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A Sufficient and Necessary Condition of the Existence of WENO-Like Linear Combination for Finite Difference Schemes

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Abstract. In the finite difference WENO (weighted essentially non-oscillatory) method, the final scheme on the whole stencil was constructed by linear combinations of highest order accurate schemes on sub-stencils, all of which share the same total count of grid points. The linear combination method which the original WENO applied was generalized to arbitrary positive-integer-order derivative on an arbitrary (uniform or non-uniform) mesh, still applying finite difference method. The possibility of expressing the final scheme on the whole stencil as a linear combination of highest order accurate schemes on WENO-like sub-stencils was investigated. The main results include: (a) the highest order of accuracy a finite difference scheme can achieve and (b) a sufficient and necessary condition that the linear combination exists. This is a sufficient and necessary condition for all finite difference schemes in a set (rather than a specific finite difference scheme) to have WENO-like linear combinations. After the proofs of the results, some remarks on the WENO schemes and TENO (targeted essentially non-oscillatory) schemes were given.

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1 Introduction

In nonlinear hyperbolic conservation systems (e.g. Euler equations of inviscid compressible flow), the solution may develop discontinuities even if the initial value is smooth,

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due to the intrinsic nonlinearity. Several techniques were developed to tackle discontinuities in such problems. Some of the techniques represent the discontinuities as actual discontinuities, e.g. shock fitting [1, 2], jump recovery [3], and subcell resolution [4]. Different from the techniques listed above, the shock capturing method [5, 6] artificially spreads a discontinuity in several (typically less than 10) cells, turning the discontinuity into a large gradient zone. Such methods automatically "capture" shock waves without special treatments, thus the algorithms of such an approach are simpler. The foundation of shock capturing methods is artificial viscosity, which was developed by Von Neumann and Richtmyer [7, 8]. At present, the artificial viscosity is often introduced implicitly via the flux vector splitting (FVS) method [9].

One of the shock capturing schemes is the essentially non-oscillatory scheme [10–12], the basic idea of which is to select the "smoothest" stencil to perform calculations. Based on the essentially non-oscillatory (ENO) scheme, weighted essentially non-oscillatory (WENO) scheme [13] was developed. The WENO scheme can be considered as an improved version of the ENO scheme. When shock is detected, the WENO scheme degenerates to the ENO scheme. If shock is not present, a higher order accurate flux will be calculated using all the fluxes calculated in the ENO scheme. Such a procedure improves the scheme's resolution in smooth zones.

Later in 1996, a generic framework to design finite difference WENO schemes [14] was published. The designing framework was a great success, yet still some issues require further considerations. Firstly, the framework actually asked for a uniform mesh to directly apply the WENO schemes. When applying the WENO schemes on a non-uniform smoothly varying mesh, one must perform a transformation to make the mesh uniform [15]. Secondly, in practice, it was noted that the order of accuracy may drop near critical points [16]. Thirdly, WENO schemes typically were unnecessarily dissipative at small scales [17]. Fourthly, stability problems may occur for very-high-order WENO schemes [18].

For the first issue that the framework was designed for uniform or smoothly varying mesh, research showed that it is feasible to apply the WENO schemes on a non-uniform mesh directly, using the finite volume method [20, 21]. If one applies finite difference schemes directly on a non-uniform mesh, the order of accuracy cannot be greater than 2 with the prerequisites that (a) the derivatives are evaluated in a conservative form, i.e.

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_j = \frac{f_{j+1/2} - f_{j-1/2}}{\Delta x} \tag{1.1}$$

and (b) the numerical flux $f_{j+1/2}$ expressed as

$$f_{j+1/2} = \sum_{i=r}^{s} c_{ij} f_{j+i} \tag{1.2}$$

with the coefficients c_{ij} independent of mesh sizes [15].

For the second issue, Henrick et al. [16] proposed a method to achieve optimal order near critical points. The basic idea is to modify the nonlinear weights of the sub-stencils.

For the third issue, Hill and Pullin [17] proposed to freeze the adaptation when the ratio between the largest and the smallest calculated smoothness indicator is less than a problem-dependent threshold. This method was based on the observation that the nonlinear adaptation of WENO schemes would directly affect the effective numerical dissipation. It is also feasible to reduce the numerical dissipation by optimizing spectral properties, improving the resolution of the final scheme. Different from the original WENO schemes which apply the highest order accurate scheme in smooth regions, such spectral optimized schemes, e.g. the MDCD (minimized dispersion and controllable dissipation) WENO scheme [24], apply spectral optimized schemes (with lower order of accuracy, of course) in the smooth regions.

For the fourth issue, Gerolymos et al. [18] proposed to modify the power coefficient occurred in the framework developed by Jiang and Shu [14]. Such an approach would actually reduce the order of accuracy, making the final scheme more like ENO schemes.

Some of the modified WENO schemes mentioned above [16–18, 24] share something in common: the sub-stencils and the numerical fluxes on the sub-stencils remained unchanged, while the nonlinear weights of such numerical fluxes were modified.

Despite of the fact that the WENO schemes were designed for hyperbolic conservation laws, aiming at calculating first derivatives, the basic idea can be extended to computations of higher order derivatives. For example, it is feasible to apply the WENO-like strategy directly to compute second derivatives. Similar to computing the first derivatives using WENO schemes, Liu et al. [19] proposed to evaluate second derivatives on the sub-stencils and the final scheme was a linear combination of all the schemes on sub-stencils. Unlike first derivatives, when building WENO-like schemes for second derivatives, the linear combination required to form the final scheme may not exist even if in the context of uniform mesh [19].

Although there already exist a lot of applications of WENO schemes, the theoretical basis of the linear combination method requires more considerations: why does the linear combination always exist for 1st derivative WENO schemes? Under what situations will the linear combination exist? When the method expands to arbitrary positive-integer-order derivatives, will the same linear combination strategy always work? What about applying the linear combination method directly on a non-uniform mesh? This paper will answer such questions.

In this paper the discussions are focused on the linear combination method the WENO schemes applied to form a higher order scheme. All the discussions in this paper are limited to the finite difference framework, while the order of the derivatives is extended to arbitrary positive integer. Besides, the mesh for calculating the derivatives can be uniform or non-uniform, and the final scheme can be an optimized one without achieving highest order of accuracy. With such preconditions a sufficient and necessary condition for the existence of WENO-like linear combination (not necessarily convex combination) was derived, and a theorem on the order of accuracy of finite difference schemes was derived.

The rest of the paper is organized as follows: in Section 2 the main results (a theorem for the order of accuracy and a theorem for the existence of WENO-like linear combination) are listed. In Section 3 some auxiliary conclusions are stated and proved. In Section 4 the proofs of the main theorems are given. In Section 5 we discuss the applications of the main theorems in three different scenarios: 1st derivative and uniform meshes, 1st derivative and non-uniform meshes, and finally 2nd derivative and uniform meshes. After that some examples of the main theorems are given. The conclusions are stated in Section 6.

2 Main results

In order to introduce the main results, we prefer to introduce some definitions first.

Let T_h be the shift operator with step h, which maps $f(x)$ to $f(x+h)$:

$$T_h[f](x)=f(x+h). \tag{2.1}$$

We define *finite difference operators* and *finite difference schemes* as follows:

Definition 2.1. Suppose $h>0$. The operator

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\sum_{i=1}^{n}a_iT_{d_ih} \tag{2.2}$$

is called a finite difference operator, if $\sum_{i=1}^{n}a_i=0$ and all $d_i\in\mathbb{R}$ are distinct, i.e. $d_i=d_j\Leftrightarrow i=j$.

Considering Taylor series, it is clear that

$$T_h=I+\frac{1}{1!}hD+\frac{1}{2!}h^2D^2+\cdots+\frac{1}{n!}h^nD^n+\cdots=e^{hD} \tag{2.3}$$

and

$$T_{ah}=T_h^a=e^{ahD},\quad \forall a\in\mathbb{R}, \tag{2.4}$$

where I is the identity operator which maps $f(x)$ to itself:

$$I[f](x)=f(x), \tag{2.5}$$

and D is the differential operator, $\frac{\mathrm{d}}{\mathrm{d}x}$.

With the definition of $\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}$, we have

$$\begin{aligned}\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}&=\sum_{j=1}^{n}a_jT_{d_jh}=\sum_{j=1}^{n}a_je^{d_jhD}\\&=\sum_{j=1}^{n}a_j\sum_{i=0}^{\infty}\frac{1}{i!}d_j^ih^iD^i=\sum_{i=0}^{\infty}\frac{1}{i!}h^iD^i\sum_{j=1}^{n}a_jd_j^i\\&=\sum_{i=0}^{\infty}\frac{1}{i!}b_ih^iD^i,\end{aligned} \tag{2.6}$$

where

$$b_i = \sum_{j=1}^{n} a_j d_j^i, \quad i \in \mathbb{N}_0. \tag{2.7}$$

Here we define $0^0 = 1$.

Definition 2.2. $\frac{p!}{h^p}\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}$ is a pth order finite difference scheme of qth order of accuracy, if

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} = \frac{1}{p!}h^p D^p + \sum_{i=p+q}^{\infty} \frac{1}{i!} b_i h^i D^i, \quad b_{p+q} \neq 0. \tag{2.8}$$

In Definition 2.2, if

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} = \frac{1}{p!}h^p D^p + \sum_{i=n}^{\infty} \frac{1}{i!} b_i h^i D^i, \tag{2.9}$$

then $a_1,\cdots,a_n$ are determined uniquely. Thus we can omit the a_is in subscripts, which is stated in Definition 2.3 as follows.

Definition 2.3. $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is a pth order finite difference scheme, which satisfies

$$\tilde{D}_{p,h,d_1,\cdots,d_n} = \frac{p!}{h^p}\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} \quad (1 \leqslant p \leqslant n), \tag{2.10}$$

where

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} = \frac{1}{p!}h^p D^p + \sum_{i=n}^{\infty} \frac{1}{i!} b_i h^i D^i. \tag{2.11}$$

Note that in Definition 2.3, the order of accuracy of $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is not mentioned, since $b_n \neq 0$ may or may not hold.

Usually, $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is of $(n-p)$th order of accuracy. On the other hand, it is possible that $\tilde{D}_{p,h,d_1,\cdots,d_n}$ has an order of accuracy greater than $(n-p)$.

Example 2.1.

$$\frac{h^2}{2!}\tilde{D}_{2,h,-1,0,1} = \sum_{i=1}^{\infty} \frac{1}{(2i)!} h^{2i} D^{2i} = \frac{1}{2!}h^2 D^2 + \frac{1}{4!}h^4 D^4 + \cdots.$$

By Definition 2.2 and Definition 2.3, $\tilde{D}_{2,h,-1,0,1}$ is of 2nd order of accuracy. However, in this case, we have that $n=3$ and $p=2$, so $2 > n-p = 1$.

Due to the uncertainty of the order of accuracy, we first define *trivial* and *nontrivial* for the highest-order-accurate scheme $\tilde{D}_{p,h,d_1,\cdots,d_n}$ as follows:

Definition 2.4. $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is trivial, if its order of accuracy is $(n-p)$; otherwise, $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is nontrivial.

Then let us consider a set of finite difference operators, $V_{h,p,q,d_1,\cdots,d_n}$, as stated in the following definition.

Definition 2.5. Suppose p,q are positive integers satisfying $p<q$. The set $V_{h,p,q,d_1,\cdots,d_n}$ is defined as

$$\left\{\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}:\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\lambda_p h^p D^p+\sum_{i=q}^{\infty}\lambda_i h^i D^i,\ \lambda_j\in\mathbb{R},\ j=p \text{ or } j\geqslant q\right\}. \tag{2.12}$$

It is easy to verify that $V_{h,p,q,d_1,\cdots,d_n}$ is a vector space over field $\mathbb{R}$.

In practical problems e.g. computing numerical solutions for hyperbolic conservation laws, we are often more interested in a subset of the vector space $V_{h,p,q,d_1,\cdots,d_n}$ rather than the vector space itself. Thus here goes the definition of *concerned zone* of $V_{h,p,q,d_1,\cdots,d_n}$:

Definition 2.6.

$$C_{h,p,q,d_1,\cdots,d_n}=\left\{\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}:\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\frac{1}{p!}h^p D^p+\sum_{i=q}^{\infty}x_i\frac{1}{i!}h^i D^i,\ x_i\in\mathbb{R}\right\} \tag{2.13}$$

is the concerned zone of $V_{h,p,q,d_1,\cdots,d_n}$.

