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Abstract

In this paper we enhance the well-known fifth order WENO shock-capturing scheme by using deep learning techniques. This fine-tuning of an existing algorithm is implemented by training a rather small neural network to modify the smoothness indicators of the WENO scheme in order to improve the numerical results especially at discontinuities. In our approach no further post-processing is needed to ensure the consistency of the method. Moreover, the formal order of accuracy of the resulting scheme can be proven.

We demonstrate our findings with the inviscid Burgers' equation, the Buckley-Leverett equation and the 1-D Euler equations of gas dynamics. Hereby we investigate the classical Sod problem and the Lax problem and show that our novel method outperforms the classical fifth order WENO schemes in simulations where the numerical solution is too diffusive or tends to overshoot at shocks. Finally, the straight-forward extension of the method to two-dimensional problems is included and illustrated using the 2D Burgers' equation.

Keywords: Weighted essentially non-oscillatory method, Hyperbolic conservation laws, Smoothness indicators, Deep Learning, Neural Networks 2000 MSC: 65M06, 68T07, 76L05

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1 1. Introduction

Typically, numerical fluid mechanics deals with nonlinear hyperbolic partial differential equations (PDEs). In its simplest one-dimensional form, these equations can be represented as

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0, \qquad t > 0, \tag{1}$$

where x represents space, t denotes time, u(x,t) is conserved quantity and 5 f(u(x,t)) is its flux. It is well-known that discontinuities may develop after 6 a finite time regardless of the smoothness of the initial or boundary data. 7 Hence, suitable numerical methods must be designed for these problems, es-8 pecially to approximate discontinuous solutions. First in 1980, Crandall and 9 Majda [1] proposed the class of *monotone schemes* that are nonlinearly sta-10 ble in the L_1 norm and satisfy certain entropy conditions. It can be proven 11 that the corresponding solutions converge to bounded variation entropy so-12 lutions including error estimates. However, these schemes are only first order 13 accurate and by the fundamental Godunov theorem [2] it is known that one 14 has to consider nonlinear non-oscillatory schemes to overcome this accuracy 15 barrier. 16

In this direction so-called *shock-capturing schemes* were developed that 17 were able to resolve sharply a shock or a steep gradient region without intro-18 ducing too much diffusion or overshoot behaviour [3]. Additionally, to remedy 19 the above mentioned drawback, at regions with smooth flow these schemes 20 exhibit a rather high order of convergence. The well-known representative of 21 this class of methods are the essentially non-oscillatory (ENO) schemes [4] 22 with high order accuracy in smooth regions and sharply resolving shocks in 23 an essentially non-oscillatory way using a smoothness indicator function, see 24 e.g. [5]. Later on Jiang and Shu [6] further improved these schemes and pro-25 posed a weighted ENO (in the sequel abbreviated with WENO-JS) scheme, 26 that is still regarded as a state-of-the-art solution approach. 27

In order to achieve higher order accuracy for WENO schemes, the sten-28 cil for the spatial reconstruction needs to be enlarged and to keep it in a 29 compact size Qiu and Shu [7, 8] developed the Hermite WENO (HWENO) 30 schemes. In order to further increase the efficiency, Pirozzoli [9] developed 31 a hybrid compact-WENO scheme using up-wind schemes in the smooth re-32 gions. Alternatively, Hill and Pullin [10] designed another hybrid WENO 33 scheme, combining special centered difference schemes with WENO methods, 34 cf. [11, 12] for most recent approaches. 35

Subsequently, different new strategies were developed by modifying the 36 WENO-JS schemes, i.e. by altering by smoothness indicators [13, 14, 15, 16, 37 17, 18] or by modifying the nonlinear weights [19]. Besides, another goal in 38 optimizing these schemes was to minimize the dispersion error (dispersion-39 relation-preserving (DRP) schemes) [20, 21], also combined with the WENO 40 approach leading to optimized WENO (OWENO) schemes [22]. Since clas-41 sical WENO methods are too dissipative for direct numerical simulations 42 (DNS) of turbulence, a goal was to reduce the dissipation by including an 43 automatic dissipation adjustment [23]. In 2016 Fu, Hu and Adams [24] pro-44 posed a family of high-order targeted ENO (TENO) schemes that are par-45 ticularly suitable for DNS. These methods reduce the numerical dissipation 46 by an ENO-like stencil selection and increase the numerical robustness by 47 assembling a set of low-order candidate stencils with increasing width, see 48 also the extensions in [25, 26]. For a detailed review on WENO schemes we 40 refer to [27]. 50

