$ for polynomials of degree $\leq p$,

$$ (Du)_i = \sum_j D_{ij}u_j = \sum_j D_{ij}u(x_j) $$

$$ = \sum_j D_{ij}\left(u(x_i) + u'(x_i)(x_j - x_i) + \cdots + \frac{1}{(p+1)!} u^{(p+1)}(x_i)(x_j - x_i)^{p+1} + O(h^{p+2})\right) $$

$$ = u'(x_i) + u^{(p+1)}(x_i)\sum_j \frac{1}{(p+1)!} D_{ij}(x_j - x_i)^{p+1} + O(h^{p+1}). $$

Here, $C_i^D h^p = O(h^p)$, since $D$ scales as $h^{-1}$. \qed

This can be used to prove one of the main observations of this article.

**Theorem 3.6.** If $D$ is a discrete derivative operator of order $p > 2$, there can be no averaging operator $A$ of order $p$ such that there is a product rule of the form $D(uv) = (Au)(Dv) + (Du)(Av)$.

**Proof.** Consider the asymptotic expansions

$$ (D(uv))_i = (uv)'(x_i) + (uv)^{(p+1)}(x_i)C_i^D h^p + O(h^{p+1}) $$

and

$$ (Au)(Dv) + (Du)(Av) = \left(u(x_i) + C_i^A(u)h^p\right)\left(v'(x_i) + v^{(p+1)}(x_i)C_i^D h^p\right) $$

$$ + \left(u'(x_i) + u^{(p+1)}(x_i)C_i^D h^p\right)\left(v(x_i) + C_i^A(v)h^p\right) + O(h^{p+1}), $$

where $C_i^A(u)$ is the leading order coefficient for $A$ and may depend on the function $u$ and its derivatives. Thus, the product rule can only hold if

$$ (uv)^{(p+1)}(x_i)C_i^D = \left(u(x_i)v^{(p+1)}(x_i) + u^{(p+1)}(x_i)v(x_i)\right)C_i^D + u'(x_i)C_i^A(v) + v'(x_i)C_i^A(u). $$

Since

$$ (uv)^{(p+1)}(x_i) = \sum_{k=0}^{p+1} \binom{p+1}{k} u^{(k)}(x_i)v^{(p+1-k)}(x_i), $$

the terms with $k = 0$ and $k = p + 1$ match the braces on the left hand side of (21), but the remaining terms can only match if $p \leq 2$, since the remaining sum cannot be factored as on the right hand side. \qed
Remark 3.7. Using polynomial collocation methods on Lobatto Legendre or Gauss Legendre nodes in $[-1, 1]$, a discrete product rule holds for $p = 1$, i.e. for two nodes, since they are of the same form as the classical finite difference derivative operator. However, for $p = 2$, there can be no product rule. Indeed, for Lobatto nodes $\{-1, 0, 1\}$ and $u(x) = (1 + x)^2 = v(x)$, the discrete derivatives of $u$ and $v$ at $-1$ are zero (since they are exact), but the discrete derivative of $uv$ at $-1$ is
\[(Du v)_{-1} = \frac{3}{2} u_{-1} v_{-1} + 2 u_{0} v_{0} - \frac{1}{2} u_{1} v_{1} = 0 + 2 \cdot 1^2 - \frac{1}{2} \cdot 4^2 = -6 \not= 0. \tag{23}\]
A similar argument holds for Gauss Legendre nodes.

Since the product rule is a special case of the chain rule with vector valued functions $u$, a general chain rule is also excluded for discrete derivative operators of higher order of accuracy. However, this argument does not forbid a chain rule for scalar valued functions. Nevertheless, this case is also excluded by the second main observation of this article.

Theorem 3.8. If $D$ is a discrete derivative operator of order $p > 2$, there can be no general averaging operator $A_f$ of order $p$ such that there is a chain rule of the form $D(f(u)) = (A_f u)(Du)$.