We have the following theorem for $\tilde{D}_{p,h,d_1,\cdots,d_n}$:

Theorem 2.1. *A nontrivial $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is of $(n-p+1)$th order of accuracy.*

For the concerned zone $C_{h,p,q,d_1,\cdots,d_n}$, we have the following theorem.

Theorem 2.2. *Suppose*

$$S=\left\{\tilde{D}_{p,h,d_1,\cdots,d_q},\tilde{D}_{p,h,d_2,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_n}\right\}, \tag{2.14}$$

$\operatorname{span}S\supseteq C_{h,p,q,d_1,\cdots,d_n}$ *if and only if*

$$\tilde{D}_{p,h,d_2,\cdots,d_q},\tilde{D}_{p,h,d_3,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_i,\cdots,d_{i+q-2}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_{n-1}}$$

are trivial.

3 Auxiliary statements

Firstly we would like to introduce Newton's inequalities, which played an important role in the proof of Theorem 2.1.

Lemma 3.1 (Newton's inequalities). *Suppose $a_i \in \mathbb{R}$ where $1 \leqslant i \leqslant n$, $n \in \mathbb{Z}^+$. Let σ_k denote the kth elementary symmetric function in $a_1,\cdots,a_n$. Then the elementary symmetric means, given by*

$$S_k = \frac{\sigma_k}{\binom{n}{k}} \tag{3.1}$$

satisfy the inequality

$$S_{k-1}S_{k+1} \leqslant S_k^2. \tag{3.2}$$

Particularly, if all a_is are distinct, i.e. $a_i = a_j \Leftrightarrow i = j$, then equality would not hold.

To check whether $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is trivial, we need the following two propositions.

Proposition 3.1. Suppose $x_1,\cdots,x_n$ are n distinct real numbers, and $c_1,\cdots,c_n \in \mathbb{R}$ are n constants. For all non-negative integer k, let

$$s_k = \sum_{i=1}^{n} c_i x_i^k. \tag{3.3}$$

Then s_k satisfies

$$\sum_{i=0}^{n} a_i s_{k+i} = 0, \tag{3.4}$$

where $a_0,a_1,\cdots,a_n$ are coefficients of a polynomial which has $x_1,\cdots,x_n$ as its roots, i.e.

$$\sum_{j=0}^{n} a_j x_i^j = 0, \quad 1 \leqslant i \leqslant n. \tag{3.5}$$

Proof. From (3.5), we have

$$\begin{aligned} 0 &= \sum_{i=1}^{n} c_i x_i^k \sum_{j=0}^{n} a_j x_i^j = \sum_{i=1}^{n}\sum_{j=0}^{n} a_j c_i x_i^{k+j} \\ &= \sum_{j=0}^{n} a_j \sum_{i=1}^{n} c_i x_i^{k+j} = \sum_{j=0}^{n} a_j s_{k+j} \end{aligned} \tag{3.6}$$

and the proposition follows. □

Proposition 3.2. Suppose $s_i \in \mathbb{R}$ $(0 \leqslant i \leqslant n)$ satisfy

$$\prod_{i=1}^{n}(x - d_i) = \sum_{i=0}^{n} s_i x^i, \tag{3.7}$$

then $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is nontrivial if and only if

$$s_p = 0. \tag{3.8}$$

Proof. By Definition 2.3,

$$\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_n}=\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\frac{1}{p!}h^pD^p+\sum_{i=n}^{\infty}\frac{1}{i!}b_ih^iD^i, \tag{3.9}$$

where

$$b_i=\sum_{j=1}^{n}a_jd_j^i \quad (i\in\mathbb{Z}^+\cup\{0\}). \tag{3.10}$$

Definition 2.3 gives

$$b_0=\cdots=b_{p-1}=0, \quad b_p=1, \quad b_{p+1}=\cdots=b_{n-1}=0. \tag{3.11}$$

By Proposition 3.1,

$$\sum_{i=0}^{n}s_ib_i=0, \tag{3.12}$$

substituting (3.11) into (3.12) gives (note that $s_n=1$)

$$s_p+b_n=0. \tag{3.13}$$

Thus $b_n=-s_p$. By Definition 2.4, $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is nontrivial if and only if $b_n=0$, and the proposition follows. □

From Definition 2.1, it is clear that

Proposition 3.3. Swapping d_i,d_j and a_i,a_j simultaneously will not change the operator

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n},$$

i.e.

$$\Delta_{h,d_1,\cdots,d_i,\cdots,d_j,\cdots,d_n,a_1,\cdots,a_i,\cdots,a_j,\cdots,a_n}=\Delta_{h,d_1,\cdots,d_j,\cdots,d_i,\cdots,d_n,a_1,\cdots,a_j,\cdots,a_i,\cdots,a_n}. \tag{3.14}$$

With Definition 2.3 and Proposition 3.3, it is clear that

Proposition 3.4. Swapping d_i,d_j in $\tilde{D}_{p,h,d_1,\cdots,d_n}$ will not change the operator, i.e.

$$\tilde{D}_{p,h,d_1,\cdots,d_i,\cdots,d_j,\cdots,d_n}=\tilde{D}_{p,h,d_1,\cdots,d_j,\cdots,d_i,\cdots,d_n}. \tag{3.15}$$

In Definition 2.3, for the special case that $p=n$, we have

Proposition 3.5. $\tilde{D}_{n,h,d_1,\cdots,d_n}$ is trivial.

Proof. By Definition 2.3, $\exists a_1,\cdots,a_n\in\mathbb{R}$ such that

$$\frac{h^n}{n!}\tilde{D}_{n,h,d_1,\cdots,d_n}=\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\sum_{i=n}^{\infty}c_i\frac{1}{i!}h^iD^i. \tag{3.16}$$

Comparing the coefficients of $D^i\,(0\leqslant i\leqslant n-1)$, we have

$$\begin{pmatrix} 1 & \cdots & 1 \\ d_1 & \cdots & d_n \\ \vdots & \ddots & \vdots \\ d_1^{n-1} & \cdots & d_n^{n-1} \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = \mathbf{0}. \tag{3.17}$$

The solution gives

$$a_1=\cdots=a_n=0, \tag{3.18}$$

i.e.

$$\frac{h^n}{n!}\tilde{D}_{n,h,d_1,\cdots,d_n}=0=\frac{1}{n!}h^nD^n+\left(-\frac{1}{n!}h^nD^n\right). \tag{3.19}$$

Thus $\tilde{D}_{n,h,d_1,\cdots,d_n}$ is trivial by Definition 2.4. □

Lemma 3.2. *If*

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}-\Delta_{h,d_1,\cdots,d_n,b_1,\cdots,b_n}=\sum_{i=n}^{\infty}\frac{1}{i!}c_ih^iD^i, \tag{3.20}$$

then

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\Delta_{h,d_1,\cdots,d_n,b_1,\cdots,b_n}. \tag{3.21}$$

Proof. Let

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\sum_{i=0}^{\infty}\frac{1}{i!}x_ih^iD^i \tag{3.22}$$

and

$$\Delta_{h,d_1,\cdots,d_n,b_1,\cdots,b_n}=\sum_{i=0}^{\infty}\frac{1}{i!}y_ih^iD^i, \tag{3.23}$$

where

$$\begin{cases} x_i=\sum_{j=1}^{n}a_jd_j^i, \\ y_i=\sum_{j=1}^{n}b_jd_j^i. \end{cases} \tag{3.24}$$

Then

$$\begin{aligned} \sum_{i=n}^{\infty}\frac{1}{i!}c_ih^iD^i &= \Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}-\Delta_{h,d_1,\cdots,d_n,b_1,\cdots,b_n} \\ &= \sum_{i=0}^{\infty}\frac{1}{i!}x_ih^iD^i-\sum_{i=0}^{\infty}\frac{1}{i!}y_ih^iD^i \\ &= \sum_{i=0}^{\infty}\frac{1}{i!}(x_i-y_i)h^iD^i, \end{aligned} \tag{3.25}$$

so we have

$$x_0-y_0=x_1-y_1=\cdots=x_{n-1}-y_{n-1}=0, \tag{3.26}$$

i.e.

$$\begin{pmatrix} 1 & 1 & \cdots & 1 \\ d_1 & d_2 & \cdots & d_n \\ \vdots & \vdots & \ddots & \vdots \\ d_1^{n-1} & d_2^{n-1} & \cdots & d_n^{n-1} \end{pmatrix} \begin{pmatrix} a_1-b_1 \\ a_2-b_2 \\ \vdots \\ a_n-b_n \end{pmatrix} = \mathbf{0}. \tag{3.27}$$

All the d_is are distinct by definition, so the only solution is

$$a_1-b_1=a_2-b_2=\cdots=a_n-b_n=0, \tag{3.28}$$

which completes the proof. □

With the help of Lemma 3.2, we have

Proposition 3.6. The dimension of $V_{h,p,q,d_1,\cdots,d_n}$ is $(n-q+1)$.

Proof. Let us consider the $(n-q+1)$ different operators in $V_{h,p,q,d_1,\cdots,d_n}$:

$$\begin{cases} \Delta_1 = h^p D^p + \sum_{i=n}^{\infty} \lambda_{1,i} h^i D^i, \\ \Delta_2 = h^q D^q + \sum_{i=n}^{\infty} \lambda_{2,i} h^i D^i, \\ \Delta_3 = h^{q+1} D^{q+1} + \sum_{i=n}^{\infty} \lambda_{3,i} h^i D^i, \\ \qquad \cdots \\ \Delta_{n-q+1} = h^{n-1} D^{n-1} + \sum_{i=n}^{\infty} \lambda_{n-q+1,i} h^i D^i. \end{cases} \tag{3.29}$$

If there exist $\mu_1,\mu_2,\cdots,\mu_{n-q+1}\in\mathbb{R}$ such that

$$\sum_{i=1}^{n-q+1} \mu_i \Delta_i = 0 = 0\cdot h^p D^p + 0\cdot h^q D^q + \cdots + 0\cdot h^{n-1} D^{n-1}, \tag{3.30}$$

then $\mu_1,\mu_2,\cdots,\mu_{n-q+1}$ satisfy

$$\begin{cases} \mu_1 = 0, \\ \mu_2 = 0, \\ \quad \cdots \\ \mu_{n-q+1} = 0, \end{cases} \tag{3.31}$$

i.e. $\mu_1=\mu_2=\cdots=\mu_{n-q+1}=0$. Thus the $(n-q+1)$ operators are linearly independent.

On the other hand, $\forall\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}\in V_{h,p,q,d_1,\cdots,d_n}$, if we re-express $\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}$ as

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\lambda_p h^p D^p+\sum_{i=q}^{\infty}\lambda_i h^i D^i, \tag{3.32}$$

then

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}-\left(\lambda_p\Delta_1+\sum_{i=q}^{n-1}\lambda_i\Delta_{i-q+2}\right)=\sum_{i=n}^{\infty}c_i h^i D^i. \tag{3.33}$$

By Lemma 3.2,

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\lambda_p\Delta_1+\sum_{i=q}^{n-1}\lambda_i\Delta_{i-q+2}, \tag{3.34}$$

i.e. any element in $V_{h,p,q,d_1,\cdots,d_n}$ can be written as a linear combination of $\Delta_1,\cdots,\Delta_{n-q+1}$. Thus $\{\Delta_1,\cdots,\Delta_{n-q+1}\}$ is a basis of $V_{h,p,q,d_1,\cdots,d_n}$, and the dimension of $V_{h,p,q,d_1,\cdots,d_n}$ is $(n-q+1)$. □

Although in practical problems, e.g. numerical simulation for hyperbolic conservation laws, we are more interested in the *concerned zone*, the following proposition shows that $C_{h,p,q,d_1,\cdots,d_n}$ and $V_{h,p,q,d_1,\cdots,d_n}$ are closely related:

Proposition 3.7. Suppose

$$S=\left\{\tilde{D}_{p,h,d_1,\cdots,d_q},\tilde{D}_{p,h,d_2,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_n}\right\}, \tag{3.35}$$

$\mathrm{span}S\supseteq C_{h,p,q,d_1,\cdots,d_n}$ if and only if S is a basis of $V_{h,p,q,d_1,\cdots,d_n}$.

Proof. If S is a basis of the vector space $V_{h,p,q,d_1,\cdots,d_n}$, then the span of S is exactly $V_{h,p,q,d_1,\cdots,d_n}$, which has $C_{h,p,q,d_1,\cdots,d_n}$ as one of its subsets.