Recently, machine learning was widely used to compute the solution of 51 PDEs. We refer to [28, 29, 30], where the neural network algorithm is used 52 to approximate a solution of a particular PDE problem. Following that 53 approach, the solution of a particular PDE is a result of a neural network 54 training procedure. Another idea is to improve a specific numerical scheme 55 using neural networks. The training of a neural network is made offline and 56 results in a new numerical scheme applicable to a wider class of problems. 57 This idea was recently used by Beck et al. [31] for discontinuous Galerkin 58 methods or in [32] for learning iterative PDE solvers and we also follow this 59 approach. Bar-Sinai et al. [33] use neural networks and learn from high 60 resolution solutions to approximate a spatial derivative on a coarse grid. We 61 refer the reader also to [34, 35, 36] for other work in this direction. 62

In [37] deep reinforcement learning is applied to design a new numerical 63 scheme to solve hyperbolic conservation laws. Authors apply their method for 64 solving of the Burgers' equation and compare their results with the standard 65 WENO scheme. The recent work of Stevens and Colonius [38] introduces 66 new WENO-NN scheme based on neural network algorithm. In their work, 67 the finite-volume coefficients of the WENO-JS scheme are perturbed, while 68 maintaining the original smoothness indicators and nonlinear weights. How-69 ever, the resulting scheme presented in their paper has only first order of 70 accuracy. Another neural network based WENO scheme was developed by 71 Liu and Wen [39], where the new smoothness indicators are an output of the 72 neural network algorithm. However, in this case the formal order of accu-73

racy of the reconstruction of the resulting method can neither be analytically
proven, nor guaranteed. For a detailed discussion on the formal order of accuracy (in contrast to the term "convergence") for WENO methods, see e.g.
[40, 41].

We implement in our work another WENO extension based on deep learn-78 ing. This approach is used to improve the classic WENO-JS and WENO-Z 79 [13] scheme in this paper, but could be efficiently applied also to other WENO 80 methods. For this purpose we will train a rather small neural network to 81 perturb the smoothness indicator functions of the WENO-JS scheme. As 82 we do not develop any new smoothness indicators as in [39], but only their 83 multiplicative perturbations, we are able to prove the formal order of accu-84 racy of the resulting scheme. We call this new scheme WENO-DS (Deep 85 Smoothness), as we modify the smoothness indicators using deep neural net-86 works. This scheme has less diffusion and less overshoot in shocks than the 87 WENO-JS and the WENO-Z scheme, while maintaining high order accuracy 88 in smooth regions. 89

Finally, let us note that the use of WENO methods is not limited to 90 hyperbolic PDEs, see e.g. [42] for an application to parabolic PDEs in finance. 91 The paper is structured as follows. In Section 2 we introduce the WENO-92 JS and WENO-Z schemes under consideration in detail. Next, in Section 3 93 we introduce our deep learning approach, where neural networks are used to 94 further improve WENO methods without any post-processing. The corres-95 ponding proofs of the formal order of accuracy for two WENO schemes are 96 given in Section 4. Then we present our numerical results in Section 5, which 97 illustrate the improvements of our proposed method. Finally, we conclude 98 our work in Section 6. 99