Proof. By the argument above, it suffices to consider scalar valued functions. In this case,
\begin{align*}
(D f(u))_i &= f'(u_i) u'(x_i) + (f(u))^{(p+1)}(x_i) C_i^D h^p + O(h^{p+1}),
(A_f u)(Du)_i &= \left( f'(u_i) + C_i^A (f'(u)) h^p \right) \left( u'(x_i) + u^{(p+1)}(x_i) C_i^D h^p \right) + O(h^{p+1}). \tag{24}\end{align*}
Expressing $(f(u))^{(p+1)}(x_i)$ using the formula of Faà di Bruno [18, Lemma II.2.8], it is clear that $u'(x_i)$ cannot be factored out of the remaining terms after subtracting $f'(u_i) u^{(p+1)}(x_i)$ if $p > 2$. \hfill \* 

Remark 3.9. A product rule for classical difference operators with error term of the form
\[(Du v)_i = u_i (Du)_i + (\partial_x u)_i (Av)_i + e_i \tag{25}\]
has been used in [27, Lemma 3.1 and Lemma 3.2]. If $u$ is smooth, $(\partial_x u)_i$ is the derivative at $x_i$ and $\|e\| \leq Ch\|v\|$ for some constant $C > 0$. The averaging operator $A$ is linear and of the same order of accuracy as the derivative operator $D$. \hfill \* 

Remark 3.10. The investigation of discrete product and chain rules is also somewhat loosely related to the entropy stability and conservation theory initiated by Tadmor [41, 42]. Indeed, instead of a chain rule of the form $\partial_x f(u) = f'(u) \partial_x u$, a discrete version of $U'(u) \cdot \partial_x u = \partial_x F(u)$ is used, where $U$ is the entropy fulfilling $U'(u) \cdot f'(u) = F'(u)$. Such approximations can be found for arbitrary order, cf. [4, 10, 23, 29, 37]. Basically, schemes of lower order can be extrapolated if regular grids are used, cf. [30, Section 3.2]. Nevertheless, they can be used also on certain irregular grids. \hfill \* 

4 Entropy Stability of Discrete Second Derivatives

In order to regularise a hyperbolic conservation law $\partial_t u + \partial_x f(u) = 0$, where $u$ are the conserved variables and $f(u)$ is the flux, a parabolic term can be added to the right-hand side, resulting in
\[
\partial_t u(t, x) + \partial_x f(u(t, x)) = \partial_x (\varepsilon(x) \partial_x u(t, x)), \tag{26}\]
where $\varepsilon \geq 0$ controls the amount of viscosity. An entropy is a convex function $U$ satisfying $U'(u) \cdot f'(u) = F'(u)$, where $F$ is the corresponding entropy flux. Thus, smooth solutions of the conservation law fulfil the additional conservation law
\[
\partial_t U(u) = U'(u) \cdot \partial_t u = -U'(u) \cdot f'(u) \cdot \partial_x u = -\partial_x F(u) \tag{27}\]
and an entropy inequality $\partial_t U + \partial_x F \leq 0$ is required for weak solutions, cf. [5, Chapter IV]. The viscosity term on the right-hand side induces a global entropy inequality for sufficiently smooth solutions. Indeed, in a periodic domain $\Omega$,

$$\int_{\Omega} U' \cdot \partial_x (\varepsilon \partial_x u) \, dx = - \int_{\Omega} \varepsilon (\partial_x U') \cdot \partial_x u \, dx = - \int_{\Omega} \varepsilon (\partial_x u) \cdot U'' \cdot \partial_x u \, dx \leq 0, \quad (28)$$

since $U$ is convex and $\varepsilon \geq 0$. In a non-periodic domain $\Omega$, if $\varepsilon$ vanishes on $\partial \Omega$, the same result holds. Otherwise, there will be additional boundary terms.

The computation given above for smooth solutions relies on the chain rule. Thus, it might be conjectured that a similar result holds for second order difference approximations of the Laplace operator (with possibly varying coefficients) but that there is no analogue for higher order difference approximations to the second derivative.

### 4.1 Second Order Derivative Operators

In a periodic domain, the classical second order difference approximation to the Laplace operator is given by

$$(D_2 u)_i = \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}. \quad (29)$$

Thus, multiplying pointwise by $U'(u_i) = U'_i$ and summing up all terms yields due to the periodicity of the domain

$$h^2 \sum_i U'_i \cdot (D_2 u)_i = \sum_i U'_i \cdot (u_{i+1} - u_i) - \sum_i U'_i \cdot (u_i - u_{i-1}) = - \sum_i (U'_{i+1} - U'_i) \cdot (u_{i+1} - u_i) \leq 0, \quad (30)$$

since $U'$ is monotone. Indeed, due to the convexity of $U$,

$$(u_{i+1} - u_i) \cdot (U'(u_{i+1}) - U'(u_i)) = \int_0^1 (u_{i+1} - u_i) \cdot U''(u_i + s(u_{i+1} - u_i)) \cdot (u_{i+1} - u_i) \, ds \geq 0. \quad (31)$$

This is exactly the chain rule for classical difference approximations.