If S is not a basis of $V_{h,p,q,d_1,\cdots,d_n}$, then there exists $\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}\in V_{h,p,q,d_1,\cdots,d_n}$ which is not in the span of S. More specifically, suppose

$$\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\lambda_p\frac{1}{p!}h^p D^p+\sum_{i=q}^{\infty}\lambda_i\frac{1}{i!}h^i D^i. \tag{3.36}$$

We will show that there exists an operator Δ_0 which is in $C_{h,p,q,d_1,\cdots,d_n}$ but is not in the span of S.

If $\lambda_p=0$, then let

$$\Delta_0=\frac{h^p}{p!}\tilde{D}_{h,d_1,\cdots,d_q}+\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}. \tag{3.37}$$

If $\lambda_p\neq 0$, then let

$$\Delta_0=\frac{1}{\lambda_p}\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}. \tag{3.38}$$

In either case it is easy to verify that $\Delta_0\in C_{h,p,q,d_1,\cdots,d_n}$, and Δ_0 is not in the span of S. Thus $C_{h,p,q,d_1,\cdots,d_n}$ is not a subset of the span of S. □

Lemma 3.3. *Suppose $d_1,d_2,\cdots,d_n\in\mathbb{R}$ are distinct. If $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is nontrivial, then $\tilde{D}_{p,h,d_1,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_n}$.*

Proof. By Definition 2.3, there exist $a_1,\cdots,a_n$ and $b_1,\cdots,b_{n-1}$ such that

$$\begin{cases} \frac{1}{p!}h^p\tilde{D}_{p,h,d_1,\cdots,d_n}=\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}=\frac{1}{p!}h^pD^p+\sum_{i=n}^{\infty}\frac{1}{i!}x_ih^iD^i, \\ \frac{1}{p!}h^p\tilde{D}_{p,h,d_2,\cdots,d_n}=\Delta_{h,d_2,\cdots,d_n,b_1,\cdots,b_{n-1}}=\frac{1}{p!}h^pD^p+\sum_{i=n}^{\infty}\frac{1}{i!}y_ih^iD^i. \end{cases} \tag{3.39}$$

Thus

$$\begin{aligned} \Delta_{h,d_1,d_2,\cdots,d_n,0,b_1,\cdots,b_{n-1}}-\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}&=\Delta_{h,d_2,\cdots,d_n,b_1,\cdots,b_{n-1}}-\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} \\ &=\sum_{i=n}^{\infty}\frac{1}{i!}(y_i-x_i)h^iD^i. \end{aligned} \tag{3.40}$$

By Lemma 3.2,

$$\Delta_{h,d_1,d_2,\cdots,d_n,0,b_1,\cdots,b_{n-1}}=\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n}, \tag{3.41}$$

i.e. $\tilde{D}_{p,h,d_1,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_n}$. □

Corollary 3.1. *If $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is nontrivial, then $\tilde{D}_{p,h,d_1,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_{n+1}}$.*

Proof. By Lemma 3.3,

$$\tilde{D}_{p,h,d_1,d_2,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_n}=\tilde{D}_{p,h,d_{n+1},d_2,\cdots,d_n}. \tag{3.42}$$

By Proposition 3.4,

$$\tilde{D}_{p,h,d_{n+1},d_2,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_n,d_{n+1}}. \tag{3.43}$$

Thus

$$\tilde{D}_{p,h,d_1,d_2,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_n,d_{n+1}}, \tag{3.44}$$

which completes the proof. □

Lemma 3.4. *There exists $\lambda\in\mathbb{R}^*$ such that*

$$\lambda\left(\tilde{D}_{p,h,d_2,\cdots,d_{n+1}}-\tilde{D}_{p,h,d_1,\cdots,d_n}\right)=\tilde{D}_{n,h,d_1,\cdots,d_{n+1}} \tag{3.45}$$

if and only if $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is trivial.

Proof. Let us start with the assumption that $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is nontrivial. In such case Corollary 3.1 gives

$$\tilde{D}_{p,h,d_1,\cdots,d_n}=\tilde{D}_{p,h,d_2,\cdots,d_{n+1}} \tag{3.46}$$

and such λ does not exist.

If $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is trivial, then we have

$$\begin{cases} \dfrac{1}{p!}h^p\tilde{D}_{p,h,d_1,\cdots,d_n}=\dfrac{1}{p!}h^pD^p+\sum\limits_{i=n}^{\infty}\dfrac{1}{i!}x_ih^iD^i, \\ \dfrac{1}{p!}h^p\tilde{D}_{p,h,d_2,\cdots,d_{n+1}}=\dfrac{1}{p!}h^pD^p+\sum\limits_{i=n}^{\infty}\dfrac{1}{i!}y_ih^iD^i. \end{cases} \tag{3.47}$$

We will prove that $x_n\neq y_n$. If $x_n=y_n$, then there exists $a_1,\cdots,a_n$ and $b_1,\cdots,b_n$ such that

$$\begin{aligned} \frac{1}{p!}h^p\tilde{D}_{p,h,d_2,\cdots,d_{n+1}}-\frac{1}{p!}h^p\tilde{D}_{p,h,d_1,\cdots,d_n}&=\Delta_{h,d_2,\cdots,d_{n+1},b_1,\cdots,b_n}-\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} \\ &=\Delta_{h,d_1,d_2,\cdots,d_{n+1},0,b_1,\cdots,b_n}-\Delta_{h,d_1,\cdots,d_n,d_{n+1},a_1,\cdots,a_n,0} \\ &=\sum_{i=n+1}^{\infty}\frac{1}{i!}(y_i-x_i)h^iD^i. \end{aligned} \tag{3.48}$$

By Lemma 3.2, we have

$$a_1=0,\quad a_{i+1}=b_i,\quad b_n=0\quad (1\leqslant i\leqslant n-1). \tag{3.49}$$

Thus

$$\begin{aligned} \frac{1}{p!}h^pD^p+\sum_{i=n}^{\infty}\frac{1}{i!}x_ih^iD^i=\frac{1}{p!}h^p\tilde{D}_{p,h,d_1,\cdots,d_n} \\ =\Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} \\ =\Delta_{h,d_2,\cdots,d_n,a_2,\cdots,a_n}. \end{aligned} \tag{3.50}$$

By Definition 2.3, $\frac{p!}{h^p}\Delta_{h,d_2,\cdots,d_n,a_2,\cdots,a_n}=\tilde{D}_{p,h,d_2,\cdots,d_n}$. On the other hand, by Definition 2.4, the scheme $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is nontrivial, which contradicts with the assumption that $\tilde{D}_{p,h,d_2,\cdots,d_n}$ is trivial. The contradiction shows that $x_n=y_n$ can not hold, thus $x_n\neq y_n$.

Since $x_n\neq y_n$, we have

$$\begin{aligned} \frac{1}{y_n-x_n}\frac{1}{p!}h^p\left(\tilde{D}_{p,h,d_2,\cdots,d_{n+1}}-\tilde{D}_{p,h,d_1,\cdots,d_n}\right)&=\Delta_{h,d_1,\cdots,d_{n+1},c_1,\cdots,c_{n+1}} \\ &=\frac{1}{n!}h^nD^n+\sum_{i=n+1}^{\infty}\frac{1}{i!}\frac{y_i-x_i}{y_n-x_n}h^iD^i. \end{aligned} \tag{3.51}$$

By Definition 2.3,

$$\frac{n!}{h^n}\Delta_{h,d_1,\cdots,d_{n+1},c_1,\cdots,c_{n+1}}=\tilde{D}_{n,h,d_1,\cdots,d_{n+1}}, \tag{3.52}$$

thus there exists $\lambda=\frac{1}{y_n-x_n}\frac{n!}{p!}h^{p-n}$ such that

$$\lambda\left(\tilde{D}_{p,h,d_2,\cdots,d_{n+1}}-\tilde{D}_{p,h,d_1,\cdots,d_n}\right)=\tilde{D}_{n,h,d_1,\cdots,d_{n+1}}. \tag{3.53}$$

Clearly $\lambda\neq 0$, since $h\neq 0$ by Definition 2.1. □

Particularly, $\tilde{D}_{n-1,h,d_2,\cdots,d_n}$ is always trivial (see Proposition 3.5), thus we have

Corollary 3.2. *There exists* $\lambda \in \mathbb{R}^*$ *such that*

$$\lambda\left(\tilde{D}_{n-1,h,d_2,\cdots,d_{n+1}} - \tilde{D}_{n-1,h,d_1,\cdots,d_n}\right) = \tilde{D}_{n,h,d_1,\cdots,d_{n+1}}. \tag{3.54}$$

4 Proof of the main theorems

In this section we prove Theorems 2.1 and 2.2.

4.1 Proof of Theorem 2.1

Proof of Theorem 2.1. Consider the operator $\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_n}$. By Definition 2.3,

$$\begin{aligned}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_n} &= \Delta_{h,d_1,\cdots,d_n,a_1,\cdots,a_n} \\ &= \sum_{i=0}^{\infty}\frac{1}{i!}b_i h^i D^i \\ &= \frac{1}{p!}h^p D^p + \sum_{i=n}^{\infty}\frac{1}{i!}b_i h^i D^i,\end{aligned} \tag{4.1}$$

where

$$b_i = \sum_{j=1}^{n} a_j d_j^i. \tag{4.2}$$

By Definition 2.4,

$$b_n = 0. \tag{4.3}$$

We will prove that $b_{n+1} \neq 0$ as follows:

Consider the following n-degree polynomial

$$\varphi(x) = \prod_{j=1}^{n}(x-d_j) = \sum_{i=0}^{n} s_i x^i. \tag{4.4}$$

It is clear that $s_n = 1$.

The definition of $\tilde{D}_{p,h,d_1,\cdots,d_n}$ gives

$$b_0 = \cdots = b_{p-1} = 0, \quad b_p = 1, \quad b_{p+1} = \cdots = b_{n-1} = 0. \tag{4.5}$$

So by Proposition 3.1, we have

$$0 = \sum_{i=0}^{n} s_i b_i = s_p b_p + s_n b_n = s_p + b_n \tag{4.6}$$

and

$$0=\sum_{i=0}^{n} s_i b_{i+1} = s_{p-1}b_p + s_{n-1}b_n + s_n b_{n+1} = s_{p-1} + s_{n-1}b_n + b_{n+1}. \tag{4.7}$$

If $b_{n+1}=0$, then from (4.6) and (4.7), together with (4.3), it is clear that

$$s_p = s_{p-1} = 0, \tag{4.8}$$

which contradicts Lemma 3.1. The contradiction shows that $b_{n+1}\neq 0$, so $\tilde{D}_{p,h,d_1,\cdots,d_n}$ is of $(n-p+1)$th order of accuracy. □

4.2 Proof of Theorem 2.2

Proposition 4.1. Suppose $d_1,\cdots,d_n \in \mathbb{R}$ are distinct. There exists $\lambda_1,\cdots,\lambda_{n-q}\in\mathbb{R}$ such that

$$\sum_{i=1}^{n-q} \lambda_i \tilde{D}_{q,h,d_i,\cdots,d_{q+i}} = \tilde{D}_{n-1,h,d_1,\cdots,d_n} \quad (1\leqslant q \leqslant n-1). \tag{4.9}$$

Proof. Let $n-q=k$, then $1\leqslant k\leqslant n-1$. We proceed by mathematical induction on k.

Firstly, for the base case that $k=1$, the equality becomes

$$\lambda_1 \tilde{D}_{n-1,h,d_1,\cdots,d_n} = \tilde{D}_{n-1,h,d_1,\cdots,d_n}. \tag{4.10}$$

The claim is true since $\lambda_1 = 1 \in \mathbb{R}$ makes the equality hold.