100 2. The WENO Scheme

Let $\{I_i\}$ be the partition of a spatial domain with the *i*-th cell $I_i = [x_{i-\frac{1}{2}}, x_{i+\frac{1}{2}}]$. We consider a uniform grid defined by the points $x_i = x_0 + i\Delta x$, $i = 0, \ldots, N$, which are the centers of the cells with cell boundaries defined by $x_{i+\frac{1}{2}} = x_i + \frac{\Delta x}{2}$. The value of a function f at x_i is indicated by $f_i = f(x_i)$. The spatial discretization of one-dimensional conservation laws (1) yields a system of ordinary differential equations (ODEs) and the resulting semidiscrete scheme is $du_i = 1$ ($\hat{x}_i = \hat{x}_i$)

$$\frac{du_i}{dt} = -\frac{1}{\Delta x} \left(\hat{f}_{i+\frac{1}{2}} - \hat{f}_{i-\frac{1}{2}} \right), \tag{2}$$

where \hat{f} is a numerical approximation of the flux function f. Following [6], if we define a function h implicitly by

$$f(u(x)) = \frac{1}{\Delta x} \int_{x-\frac{\Delta x}{2}}^{x+\frac{\Delta x}{2}} h(\xi) d\xi, \qquad (3)$$

 $_{110}$ then (2) is approximated by

$$f'(u(x_i)) = \frac{1}{\Delta x} \left(h_{i+\frac{1}{2}} - h_{i-\frac{1}{2}} \right), \qquad h_{i\pm\frac{1}{2}} = h(x_{i\pm\frac{1}{2}}), \tag{4}$$

where $h_{i\pm\frac{1}{2}}$ approximates the numerical flux $\hat{f}_{\pm\frac{1}{2}}$ with fifth order of accuracy

$$\hat{f}_{i\pm\frac{1}{2}} = h_{i\pm\frac{1}{2}} + O(\Delta x^5).$$
(5)

¹¹² Further, the *flux splitting method* is applied, thus we write

$$f(u) = f^+(u) + f^-(u)$$
, where $\frac{df^+(u)}{du} \ge 0$ and $\frac{df^-(u)}{du} \le 0$. (6)

¹¹³ The numerical flux $\hat{f}_{i\pm\frac{1}{2}}$ is then represented by $\hat{f}_{i\pm\frac{1}{2}} = \hat{f}^+_{i\pm\frac{1}{2}} + \hat{f}^-_{i\pm\frac{1}{2}}$ and the ¹¹⁴ final scheme is formed as

$$\frac{du_i}{dt} = -\frac{1}{\Delta x} \left[\left(\hat{f}^+_{i+\frac{1}{2}} - \hat{f}^+_{i-\frac{1}{2}} \right) + \left(\hat{f}^-_{i+\frac{1}{2}} - \hat{f}^-_{i-\frac{1}{2}} \right) \right].$$
(7)

¹¹⁵ Next, only the construction of $\hat{f}_{i\pm\frac{1}{2}}^+$ is considered. The negative part can be ¹¹⁶ then obtained using symmetry (see e.g. [43]).

117 2.1. Fifth order WENO scheme

For a construction of $\hat{f}_{i+\frac{1}{2}}$, the fifth order WENO method uses a 5-point stencil

$$S(i) = \{x_{i-2}, \dots, x_{i+2}\}$$
(8)

¹²⁰ divided into three candidate substencils, which are given by

$$S^{m}(i) = \{x_{i+m-2}, x_{i+m-1}, x_{i+m}\}, \quad m = 0, 1, 2.$$
(9)

¹²¹ To form the numerical flux over the entire 5-point stencil, the numerical flux ¹²² for each of these substencils $\hat{f}_{i+\frac{1}{2}}^m = h_{i+\frac{1}{2}} + O(\Delta x^3)$ is calculated. These fluxes ¹²³ are then averaged in such a way, that fifth order accuracy is ensured in the smooth regions. In regions with discontinuities, the weights should partly
remove the contribution of these stencils so that the solution near the shock
can be approximated in more stable manner.