If a variable coefficient $\varepsilon \geq 0$ is considered in a periodic domain, a second order approximation to $\partial_x (\varepsilon \partial_x u)$ is given by

$$(D_2^\varepsilon u)_i = \frac{\varepsilon_i + \varepsilon_{i+1}}{2} u_{i+1} - \frac{\varepsilon_{i-1} + 2\varepsilon_i + \varepsilon_{i+1}}{2} u_i + \frac{\varepsilon_{i-1} + \varepsilon_i}{2} u_{i-1}, \quad (32)$$

cf. [25]. Using again the periodicity and the convexity of $U$,

$$h^2 \sum_i U'_i \cdot (D_2^\varepsilon u)_i = \sum_i \frac{\varepsilon_i + \varepsilon_{i+1}}{2} U'_i \cdot (u_{i+1} - u_i) - \sum_i \frac{\varepsilon_{i-1} + \varepsilon_i}{2} U'_i \cdot (u_i - u_{i-1}) = - \sum_i \frac{\varepsilon_i + \varepsilon_{i+1}}{2} (U'_{i+1} - U'_i) \cdot (u_{i+1} - u_i) \leq 0. \quad (33)$$

Summation-by-parts operators for second derivatives with variable coefficients have been developed in [25]. The second order discrete derivative in the interior is given by (32) and equipped with the boundary closures

$$(D_2^\varepsilon u)_0 = (2\varepsilon_0 - \varepsilon_1)u_0 + (-3\varepsilon_0 + \varepsilon_1)u_1 + \varepsilon_0 u_3, \quad (D_2^\varepsilon u)_N = (2\varepsilon_N - \varepsilon_{N-1})u_N + (-3\varepsilon_N + \varepsilon_{N-1})u_{N-1} + \varepsilon_N u_{N-2}. \quad (34)$$

If the variable coefficient $\varepsilon$ vanishes at the boundary, i.e. if $\varepsilon_0 = 0 = \varepsilon_N$, these boundary closures become

$$(D_2^\varepsilon u)_0 = \varepsilon_1(u_1 - u_0), \quad (D_2^\varepsilon u)_N = -\varepsilon_{N-1}(u_N - u_{N-1}). \quad (35)$$
Since the discrete integral is given as a quadrature with weights on the diagonal of the mass/norm matrix $H = \text{diag}(1/2, 1, \ldots, 1, 1/2)$, the discrete equivalent of the integral $\int_\Omega U' \cdot \partial_x (\varepsilon \partial_x u)$ is

$$
\sum_{i=0}^{N} H_i U_i' \cdot (D_2^\varepsilon u)_i
$$

$$
= \frac{1}{2} \varepsilon_1 U_0' \cdot (u_1 - u_0) - \frac{1}{2} \varepsilon_{N-1} U_{N}' \cdot (u_N - u_{N-1})
+ \sum_{i=1}^{N-1} \frac{\varepsilon_i + \varepsilon_{i+1}}{2} U_i' \cdot (u_{i+1} - u_i) - \sum_{i=1}^{N-1} \frac{\varepsilon_i - \varepsilon_{i+1}}{2} U_i' \cdot (u_i - u_{i-1})
= \frac{\varepsilon_0 + \varepsilon_1}{2} U_0' \cdot (u_1 - u_0) - \frac{\varepsilon_{N-1} + \varepsilon_N}{2} U_N' \cdot (u_N - u_{N-1})
+ \sum_{i=1}^{N-1} \frac{\varepsilon_i + \varepsilon_{i+1}}{2} U_i' \cdot (u_{i+1} - u_i) - \sum_{i=0}^{N-2} \frac{\varepsilon_i + \varepsilon_{i+1}}{2} U_{i+1}' \cdot (u_{i+1} - u_i)
= - \sum_{i=0}^{N} \frac{\varepsilon_i + \varepsilon_{i+1}}{2} (U_{i+1}' - U_i') \cdot (u_{i+1} - u_i)
\leq 0.
\tag{36}
$$

This proves

**Theorem 4.1.** The discretisations of the second derivative operator $\partial_x (\varepsilon \partial_x \cdot)$ with possibly varying coefficients $\varepsilon \geq 0$ given above in periodic domains or on bounded domains with $\varepsilon_0 = 0 = \varepsilon_N$ are entropy dissipative for every convex entropy.