Secondly, for the inductive step, suppose the claim is true for $k=k_0<n-1$, i.e. $\exists \lambda_1,\cdots,\lambda_{k_0}\in\mathbb{R}$ such that

$$\sum_{i=1}^{k_0} \lambda_i \tilde{D}_{n-k_0,h,d_i,\cdots,d_{n-k_0+i}} = \tilde{D}_{n-1,h,d_1,\cdots,d_n}. \tag{4.11}$$

By Corollary 3.2, $\exists \mu_i \in \mathbb{R}^*$ such that

$$\tilde{D}_{n-k_0,h,d_i,\cdots,d_{n-k_0+i}} = \mu_i \left(\tilde{D}_{n-k_0-1,h,d_{i+1},\cdots,d_{n-k_0+i}} - \tilde{D}_{n-k_0-1,h,d_i,\cdots,d_{n-k_0-1+i}} \right). \tag{4.12}$$

So

$$\begin{aligned}
\tilde{D}_{n-1,h,d_1,\cdots,d_n} &= \sum_{i=1}^{k_0} \lambda_i \tilde{D}_{n-k_0,h,d_i,\cdots,d_{n-k_0+i}} \\
&= \sum_{i=1}^{k_0} \lambda_i \mu_i \left(\tilde{D}_{n-k_0-1,h,d_{i+1},\cdots,d_{n-k_0+i}} - \tilde{D}_{n-k_0-1,h,d_i,\cdots,d_{n-k_0-1+i}} \right) \\
&= \sum_{i=2}^{k_0+1} \lambda_{i-1}\mu_{i-1} \tilde{D}_{n-k_0-1,h,d_i,\cdots,d_{n-k_0-1+i}} \\
&\quad - \sum_{i=1}^{k_0} \lambda_i \mu_i \tilde{D}_{n-k_0-1,h,d_i,\cdots,d_{n-k_0-1+i}}.
\end{aligned} \tag{4.13}$$

Let $\lambda_0=\mu_0=\lambda_{k_0+1}=\mu_{k_0+1}=0$, then

$$\tilde{D}_{n-1,h,d_1,\cdots,d_n}=\sum_{i=1}^{k_0+1}(\lambda_{i-1}\mu_{i-1}-\lambda_i\mu_i)\tilde{D}_{n-k_0-1,h,d_i,\cdots,d_{n-k_0-1+i}}. \tag{4.14}$$

Thus the claim is true for $k=k_0+1$, which completes the inductive step. □

Proposition 4.2. The $(n-q+1)$ operators $\tilde{D}_{p,h,d_1,\cdots,d_q},\tilde{D}_{p,h,d_2,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_n}$ form a basis of $V_{h,p,q,d_1,\cdots,d_n}$ if and only if $\tilde{D}_{p,h,d_2,\cdots,d_q},\tilde{D}_{p,h,d_3,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_{n-1}}$ are trivial.

Proof. If

$$\tilde{D}_{p,h,d_2,\cdots,d_q},\ \tilde{D}_{p,h,d_3,\cdots,d_{q+1}},\ \cdots,\ \tilde{D}_{p,h,d_{n-q+1},\cdots,d_{n-1}} \tag{4.15}$$

are trivial, then by Lemma 3.4, $\exists\lambda_1,\lambda_2,\cdots,\lambda_{n-q}\in\mathbb{R}$ such that

$$\lambda_i\left(\tilde{D}_{p,h,d_{i+1},\cdots,d_{i+q}}-\tilde{D}_{p,h,d_i,\cdots,d_{i+q-1}}\right)=\tilde{D}_{q,h,d_i,\cdots,d_{i+q}}. \tag{4.16}$$

$\forall\Delta_0\in V_{h,p,q,d_1,\cdots,d_n}$, suppose

$$\Delta_0=a_{pp}\frac{h^p}{p!}D^p+\sum_{i=q}^{\infty}a_{pi}\frac{h^i}{i!}D^i. \tag{4.17}$$

We can rewrite Δ_0 as

$$\Delta_0=a_{pp}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_q}+R_q, \tag{4.18}$$

where

$$R_q=\Delta_0-a_{pp}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_q}=\sum_{i=q}^{\infty}a_{qi}\frac{h^i}{i!}D^i. \tag{4.19}$$

And R_q can be expressed as

$$R_q=a_{qq}\frac{h^q}{q!}\tilde{D}_{q,h,d_1,\cdots,d_{q+1}}+R_{q+1}, \tag{4.20}$$

where

$$R_{q+1}=R_q-a_{qq}\frac{h^q}{q!}\tilde{D}_{q,h,d_1,\cdots,d_{q+1}}=\sum_{i=q+1}^{\infty}a_{q+1,i}\frac{h^i}{i!}D^i. \tag{4.21}$$

Repeat the procedure, then we get

$$\Delta_0=a_{pp}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_q}+\sum_{i=q}^{n-1}a_{ii}\frac{h^i}{i!}\tilde{D}_{i,h,d_1,\cdots,d_{i+1}}+R_n, \tag{4.22}$$

where

$$R_n=\Delta_0-\left(a_{pp}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_q}+\sum_{i=q}^{n-1}a_{ii}\frac{h^i}{i!}\tilde{D}_{i,h,d_1,\cdots,d_{i+1}}\right)=\sum_{i=n}^{\infty}a_{ni}\frac{h^i}{i!}D^i. \tag{4.23}$$

By Lemma 3.2,

$$\Delta_0 = a_{pp}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_q} + \sum_{i=q}^{n-1} a_{ii}\frac{h^i}{i!}\tilde{D}_{i,h,d_1,\cdots,d_{i+1}}. \tag{4.24}$$

By Proposition 4.1, $\tilde{D}_{i,h,d_1,\cdots,d_{i+1}}$ can be expressed as a linear combination of

$$\tilde{D}_{q,h,d_1,\cdots,d_{q+1}},\cdots,\tilde{D}_{q,h,d_{i-q+1},\cdots,d_{i+1}} \quad (q \leqslant i \leqslant n-1). \tag{4.25}$$

Thus $\exists \mu_1,\cdots,\mu_{n-q} \in \mathbb{R}$ such that

$$\Delta_0 = a_{pp}\frac{h^p}{p!}\tilde{D}_{p,h,d_1,\cdots,d_q} + \sum_{i=1}^{n-q} \mu_i \tilde{D}_{q,h,d_i,\cdots,d_{q+i}}. \tag{4.26}$$

Note that $\tilde{D}_{q,h,d_i,\cdots,d_{q+i}} = \lambda_i\left(\tilde{D}_{p,h,d_{i+1},\cdots,d_{i+q}} - \tilde{D}_{p,h,d_i,\cdots,d_{i+q-1}}\right)$, so $\forall \Delta_0 \in V_{h,p,q,d_1,\cdots,d_n}$ can be expressed as a linear combination of the $(n-q+1)$ operators, i.e.

$$\tilde{D}_{p,h,d_1,\cdots,d_q}, \tilde{D}_{p,h,d_2,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_n}. \tag{4.27}$$

By Proposition 3.6, $V_{h,p,q,d_1,\cdots,d_n}$ is $(n-q+1)$-dimensional, thus the $(n-q+1)$ operators form a basis of $V_{h,p,q,d_1,\cdots,d_n}$.

If at least one of the operators among $\tilde{D}_{p,h,d_2,\cdots,d_q}, \tilde{D}_{p,h,d_3,\cdots,d_{q+1}},\cdots,\tilde{D}_{p,h,d_{n-q+1},\cdots,d_{n-1}}$ is nontrivial, without loss of generality, suppose $\tilde{D}_{p,h,d_2,\cdots,d_q}$ is nontrivial. Then by Corollary 3.1, $\tilde{D}_{p,h,d_1,\cdots,d_q} = \tilde{D}_{p,h,d_2,\cdots,d_{q+1}}$. Thus the $(n-q+1)$ operators are linearly dependent, and cannot form a basis of $V_{h,p,q,d_1,\cdots,d_n}$. ☐

Proof of Theorem 2.2. Use Proposition 3.7 and Proposition 4.2, the theorem immediately follows. ☐

5 Discussion

Firstly we will discuss the existence of WENO-like linear combination for 1st derivative and uniform meshes in Section 5.1, for 1st derivative and non-uniform meshes in Section 5.2, and then for 2nd derivative and uniform meshes in Section 5.3. Finally we would like to present some examples of Theorem 2.1 and Theorem 2.2 in Section 5.4.

5.1 1st derivative and uniform meshes

When our scope is limited to the 1st order derivatives and uniform meshes, the linear combination strategy will always work. More specifically, there are two different strategies to construct high order accurate schemes. We will discuss the strategies in detail.

5.1.1 Construct high order accurate schemes directly

Using the polynomial $\varphi(x)$ defined in the proof of Theorem 2.1, together with Lemma 3.1, it is easy to show that

Proposition 5.1. $\tilde{D}_{1,h,d_1,\cdots,d_n}$ is nontrivial if and only if

$$\sum_{i=1}^{n}\frac{1}{d_i}=0. \tag{5.1}$$

Proof. By (4.6),

$$b_n=-s_1. \tag{5.2}$$

So

$$\tilde{D}_{1,h,d_1,\cdots,d_n} \text{ is nontrivial } \Leftrightarrow b_n=0 \Leftrightarrow s_1=0. \tag{5.3}$$

When $s_1=0$, one must have $s_0\neq 0$ (by Lemma 3.1). Thus

$$0=\frac{s_1}{s_0}=-\sum_{i=1}^{n}\frac{1}{d_i}, \tag{5.4}$$

i.e.

$$\sum_{i=1}^{n}\frac{1}{d_i}=0. \tag{5.5}$$

On the other hand, if (5.5) holds, then one must have

$$d_i\neq 0, \quad 1\leqslant i\leqslant n. \tag{5.6}$$

So

$$s_1=-s_0\sum_{i=1}^{n}\frac{1}{d_i}=0. \tag{5.7}$$

Thus

$$s_1=0 \Leftrightarrow \sum_{i=1}^{n}\frac{1}{d_i}=0, \tag{5.8}$$

which completes the proof. □

Corollary 5.1. *$\tilde{D}_{1,h,d_1,\cdots,d_n}$ is trivial if $d_1,d_2,\cdots,d_n$ are consecutive integers.*

Proof. If $0\in\{d_1,\cdots,d_n\}$, then by Proposition 5.1, $\tilde{D}_{1,h,d_1,\cdots,d_n}$ is trivial.

If $0\notin\{d_1,\cdots,d_n\}$, then all the d_is must have the same sign, since they are consecutive integers. Thus

$$\sum_{i=1}^{n}\frac{1}{d_i}\neq 0. \tag{5.9}$$

And $\tilde{D}_{1,h,d_1,\cdots,d_n}$ is trivial, again by Proposition 5.1. □

Corollary 5.1 is helpful for the current discussion.

By Corollary 5.1, together with Theorem 2.2, it immediately follows that the schemes

$$\tilde{D}_{1,h,d_k,\cdots,d_{k+q-2}} \quad (2 \leqslant k \leqslant n-q+1) \tag{5.10}$$

are trivial (under the assumption of uniform mesh, the d_is can be taken as consecutive integers), and the optimized scheme on the wide stencil can always be expressed as a linear combination of schemes on WENO-like sub-stencils. Particularly, the 5th order WENO scheme [15] and the MDCD WENO scheme [24] can be considered as examples of Theorem 2.2.

5.1.2 Construct high order accurate schemes gradually

On the other hand, for the special case $n=q+1$ in Theorem 2.2, we have

Corollary 5.2. *There exist* $\lambda,\mu \in \mathbb{R}^*$ *such that*

$$\lambda \tilde{D}_{1,h,d_1,\cdots,d_q} + \mu \tilde{D}_{1,h,d_2,\cdots,d_{q+1}} = \tilde{D}_{1,h,d_1,\cdots,d_{q+1}} \tag{5.11}$$

if $d_1,d_2,\cdots,d_{q+1}$ *are consecutive integers.*

Proof. From Corollary 5.1,

$$\tilde{D}_{1,h,d_2,\cdots,d_q} \tag{5.12}$$

is trivial. Then by Theorem 2.2,

$$\operatorname{span}\left\{\tilde{D}_{1,h,d_1,\cdots,d_q}, \tilde{D}_{1,h,d_2,\cdots,d_{q+1}}\right\} \supseteq C_{h,1,q,d_1,\cdots,d_{q+1}}. \tag{5.13}$$

On the other hand, by Definition 2.6,

$$h\tilde{D}_{1,h,d_1,\cdots,d_{q+1}} \in C_{h,1,q,d_1,\cdots,d_{q+1}}. \tag{5.14}$$

Thus $\exists \lambda_1,\lambda_2 \in \mathbb{R}$ such that

$$h\tilde{D}_{1,h,d_1,\cdots,d_{q+1}} = \lambda_1 \tilde{D}_{1,h,d_1,\cdots,d_q} + \lambda_2 \tilde{D}_{1,h,d_2,\cdots,d_{q+1}}. \tag{5.15}$$

Since $h>0$, (5.15) is equivalent to

$$\tilde{D}_{1,h,d_1,\cdots,d_{q+1}} = \frac{\lambda_1}{h} \tilde{D}_{1,h,d_1,\cdots,d_q} + \frac{\lambda_2}{h} \tilde{D}_{1,h,d_2,\cdots,d_{q+1}}. \tag{5.16}$$

Clearly $\lambda_{1,2} \neq 0$, since $\tilde{D}_{1,h,d_1,\cdots,d_q}$, $\tilde{D}_{1,h,d_2,\cdots,d_{q+1}}$, $\tilde{D}_{1,h,d_1,\cdots,d_{q+1}}$ are trivial.