Let $\hat{f}^m(x)$ be the polynomial approximation of h(x) on each of the substencils (9). Then, evaluated at $i + \frac{1}{2}$ we obtain

$$\hat{f}^m(x_{i+\frac{1}{2}}) = \hat{f}^m_{i+\frac{1}{2}} = \sum_{j=0}^2 c_{m,j} f_{i+m-2+j}, \quad i = 0, \dots, N,$$
 (10)

where $c_{m,j}$ are the Lagrangian interpolation coefficients, dependent on m (see 130 [6]). They take an explicit form

$$\hat{f}_{i+\frac{1}{2}}^{0} = \frac{2f_{i-2} - 7f_{i-1} + 11f_{i}}{6},$$

$$\hat{f}_{i+\frac{1}{2}}^{1} = \frac{-f_{i-1} + 5f_{i} + 2f_{i+1}}{6},$$

$$\hat{f}_{i+\frac{1}{2}}^{2} = \frac{2f_{i} + 5f_{i+1} - f_{i+2}}{6},$$
(11)

¹³¹ and the numerical fluxes $\hat{f}_{i-\frac{1}{2}}^m$ can be obtained by shifting each index by -1. ¹³² Using the Taylor series expansion it can be shown that:

$$\begin{split} \hat{f}_{i\pm\frac{1}{2}}^{0} &= h_{i\pm\frac{1}{2}} - \frac{1}{4} f_{xxx}(0) \Delta x^{3} + O(\Delta x^{4}), \\ \hat{f}_{i\pm\frac{1}{2}}^{1} &= h_{i\pm\frac{1}{2}} + \frac{1}{12} f_{xxx}(0) \Delta x^{3} + O(\Delta x^{4}), \\ \hat{f}_{i\pm\frac{1}{2}}^{2} &= h_{i\pm\frac{1}{2}} - \frac{1}{12} f_{xxx}(0) \Delta x^{3} + O(\Delta x^{4}), \end{split}$$
(12)

where we used the short notation for the derivatives $f_x = f'(u)u_x$, etc.. Doing so, we obtain the general form of these expressions

$$\hat{f}_{i\pm\frac{1}{2}}^{m} = h_{i\pm\frac{1}{2}} + A_m \Delta x^3 + O(\Delta x^4), \tag{13}$$

¹³⁵ with A_m being independent of Δx .

Then, the convex combination of the interpolated values $\hat{f}_{i\pm\frac{1}{2}}^m$ given by

$$\hat{f}_{i\pm\frac{1}{2}} = \sum_{j=0}^{2} \omega_m \, \hat{f}^m_{i\pm\frac{1}{2}} \tag{14}$$

¹³⁷ yields the WENO approximation of the value $h_{i\pm\frac{1}{2}}$, where ω_m are the non-¹³⁸ linear weights defined as, cf. [6]

$$\omega_m^{JS} = \frac{\alpha_m^{JS}}{\sum_{i=0}^2 \alpha_i^{JS}}, \quad \text{where} \quad \alpha_m^{JS} = \frac{d_m}{(\epsilon + \beta_m)^2}. \tag{15}$$

The scheme using these nonlinear weights is denoted as the WENO-JS scheme. The parameter ϵ guarantees that the denominator does not become zero, and the coefficients d_0 , d_1 and d_2 are called ideal weights, which would form the upstream fifth order central scheme for the 5-point stencil and satisfy (5). Their values are:

$$d_0 = \frac{1}{10}, \quad d_1 = \frac{6}{10}, \quad d_2 = \frac{3}{10}.$$
 (16)

The parameter β_m is called the *smoothness indicator* and is analyzed in the next section.

146 2.2. Smoothness Indicators

The role of smoothness indicators is to measure the regularity of the polynomial approximation $\hat{f}^m(x)$ in each of three substencils. As developed in [6], they are defined as:

$$\beta_m = \sum_{q=1}^2 \Delta x^{2q-1} \int_{x_{i-\frac{1}{2}}}^{x_{i+\frac{1}{2}}} \left(\frac{d^q \hat{f}^m(x)}{dx^q}\right)^2 dx.$$
(17)