### 4.2 Higher Order Derivative Operators

Since there is no discrete chain rule for higher order difference approximations to the first derivative, it might be conjectured that discrete higher order second derivatives are in general not entropy dissipative.

**Example 4.2.** Consider the classical fourth order approximation to the second derivative on a periodic domain, given by

$$h^2 (D_2 u)_i = -\frac{1}{12} (u_{i+2} + u_{i-2}) + \frac{4}{3} (u_{i+1} + u_{i-1}) - \frac{5}{2} u_i.
\tag{37}
$$

Choose the grid $x_i = i$, $i \in \{0, \ldots, 7\}$, with periodic boundary conditions, i.e. $u_0 = u_7$. Set $u = (0.21, 0.80, 0.21, 0.84, 0.75, 0.20, 0.17)$ and use entropy $U(u) = \max\{0, u - 0.19\}$. Then, $U'(u) = 0$ if $u < 0.19$ and $U'(u) = 1$ if $u > 0.19$. Finally,

$$
\sum_{i=0}^{6} U'(u_i) \cdot (D_2 u)_i = 0.0075 > 0.
\tag{38}
$$

By suitable modifications, the entropy $U$ can be made arbitrarily smooth while preserving $\sum_i U'(u_i) \cdot (D_2 u)_i > 0$.

Similar counterexamples to general entropy dissipation seem to be possible for other higher order approximations to second order derivative operators with possibly varying coefficients. It would be interesting to know whether this is a general limitation of higher order approximations similar to the results for the product and the chain rule (Theorem 3.6 and Theorem 3.8).

**Remark 4.3.** Of course, higher order approximations to second derivatives that are dissipative for a specific entropy can be constructed. Classical difference operators are negative semidefinite, i.e. they are dissipative for the $L^2$ entropy $U(u) = \frac{1}{2} u^2$ with $U'(u) = u$. For a general entropy $U$, entropy dissipative second derivatives can be constructed by using the entropy variables $w := U'(u)$ instead of the conserved variables $u$, cf. [10].
Remark 4.4. In periodic domains, the classical central finite difference approximations to the first derivative of higher order can be constructed via extrapolation from the second order operator, cf. [30, Section 3.2]. Thus, by enforcing positivity of the corresponding coefficients for the second derivative, entropy dissipative terms can be constructed similarly for higher order first derivative operators, as used in [39]. However, these are not higher order approximations of the second derivative.

5 Summary and Discussion

In this article, product and chain rules using averaged compositions have been shown to hold for second order approximations to first order derivative operators, similarly to corresponding results for functions of bounded variation (Lemma 3.1 and Lemma 3.2). While such mimetic properties may have nice implications, it is proven that such results cannot hold for higher order approximations, independently of the grid or the exact form of the discrete derivative operator (Theorem 3.6 and Theorem 3.8). Especially, this result holds also for spectral collocation and nodal discontinuous Galerkin methods.

Furthermore, the entropy dissipation induced by difference operators approximating second derivatives with varying coefficients is studied. While second order approximations are dissipative for all entropies (Theorem 4.1), such a result is not valid for higher order approximations in general. Especially, a counterexample for classical fourth order approximations is given (Example 4.2).

While these results are interesting on their own, there are several connections with other results and open questions. It is well-known that higher order schemes can be more efficient for certain problems than lower order ones [19]. However, the numerical treatment of discontinuities in solutions to hyperbolic conservation laws has to be well-considered, especially for higher order schemes. Even though a single entropy inequality can be sufficient for genuinely nonlinear scalar conservation laws [7, 21, 28], general conservation laws pose additional challenges [22]. Since certain mimetic properties discussed in this article are limited to second order schemes, suitable detection of discontinuities and corresponding adaptations of the numerical methods may be inevitable.

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