Let $\lambda = \frac{\lambda_1}{h}$ and $\mu = \frac{\lambda_2}{h}$, the corollary follows. ☐

Corollary 5.2 means that when computing 1st derivative using uniform mesh, two nth order accurate linear schemes can build a $(n+1)$th order accurate linear scheme through linear combination. This can explain the strategy the TENO schemes [25, 26] applied to gradually construct high order accurate schemes, as well as the strategy of the WENO schemes proposed by Jiang and Shu [14] (use 3rd order accurate schemes to build 4th order accurate schemes, and then use 4th order accurate schemes to build 5th order accurate schemes).

The other side of Corollary 5.2 is that, despite the mainstream WENO schemes as well as the TENO schemes are constructed in such a manner that the sub-stencils should not go across the discontinuities, it is possible to construct schemes with sub-stencils going across discontinuities and maintain the essentially non-oscillatory property.

Consider the 5th order WENO scheme for example. It is easy to verify that

$$\tilde{D}_{1,h,-3,-2,-1,0,1}=\frac{1}{4}\tilde{D}_{1,h,-3,-2,-1,0}+\frac{3}{4}\tilde{D}_{1,h,-2,-1,0,1}, \tag{5.17a}$$

$$\tilde{D}_{1,h,-2,-1,0,1,2}=\frac{1}{2}\tilde{D}_{1,h,-2,-1,0,1}+\frac{1}{2}\tilde{D}_{1,h,-1,0,1,2}. \tag{5.17b}$$

From (5.17a) and (5.17b), it is clear that we can re-express $\tilde{D}_{1,h,-3,-2,-1,0}$ and $\tilde{D}_{1,h,-1,0,1,2}$ as

$$\tilde{D}_{1,h,-3,-2,-1,0}=4\tilde{D}_{1,h,-3,-2,-1,0,1}-3\tilde{D}_{1,h,-2,-1,0,1}, \tag{5.18a}$$

$$\tilde{D}_{1,h,-1,0,1,2}=2\tilde{D}_{1,h,-2,-1,0,1,2}-\tilde{D}_{1,h,-2,-1,0,1}. \tag{5.18b}$$

In the original WENO scheme, the final scheme for characteristic waves with positive eigenvalues can be written (in derivative form rather than flux form, to illustrate the basic idea) as

$$\Delta_{WENO}=\omega_1\tilde{D}_{1,h,-3,-2,-1,0}+\omega_2\tilde{D}_{1,h,-2,-1,0,1}+\omega_3\tilde{D}_{1,h,-1,0,1,2}, \tag{5.19}$$

where

$$\omega_i\in\mathbb{R}^+,\quad \sum_{i=1}^{3}\omega_i=1,\quad 1\leqslant i\leqslant 3. \tag{5.20}$$

Substituting (5.18a), (5.18b) into (5.19), one have

$$\Delta_{WENO}=4\omega_1\tilde{D}_{1,h,-3,-2,-1,0,1}+(\omega_2-3\omega_1-\omega_3)\tilde{D}_{1,h,-2,-1,0,1}+2\omega_3\tilde{D}_{1,h,-2,-1,0,1,2}. \tag{5.21}$$

When written in flux form, (5.21) becomes

$$f_{WENO}=4\omega_1 f_{1,h,-2,-1,0,1}+(\omega_2-3\omega_1-\omega_3)f_{1,h,-1,0,1}+2\omega_3 f_{1,h,-1,0,1,2}. \tag{5.22}$$

Note that in (5.22), all the fluxes occurs on the right hand side have subscripts $-1,0,1$. This implies that when a discontinuity occurs in the region $(-h,h)$, all the 3 numerical fluxes are calculated using sub-stencils *containing* the discontinuity. However, it is derived from the original WENO scheme and is theoretically equivalent to the original

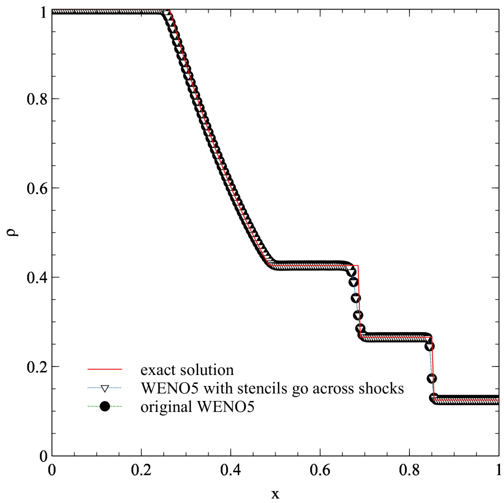

Figure 1: Sod shock tube problem, density calculated using the original WENO5 scheme and its equivalent form using stencils going across shocks simultaneously.

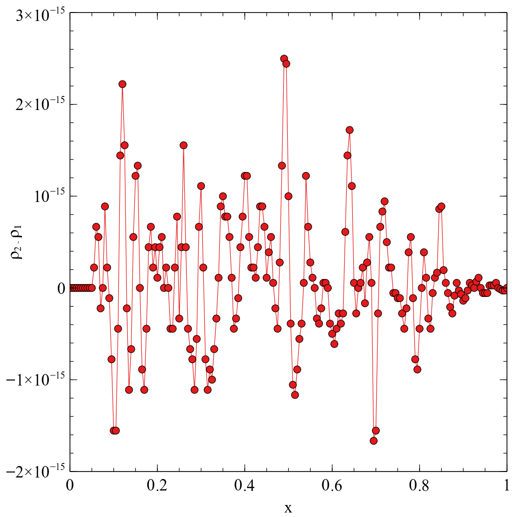

Figure 2: Absolute error of Sod problem, where ρ_1, ρ_2 represent density calculated using the original WENO5 scheme and its equivalent form respectively.

version, so the scheme given by (5.22) should maintain the essentially non-oscillatory property. When using double precision variables to carry out the calculation of Sod problem, the numerical solutions generated by the two equivalent schemes should have an absolute error around 1×10^{-15} at every discrete mesh point since this is the maximum precision that a double precision variable would allow. Numerical test on Sod problem also confirmed the fact (see Fig. 1 and Fig. 2).

5.1.3 Targeted ENO: composite utilization of both strategies

In Section 5.1.2, we mentioned the recently published TENO schemes. Here we discuss the TENO schemes in more detail. To illustrate the procedure and to reveal the general case, we picked the 8th order TENO [27]. Although in this paper the schemes are selected directly, in the following discussion we will see that these schemes *can* be expressed as linear combinations of the basis schemes.

5.1.3.1 Construct the highest order accurate schemes gradually

To construct the highest order accurate scheme on the wide stencil, we can apply the method mentioned in Section 5.1.2, i.e. increasing the order of accuracy gradually (see Fig. 3).

In Fig. 3, the upmost integers represent the omitted d_is of the circle nodes (which represent finite difference schemes) below them. By discussions in Section 5.1.2, a $(n+$

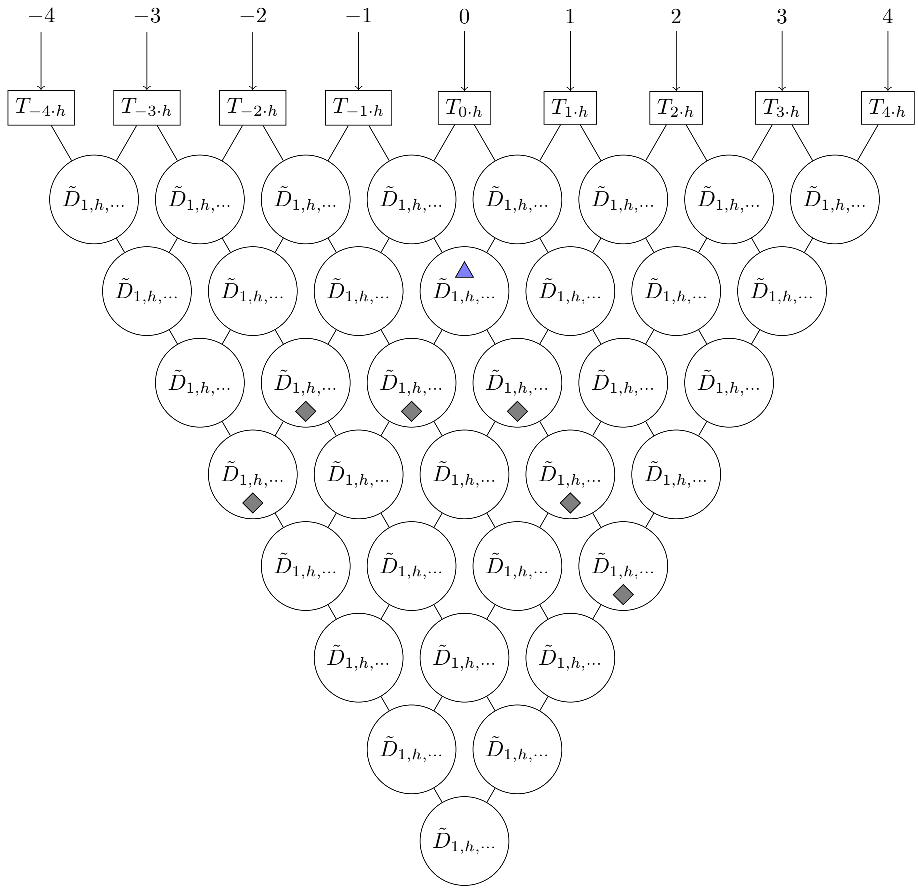

Figure 3: Construct high order accurate finite difference schemes gradually. The omitted subscripts can be determined by tracing the connections between nodes.

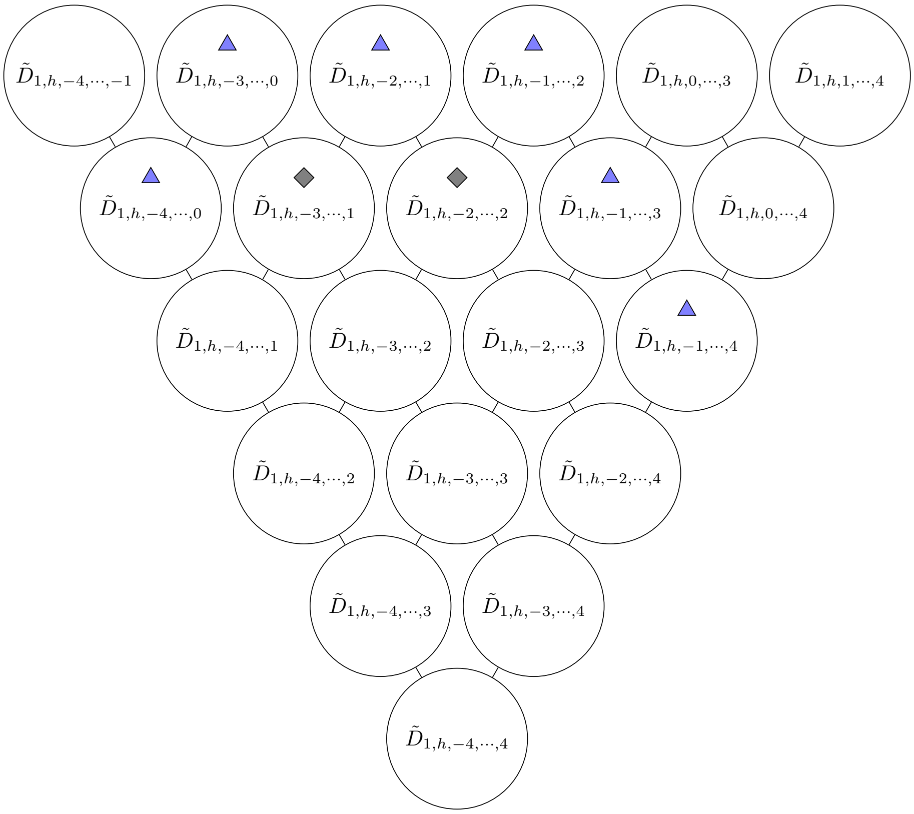

Figure 4: Construct the highest order accurate schemes in TENO8: step 1. Triangles: basis schemes. Diamonds: new schemes to construct.