¹⁵⁰ Corresponding to the flux approximation $\hat{f}_{i+\frac{1}{2}}$ they take an explicit form

$$\beta_{0} = \frac{13}{12} (f_{i-2} - 2f_{i-1} + f_{i})^{2} + \frac{1}{4} (f_{i-2} - 4f_{i-1} + 3f_{i})^{2},$$

$$\beta_{1} = \frac{13}{12} (f_{i-1} - 2f_{i} + f_{i+1})^{2} + \frac{1}{4} (-f_{i-1} + f_{i+1})^{2},$$

$$\beta_{2} = \frac{13}{12} (f_{i} - 2f_{i+1} + f_{i+2})^{2} + \frac{1}{4} (3f_{i} - 4f_{i+1} + f_{i+2})^{2},$$

(18)

¹⁵¹ and their Taylor expansions at x_i are:

$$\beta_{0} = f_{x}^{2} \Delta x^{2} + \left(\frac{13}{12}f_{xx}^{2} - \frac{2}{3}f_{x}f_{xxx}\right)\Delta x^{4} \\ + \left(-\frac{13}{6}f_{xx}f_{xxx} + \frac{1}{2}f_{x}f_{xxxx}\right)\Delta x^{5} + O(\Delta x^{6}), \\ \beta_{1} = f_{x}^{2}\Delta x^{2} + \left(\frac{13}{12}f_{xx}^{2} + \frac{1}{3}f_{x}f_{xxx}\right)\Delta x^{4} + O(\Delta x^{6}),$$
(19)
$$\beta_{2} = f_{x}^{2}\Delta x^{2} + \left(\frac{13}{12}f_{xx}^{2} - \frac{2}{3}f_{x}f_{xxx}\right)\Delta x^{4} \\ + \left(\frac{13}{6}f_{xx}f_{xxx} - \frac{1}{2}f_{x}f_{xxxx}\right)\Delta x^{5} + O(\Delta x^{6}).$$

These indicators are designed to come closer to zero for smooth parts of the solution so that the nonlinear weights ω_m come closer to the ideal weights d_m . In the case that the stencil S^m contains a discontinuity, β_m is O(1) and the corresponding weight ω_m becomes smaller, therefore the contribution of the substencil S^m is reduced.

Following the work of Henrick, Aslam and Powers [19], it can be shown that demanding (5) we obtain the sufficient conditions for the fifth order accuracy:

$$\sum_{m=0}^{2} (\omega_m^{\pm} - d_m) = O(\Delta x^6), \tag{20}$$

$$\omega_m^{\pm} - d_m = O(\Delta x^3). \tag{21}$$

Considering the overall finite difference formula

$$\hat{f}_{j+\frac{1}{2}} - \hat{f}_{j-\frac{1}{2}} = f'(x)\Delta x + O(\Delta x^6),$$

it can be shown, that (21) may be relaxed and we obtain the following sufficient and necessary conditions:

$$\sum_{m=0}^{2} (\omega_m^{\pm} - d_m) = O(\Delta x^6), \qquad (22)$$

$$\sum_{m=0}^{2} A_m (\omega_m^+ - \omega_m^-) = O(\Delta x^3),$$
(23)

$$\omega_m^{\pm} - d_m = O(\Delta x^2). \tag{24}$$

Note that due to the normalization (15), the first condition (22) (resp. (20)) is always fulfilled. The superscripts \pm on ω_m specify their use in $\hat{f}_{i+\frac{1}{2}}$ or $\hat{f}_{i-\frac{1}{2}}$. The analysis of the formal order of accuracy was performed in [6] and it was shown that if

$$\beta_m = D\left(1 + O(\Delta x^2)\right),\tag{25}$$

with D being a non-zero constant independent of m, the condition (24) is satisfied and the scheme has the expected fifth order accuracy. However, it was shown in [19] that at the critical points where the first derivative of fvanishes, the order of accuracy of the scheme from [6] decreases to the third order. Moreover, if the second derivative also vanishes, the accuracy order is further reduced to the second order. For a further explanation of this problem we refer the interested reader to [19].