1)th order accurate scheme can be expressed as a linear combination of two nth order accurate schemes if the mesh is uniform (i.e. the d_is are consecutive integers). Such relations are shown in the figure by drawing straight lines connecting the nodes, i.e. two neighbouring nodes from the same level are connected to a node in the next level. The rectangle nodes (which represent shift operators, T_{d_ih}) are connected to the integers with arrows, to represent the map $d_i \to T_{d_ih}$. Since the upmost circle nodes (i.e. the 1st order accurate schemes) are actually linear combinations of the upper rectangle nodes, the rectangle nodes are also connected to lower circle nodes with the same straight lines.

Because Fig. 3 contains many nodes, it is not easy to include all the subscripts of the schemes while keeping the whole figure at a proper width. However, we can determine the omitted subscripts by tracing the straight lines connecting the nodes. For example, in Fig. 3, the circle node marked with a triangle is $\tilde{D}_{1,h,-1,0,1}$. In Fig. 3, all the schemes used as TENO8 basis are marked with diamonds.

Now we describe the procedure to gradually construct high order accurate schemes.

For the first step (see Fig. 4), use the 3rd order accurate schemes

$$\tilde{D}_{1,h,-3,\cdots,0},\ \tilde{D}_{1,h,-2,\cdots,1},\ \tilde{D}_{1,h,-1,\cdots,2}$$

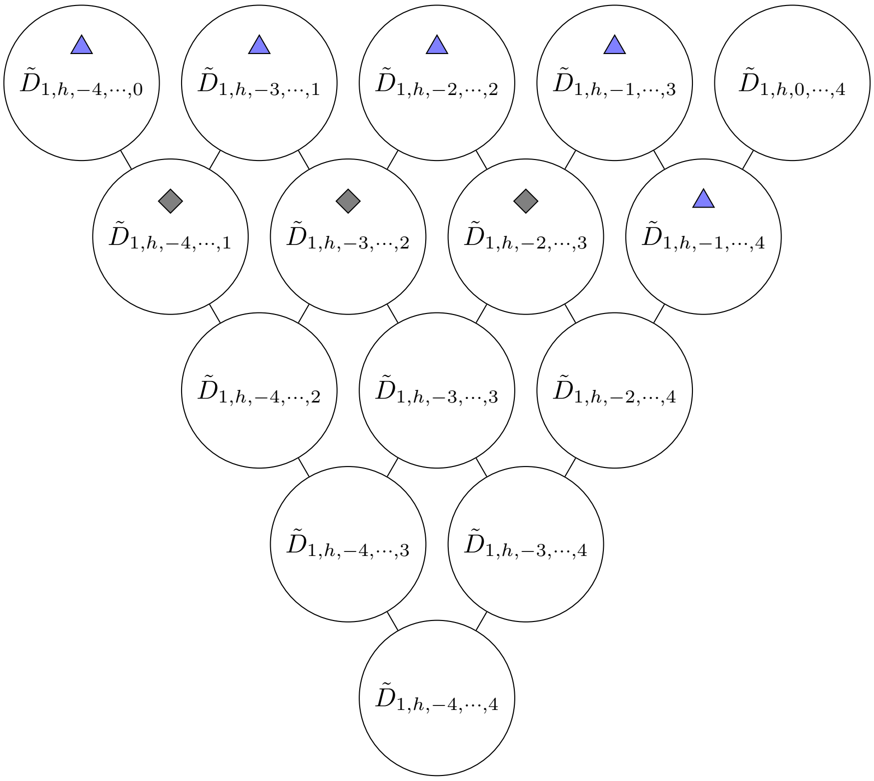

Figure 5: Construct the highest order accurate schemes in TENO8: step 2. Triangles: basis schemes. Diamonds: new schemes to construct.

to construct two 4th order accurate schemes, i.e.

$$\tilde{D}_{1,h,-3,\cdots,1},\ \tilde{D}_{1,h,-2,\cdots,2}.$$

For the second step (see Fig. 5), use the 4th order accurate schemes

$$\tilde{D}_{1,h,-4,\cdots,0},\ \tilde{D}_{1,h,-3,\cdots,1},\ \tilde{D}_{1,h,-2,\cdots,2},\ \tilde{D}_{1,h,-1,\cdots,3}$$

to construct three 5th order accurate schemes, i.e.

$$\tilde{D}_{1,h,-4,\cdots,1},\ \tilde{D}_{1,h,-3,\cdots,2},\ \tilde{D}_{1,h,-2,\cdots,3}.$$

For the third step (see Fig. 6), use the 5th order accurate schemes

$$\tilde{D}_{1,h,-4,\cdots,1},\ \tilde{D}_{1,h,-3,\cdots,2},\ \tilde{D}_{1,h,-2,\cdots,3},\ \tilde{D}_{1,h,-1,\cdots,4}$$

to construct three 6th order accurate schemes, i.e.

$$\tilde{D}_{1,h,-4,\cdots,2},\ \tilde{D}_{1,h,-3,\cdots,3},\ \tilde{D}_{1,h,-2,\cdots,4}.$$

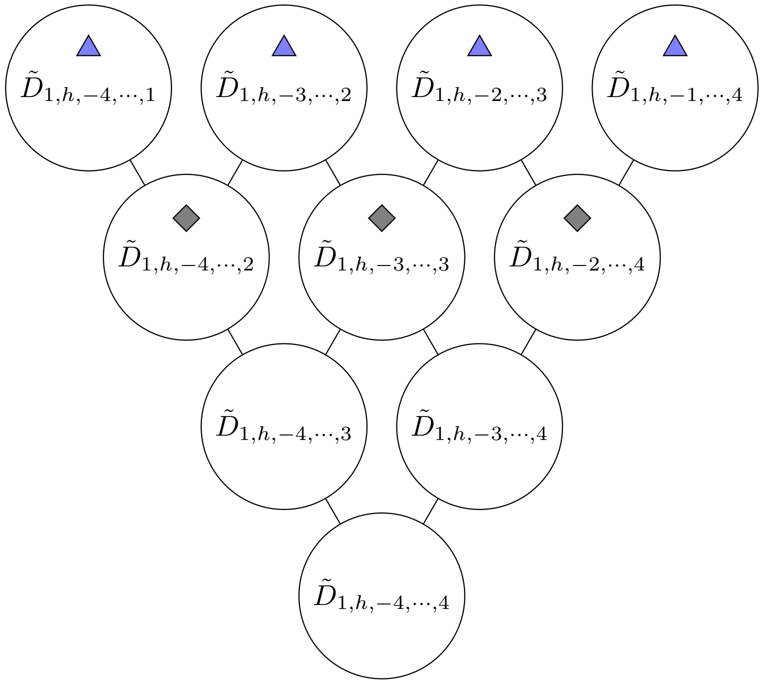

Figure 6: Construct the highest order accurate schemes in TENO8: step 3. Triangles: basis schemes. Diamonds: new schemes to construct.

For the fourth step (see Fig. 7), use the 6th order accurate schemes

$$\tilde{D}_{1,h,-4,\cdots,2},\ \tilde{D}_{1,h,-3,\cdots,3},\ \tilde{D}_{1,h,-2,\cdots,4}$$

to construct two 7th order accurate schemes, i.e.

$$\tilde{D}_{1,h,-4,\cdots,3},\ \tilde{D}_{1,h,-3,\cdots,4}.$$

For the fifth step (also the last step for current discussion, see Fig. 8), use the 7th order accurate schemes

$$\tilde{D}_{1,h,-4,\cdots,3},\ \tilde{D}_{1,h,-3,\cdots,4}$$

to construct the 8th order accurate scheme, i.e.

$$\tilde{D}_{1,h,-4,\cdots,4}.$$

Although in the published paper [27] there existed a lot of schemes (for TENO8, there were 16 such schemes in total) that were directly selected rather than constructed through the linear combination approach, by our discussion above, it is indeed feasible to express these schemes as linear combinations of the TENO8 basis schemes. All the selected schemes are marked with numbers in Fig. 9. For example, the scheme marked with 5 corresponds to $\hat{f}_{5,i+1/2}$ (see [27], pp. 731-732).

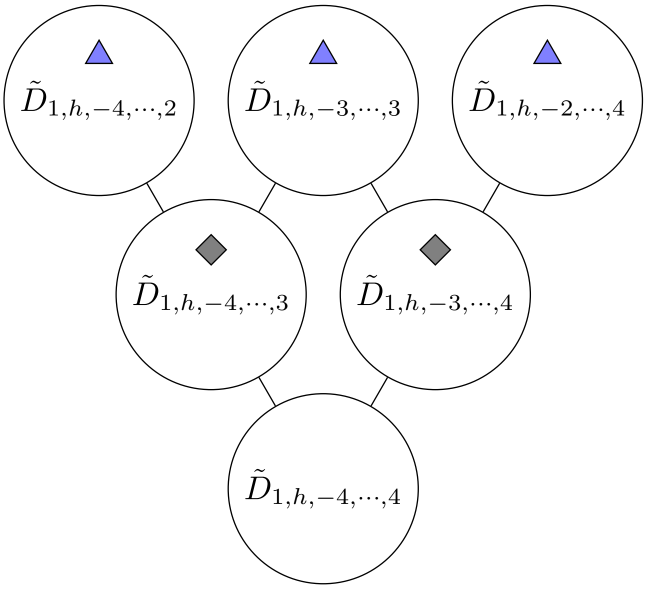

Figure 7: Construct the highest order accurate schemes in TENO8: step 4. Triangles: basis schemes. Diamonds: new schemes to construct.

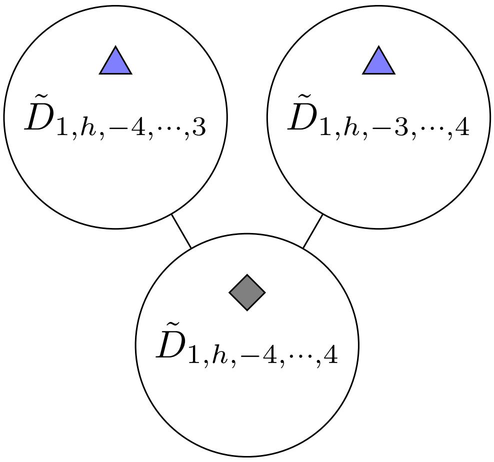

Figure 8: Construct the highest order accurate schemes in TENO8: step 5. Triangles: basis schemes. Diamond: new scheme to construct.

5.1.3.2 Construct optimized schemes directly

In the published work [27], the scheme applied to smooth regions was optimized to acquire better spectral properties. When using the 9-point stencil to evaluate the 1st derivative (or using a 8-point stencil to evaluate the numerical flux, equivalently), the highest order of accuracy is 8. The spectral optimized scheme applied on the wide stencil, however, dropped its order of accuracy to 6. Such a scheme cannot be expressed as a linear combination of two 7th order accurate schemes, but it is feasible to express

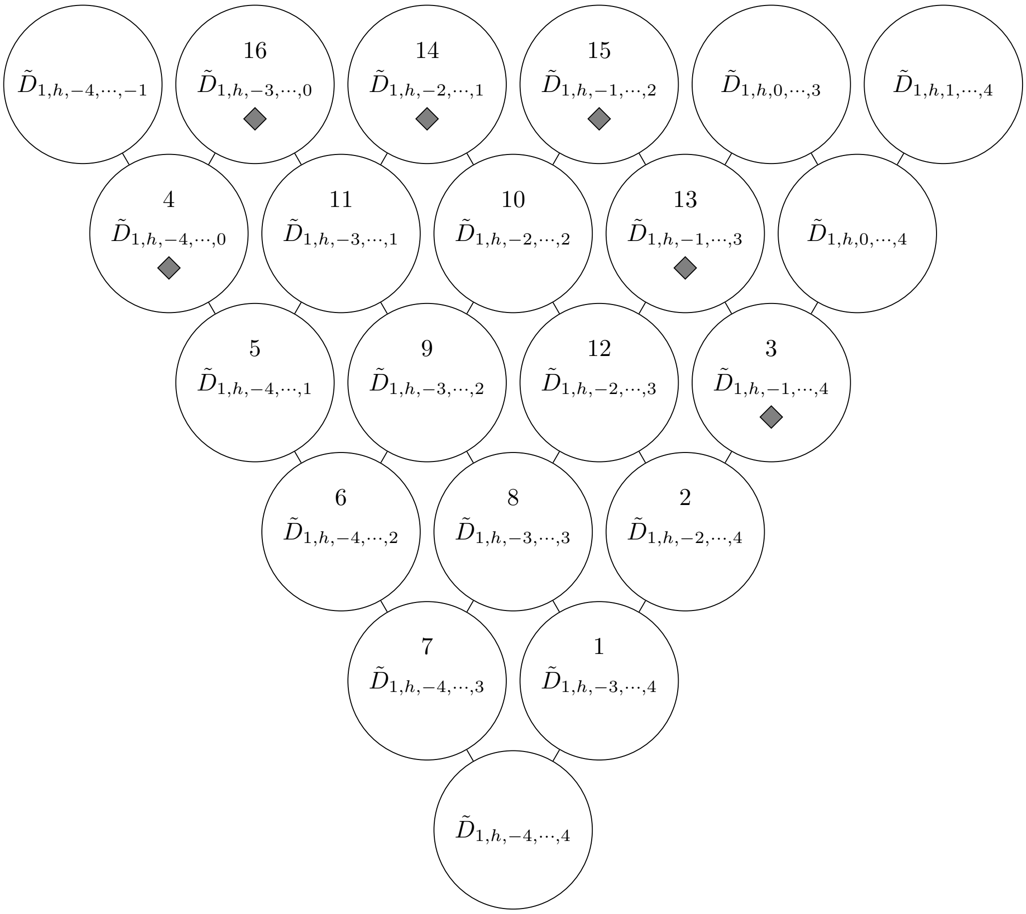

Figure 9: Correspondence between the current discussion and the published paper [27]. Schemes marked with diamonds are TENO8 basis schemes. Schemes marked with numbers are schemes that were directly selected. The numbers indicate the correspondence.

the scheme as a linear combination of three 6th order accurate schemes, i.e. $\tilde{D}_{1,h,-4,\cdots,2}$, $\tilde{D}_{1,h,-3,\cdots,3}$ and $\tilde{D}_{1,h,-2,\cdots,4}$. (see Fig. 10). The basis schemes we used here can be written as linear combinations of the TENO8 basis schemes (see Section 5.1.3.1), thus the optimized TENO8 scheme can also be written as a linear combination of the TENO8 basis schemes.

5.2 1st derivative and non-uniform meshes

There have been many works of finite difference WENO schemes based on uniform meshes. On the other hand, research on applying the WENO schemes to non-uniform meshes also exists: some of the published works were based on the finite volume framework [20, 21], while some others were based on the finite difference framework [22, 23]. Here we focus on the possibility to directly build high order accurate *finite difference* schemes on non-uniform meshes using WENO-like linear combination method.

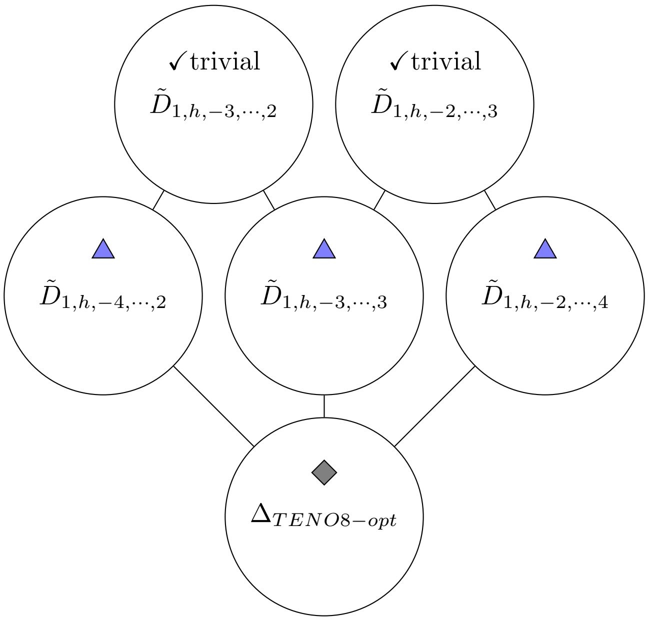

Figure 10: Construct spectral optimized TENO8 scheme. "✓trivial": schemes that need to be checked (see Theorem 2.2). Triangles: basis schemes for constructing the optimized TENO8 scheme. Diamond: the optimized TENO8 as a linear combination of basis schemes.

As a corollary of Proposition 5.1, for non-uniform meshes we have the following

Corollary 5.3. *$\tilde{D}_{1,h,d_1,\cdots,d_n}$ is trivial if $0 \in \{d_1,d_2,\cdots,d_n\}$.*

Proof. From Proposition 5.1, it immediately follows that when $\tilde{D}_{1,h,d_1,\cdots,d_n}$ is nontrivial, all the d_is must be non-zero. When $0 \in \{d_1,d_2,\cdots,d_n\}$, $\tilde{D}_{1,h,d_1,\cdots,d_n}$ must be trivial, or otherwise a contradiction would arise concerning whether the set $\{d_1,d_2,\cdots,d_n\}$ has 0 as one of its elements. □

Using Corollary 5.3 and Theorem 2.2, we have the following

Corollary 5.4. *Suppose*

$$S = \left\{ \tilde{D}_{1,h,d_1,\cdots,d_q}, \tilde{D}_{1,h,d_2,\cdots,d_{q+1}}, \cdots, \tilde{D}_{1,h,d_{n-q+1},\cdots,d_n} \right\}, \tag{5.23}$$

$n-q+1 \leqslant q$ and $0 \in \left\{ d_{n-q+1},\cdots,d_q \right\}$. Then $\mathrm{span} S \supseteq C_{h,1,q,d_1,\cdots,d_n}$.

Proof. Since $n-q+1 \leqslant q$, it follows that

$$\bigcap_{i=1}^{n-q} \{i+1,\cdots,i+j,\cdots,i+q-1\} = \{n-q+1,\cdots,q\}. \tag{5.24}$$

Since $0 \in \{d_{n-q+1},\cdots,d_q\}$, we have

$$0 \in \bigcap_{i=1}^{n-q} \{d_{i+1},\cdots,d_{i+j},\cdots,d_{i+q-1}\}. \tag{5.25}$$

By Corollary 5.3, $\tilde{D}_{1,h,d_{i+1},\cdots,d_{i+j},\cdots,d_{i+q-1}}$ is trivial ($1 \leqslant i \leqslant n-q$). Use Theorem 2.2 and the corollary follows. □

Note that in Corollary 5.4,

$$\bigcap_{i=1}^{n-q} \{i+1,\cdots,i+j,\cdots,i+q-1\} = \bigcap_{i=1}^{n-q+1} \{i,\cdots,i+j,\cdots,i+q-1\} = \{n-q+1,\cdots,q\}. \tag{5.26}$$

This implies that if the point at which the 1st derivative is evaluated occurs in all the sub-stencils, then it is feasible to construct high order accurate finite difference schemes from the sub-stencils using linear combination. Corollary 5.4 can also be used to explain the WENO5 scheme on uniform meshes, since all the sub-stencils contain the point at which the derivative is evaluated.

Furthermore, for the very same reason, the TENO schemes discussed in Section 5.1 can be extended directly to non-uniform meshes. The figures we used to illustrate the construction procedure only need to change the d_is in the subscripts. The only difference lies in the proposition we used to check the triviality of the schemes on our checklist: for uniform meshes we used Corollary 5.1 to insure the triviality, while for non-uniform meshes we used Proposition 5.3 to achieve the same goal.

5.3 2nd derivative and uniform meshes

When the linear combination method is extended to arbitrary positive-integer-order derivatives, the strategy will not always work. As it was shown in Theorem 2.2, there exist such linear combinations for all schemes whose order of accuracy is greater than a specified value if and only if some of the highest order finite difference schemes are trivial. If the condition is not satisfied, then there must exist a scheme which can not be expressed as a linear combination of the WENO-like sub-stencil schemes. When the linear combination does not exist, it is impossible to design WENO-like schemes via linear combinations.

As an example, consider the computation of 2nd derivatives on a uniform mesh with mesh size h. Thus the d_is in Theorem 2.2 are consecutive integers. We have the following

Proposition 5.2. For any positive integer k, $\tilde{D}_{2,h,-k,-k+1,\cdots,0,\cdots,k-1,k}$ is nontrivial.

Proof. Imitate the proof of Proposition 5.1. We have

$$\prod_{i=-k}^{k}(x-i) = x\prod_{i=1}^{k}(x-i)\prod_{i=1}^{k}(x+i) = x\prod_{i=1}^{k}(x^2-i^2) = xg(x^2), \tag{5.27}$$

where $g(x)$ is a polynomial of x. Thus

$$\prod_{i=-k}^{k}(x-i)=\sum_{i=0}^{k}s_{2i+1}x^{2i+1}. \tag{5.28}$$

By (4.6),

$$b_{2k+1}=-s_2=0. \tag{5.29}$$

And the proposition follows. □

Using Proposition 5.2, an example showing the non-existence of WENO-like linear combination can be constructed.

Recall that in Theorem 2.2, to make sure the linear combination exists, one must check a sequence of finite difference schemes to make sure that they are all trivial. Now Proposition 5.2 suggests a way to construct nontrivial schemes, thus we can use the proposition to make one of the schemes on our checklist nontrivial. In this way the existence of linear combination will be impossible for at least one high order accurate scheme.

For example, consider expressing the finite difference scheme $\tilde{D}_{2,h,-3,-2,-1,0,1,2,3}$ as linear combination of the following schemes:

$$\tilde{D}_{2,h,-3,-2,-1,0},\ \tilde{D}_{2,h,-2,-1,0,1},\ \tilde{D}_{2,h,-1,0,1,2},\ \tilde{D}_{2,h,0,1,2,3}.$$

By Theorem 2.2, such linear combination must exist if $\tilde{D}_{2,h,-2,-1,0},\tilde{D}_{2,h,-1,0,1},\tilde{D}_{2,h,0,1,2}$ are trivial. In fact, as Proposition 5.2 shows, $\tilde{D}_{2,h,-1,0,1}$ is nontrivial, and such linear combination does not exist. Similarly, when the sub-stencils contain 6 mesh points respectively, the scheme that needs to be checked is $\tilde{D}_{2,h,-2,-1,0,1,2}$, which is nontrivial by Proposition 5.2. Again, it is impossible to express $\tilde{D}_{2,h,-3,-2,-1,0,1,2,3}$ as linear combination of $\tilde{D}_{2,h,-3,-2,-1,0,1,2}$ and $\tilde{D}_{2,h,-2,-1,0,1,2,3}$.

When the basis schemes contain odd grid points, the schemes on our checklist contain even grid points. This time, it turns out that the schemes we need to check are always trivial:

Proposition 5.3. Let k be a positive integer. $\forall i\in\mathbb{Z}$, $\tilde{D}_{2,h,i,i+1,\cdots,i+2k-1}$ is trivial.

Proof. Let us consider the polynomial defined in Proposition 3.2. To prove that the scheme is trivial, all we have to do is to show that $s_2\neq 0$. If $i+2k-1<0$ or $i>0$, then

$$s_2=\prod_{j=i}^{i+2k-1}j\sum_{i\leqslant u<v\leqslant i+2k-1}\frac{1}{uv}\neq 0. \tag{5.30}$$

If $i\leqslant 0\leqslant i+2k-1$, we suppose $i=-n$. The inequalities imply $0\leqslant n\leqslant 2k-1$, so we have

$$\prod_{j=i}^{i+2k-1}(x-j)=x\prod_{j=1}^{n}(x+j)\prod_{j=1}^{2k-1-n}(x-j). \tag{5.31}$$

Therefore $\tilde{D}_{2,h,-n,-n+1,\cdots,2k-1-n}$ is trivial if and only if $\tilde{D}_{1,h,-n,\cdots,-1,1,\cdots,2k-1-n}$ is trivial. By Proposition 5.1, $\tilde{D}_{1,h,-n,\cdots,-1,1,\cdots,2k-1-n}$ is trivial if and only if

$$\sum_{j=1}^{n}\frac{1}{j}\neq\sum_{j=1}^{2k-1-n}\frac{1}{j}. \tag{5.32}$$

This is clearly true, since $n,k\in\mathbb{Z}$. □

Such phenomena was observed by Liu, Shu and Zhang [19]. In their paper, the possibility of expressing $\tilde{D}_{2,h,-2,-1,0,1,2}$ and $\tilde{D}_{2,h,-4,-3,-2,-1,0,1,2,3,4}$ as linear combinations of sub-stencils were also discussed. It turns out to be impossible to find the desired linear combination when the sub-stencils have even grid points. When the sub-stencils have odd grid points, the desired linear combination always exists. Proposition 5.2, Proposition 5.3 and Theorem 2.2 can explain the existence and non-existence of WENO-like linear combinations presented in the paper.

5.4 Numerical validation and visualization

5.4.1 An example for Theorem 2.1

To give an example for nontrivial highest order accurate scheme, we take advantage of Proposition 5.1 (see Section 5.1), so the scheme will be $\tilde{D}_{1,h,d_1,\cdots,d_n}$. To make the example as easy as possible, we further assume that $d_i\in\mathbb{Z}$, $1\leqslant i\leqslant n$. Since

$$\frac{1}{2}=\frac{1}{3}+\frac{1}{6}, \tag{5.33}$$

the scheme $\tilde{D}_{1,h,-2,3,6}$ can serve as an example for Theorem 2.1.

By Proposition 5.1, this scheme is nontrivial. By Theorem 2.1, this scheme is of 3rd order of accuracy. After a few calculations, we can know the specific expression of $\tilde{D}_{1,h,-2,3,6}$:

$$\tilde{D}_{1,h,-2,3,6}=\frac{1}{h}\left(-\frac{9}{40}T_{-2h}+\frac{4}{15}T_{3h}-\frac{1}{24}T_{6h}\right). \tag{5.34}$$

Now we use this scheme to compute derivatives of $\sin x$ at different locations. More specifically, we evaluate 1st derivative of $\sin x$ using the following formula:

$$\left.\frac{\mathrm{d}f}{\mathrm{d}x}\right|_{x=x_i}=\frac{1}{h}\left(-\frac{9}{40}f(x_{i-2})+\frac{4}{15}f(x_{i+3})-\frac{1}{24}f(x_{i+6})\right), \tag{5.35}$$

where

$$x_i=ih,\quad h=\frac{2\pi}{n},\quad 1\leqslant i\leqslant n,\quad n\in\mathbb{Z}^+, \tag{5.36}$$

i.e. we evaluate 1st derivative of $\sin x$ on interval $(0,2\pi]$ with a uniform mesh, which has n points equally spaced. The results are shown in Table 1, and they are highly consistent with the theoretical prediction.

Table 1: L_1 error, L_∞ error and their respective orders. Scheme: $\tilde{D}_{1,h,-2,3,6}$. Function: $\sin x$.

n	L_1	order	L_∞	order
10	1.85102572E-01	-	2.85999202E-01	-
20	2.78552314E-02	2.73230474	4.32722190E-02	2.72449811
40	3.64517074E-03	2.93389001	5.70951034E-03	2.92200218
80	4.60880882E-04	2.98352056	7.23430357E-04	2.98044098
160	5.77747420E-05	2.9958831	9.07360355E-05	2.99510661
320	7.22699576E-06	2.99897096	1.13516279E-05	2.99877643
640	9.03535566E-07	2.99974275	1.41925439E-06	2.99969409
1250	1.21275809E-07	2.99993449	1.90499389E-07	2.99991932
2500	1.51596533E-08	2.99998314	2.38127111E-08	2.99998258
5000	1.89496222E-09	2.99999577	2.97661652E-09	2.99998661
10000	2.36870610E-10	2.99999798	3.72114806E-10	2.99985367

5.4.2 An example for Theorem 2.2

Let us consider three schemes: $\tilde{D}_{1,h,-9,-1,x,y}$, $\tilde{D}_{1,h,-1,x,y,z}$, $\tilde{D}_{1,h,x,y,z,2}$. By Theorem 2.2,

$$span\{\tilde{D}_{1,h,-9,-1,x,y},\tilde{D}_{1,h,-1,x,y,z},\tilde{D}_{1,h,x,y,z,2}\}\supseteq C_{h,1,4,-9,-1,x,y,z,2} \tag{5.37}$$

if and only if $\tilde{D}_{1,h,-1,x,y}$ and $\tilde{D}_{1,h,x,y,z}$ are trivial. Suppose

$$\begin{cases} \tilde{D}_{1,h,-9,-1,x,y}=D+\frac{1}{4!}u_1h^3D^4+\frac{1}{5!}v_1h^4D^5+\cdots, \\ \tilde{D}_{1,h,-1,x,y,z}=D+\frac{1}{4!}u_2h^3D^4+\frac{1}{5!}v_2h^4D^5+\cdots, \\ \tilde{D}_{1,h,x,y,z,2}=D+\frac{1}{4!}u_3h^3D^4+\frac{1}{5!}v_3h^4D^5+\cdots. \end{cases} \tag{5.38}$$

Then (5.37) is equivalent to

$$\begin{vmatrix} 1 & 1 & 1 \\ u_1 & u_2 & u_3 \\ v_1 & v_2 & v_3 \end{vmatrix}\neq 0 \tag{5.39}$$

and by Proposition 3.2,

$$\tilde{D}_{1,h,-1,x,y} \text{ is trivial } \Leftrightarrow xy-x-y\neq 0, \tag{5.40}$$

$$\tilde{D}_{1,h,x,y,z} \text{ is trivial } \Leftrightarrow xy+yz+zx\neq 0. \tag{5.41}$$

So we compute the determinant in (5.39), as well as $xy-x-y$ and $xy+yz+zx$ which occurred in (5.40) and (5.41).

Let

$$\begin{cases} x=\dfrac{2\sqrt{3}\cos\theta+3\sqrt{2}\sin\theta}{6}x_1+\dfrac{\sqrt{6}}{6}z_1+\dfrac{\sqrt{2}}{2}, \\ y=\dfrac{2\sqrt{3}\cos\theta-3\sqrt{2}\sin\theta}{6}x_1+\dfrac{\sqrt{6}}{6}z_1-\dfrac{\sqrt{2}}{2}, \\ z=\dfrac{\sqrt{3}\cos\theta}{3}x_1-\dfrac{2\sqrt{6}}{6}z_1, \end{cases} \tag{5.42}$$

with (5.42), we have

(a) when $\theta=\arctan\sqrt{3}=\frac{\pi}{3}$, $xy+yz+zx=0$ represents an ellipse and $xy-x-y=0$ represents a hyperbola;

(b) when $\theta=\arctan\sqrt{2}$, $xy+yz+zx=0$ represents a parabola and $xy-x-y=0$ represents a hyperbola;

(c) when $\theta=\arctan\sqrt{1}=\frac{\pi}{4}$, $xy+yz+zx=0$ represents a hyperbola and $xy-x-y=0$ represents a hyperbola.

By Theorem 2.2, the contour plot of the determinant in (5.39) should have these curves as its zero contours. For all the cases mentioned above (i.e. $\theta=\arctan\sqrt{3},\arctan\sqrt{2},\arctan\sqrt{1}$), numerical tests give results consistent with theoretical predictions (see Fig. 11, Fig. 12, Fig. 13).

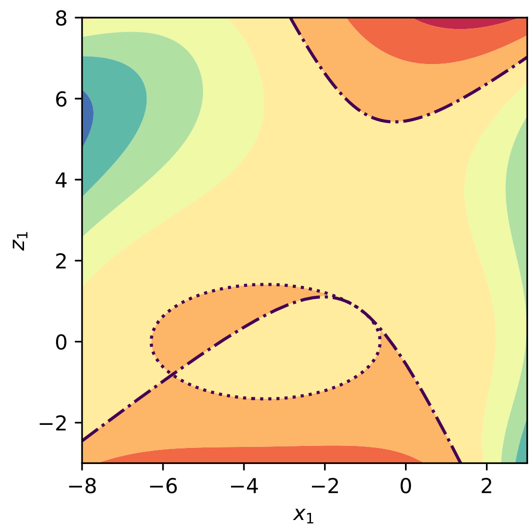

Figure 11: Contour plot of the determinant in (5.39), with $\theta=\arctan\sqrt{3}$. Dash dot line: parameters that make $\tilde{D}_{1,h,-1,x,y}$ nontrivial. Dotted line: parameters that make $\tilde{D}_{1,h,x,y,z}$ nontrivial.

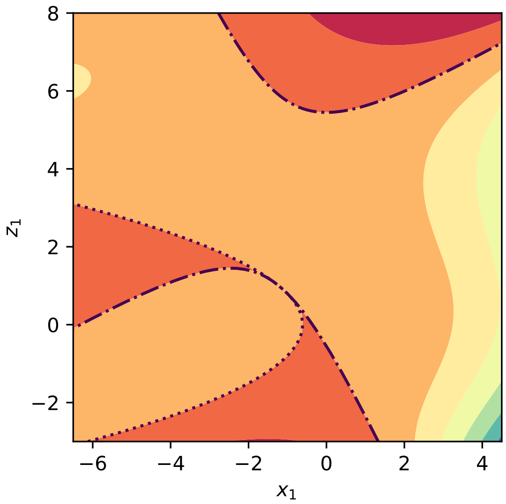

Figure 12: Contour plot of the determinant in (5.39), with $\theta = \arctan\sqrt{2}$. Dash dot line: parameters that make $\tilde{D}_{1,h,-1,x,y}$ nontrivial. Dotted line: parameters that make $\tilde{D}_{1,h,x,y,z}$ nontrivial.

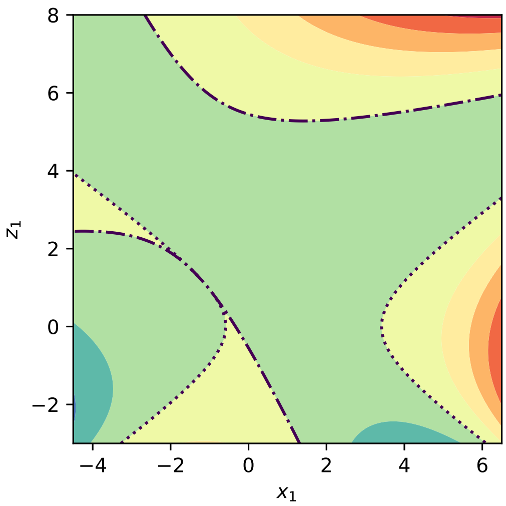

Figure 13: Contour plot of the determinant in (5.39) with $\theta = \arctan\sqrt{1}$. Dash dot line: parameters that make $\tilde{D}_{1,h,-1,x,y}$ nontrivial. Dotted line: parameters that make $\tilde{D}_{1,h,x,y,z}$ nontrivial.

6 Conclusions

The paper focused on the possibility to express finite difference schemes using the WENO-like linear combination method, with two prerequisites: (i) positive-integer-order derivatives and (ii) finite difference framework. The mesh can be uniform or non-uniform. A theorem on the order of accuracy of finite difference schemes is proved, and a sufficient and necessary condition for the existence of WENO-like linear combination is proved. After the proofs of the theorems, we discussed the linear combination method in three different application scenarios, i.e. 1st derivative and uniform meshes, 1st derivative and non-uniform meshes, and 2nd derivative and uniform meshes.

For 1st derivative and uniform meshes, the linear combination strategy will always work. Two different strategies were discussed with these preconditions, i.e. constructing target schemes directly, and constructing target schemes gradually. The spectral optimized WENO schemes (e.g. the MDCD WENO scheme) can be considered as examples of the first strategy, and the original WENO scheme (which uses the highest order accurate scheme in smooth regions) can be considered as an example of the second strategy. The spectral optimized TENO schemes can be considered as examples of composite utilization of both. Although in some published work [27] the target schemes were selected directly, by our discussion, it is indeed feasible to construct these target schemes through the linear combination approach.

Moreover, despite the mainstream WENO schemes (as well as the TENO schemes) are designed in such a manner that sub-stencils should not go across discontinuities, it is indeed possible to construct a finite difference scheme with all sub-stencils going across discontinuities and maintaining the essentially non-oscillatory property unchanged.

For 1st derivative and non-uniform meshes, as long as all the sub-stencils contain the point at which the derivative is evaluated, the WENO-like linear combination method will always work. This conclusion can also explain the existence of WENO-like linear combination for the case of 1st derivative and uniform meshes. Furthermore, the feasibility of constructing TENO schemes on non-uniform meshes was also revealed.

For 2nd derivative and uniform meshes, when the sub-stencils have even grid points, the WENO-like linear combination may not exist. When the sub-stencils have odd grid points, the WENO-like linear combination always exists. Or equivalently, when evaluating numerical fluxes, sub-stencils which contain odd grid points may lead to non-existence of WENO-like linear combination, while sub-stencils which contain even grid points will make sure the WENO-like linear combinations exist. Such phenomena was observed in previous work [19] and can be explained using Theorem 2.2.

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