168 2.3. The WENO-Z scheme

In this paper we consider the modified WENO scheme of Borges et al. [13] with a new global smoothness indicator, which is characterized by

$$\tau_5 = |\beta_0 - \beta_2|. \tag{26}$$

¹⁷¹ It is easy to see from the equations (19) that

$$\tau_5 = \left| -\frac{13}{3} f_{xx} f_{xxx} + f_x f_{xxxx} \right| \Delta x^5 + O(\Delta x^6).$$
 (27)

¹⁷² The new WENO-Z weights are then defined by

$$\omega_m^Z = \frac{\alpha_m^Z}{\sum_{i=0}^2 \alpha_i^Z}, \quad \text{where} \quad \alpha_m^Z = d_m \left[1 + \left(\frac{\tau_5}{\beta_m + \epsilon} \right)^2 \right]. \tag{28}$$

Borges et al. [13] have shown that when using these nonlinear weights, fifth order accuracy is preserved, even at the critical points where f'(u) = 0.

175 3. The Deep Learning Approach for WENO Schemes

To better capture discontinuities and avoid oscillations, we propose to apply deep learning to develop new smoothness indicators. We construct them as products of the original smoothness indicators β_m and multipliers δ_m which are outputs of a neural network algorithm. We refer to these ¹⁸⁰ new smoothness indicators as β_m^{DS} , where index DS corresponds to the new ¹⁸¹ WENO-DS scheme:

$$\beta_m^{DS} = \beta_m (\delta_m + C), \tag{29}$$

where C is a constant, whose role is crucial for the proof of consistency 182 and the formal order of accuracy and we will explain how to choose it in 183 the Section 4. We emphasize that this formulation as a multiplication is 184 very advantageous in a sense that the consistency and accuracy properties 185 can be analytically shown. In the case that the solution is smooth and the 186 original smoothness indicator β_m converges to zero, the smoothness indicator 187 β_m^{DS} behaves in the same way. If the smoothness indicator β_m is O(1), the 188 multiplier δ_m can change it so that the final scheme performs better. We 189 emphasize, that there was an attempt by Liu and Wen [39] to learn the 190 smoothness indicators directly. However, in this case the consistency and 191 accuracy analysis could not be performed. 192

In the original WENO method, the stencil (8) is used to approximate 193 the solution in x_i , and the fluxes are being reconstructed in the points $x_{i-\frac{1}{2}}$ 194 and $x_{i+\frac{1}{2}}$. To define $\hat{f}_{i-\frac{1}{2}}^m$ we use (10) and shift each index by -1. In our 195 approach we proceed as in the classical WENO method [5] and compute the 196 smoothness indicators as described in (17) in the Section 2.2. We use them 197 for a flux reconstruction $f_{i+\frac{1}{2}}$ and then by shifting each of the index by -1 we 198 compute the smoothness indicators corresponding to the flux approximation 199 $\hat{f}_{i-\frac{1}{2}}$. We denote them as $\beta_{m,i+\frac{1}{2}}$ and $\beta_{m,i-\frac{1}{2}}$, respectively. For a fixed m we could make the multiplier δ_m for $\beta_{m,i+\frac{1}{2}}$ and $\beta_{m,i-\frac{1}{2}}$ dependent on the location of the substencils corresponding to $\beta_{m,i+\frac{1}{2}}$ and $\beta_{m,i-\frac{1}{2}}$. This would result in 200 201 202 two different multipliers for $\beta_{m,i+\frac{1}{2}}$ and $\beta_{m,i-\frac{1}{2}}^2$. However, experimentally we got the superior results by using the same multiplier $\delta_{m,i}$ for both $\beta_{m,i+\frac{1}{2}}$ 203 204 and $\beta_{m,i-\frac{1}{2}}$, dependent only on the position *i* of the global stencil. The new 205 smoothness indicators are then computed as 206

$$\beta_{m,i+\frac{1}{2}}^{DS} = \beta_{m,i+\frac{1}{2}} (\delta_{m,i} + C), \beta_{m,i-\frac{1}{2}}^{DS} = \beta_{m,i-\frac{1}{2}} (\delta_{m,i} + C),$$
(30)

and the values δ_0 , δ_1 , δ_2 are obtained by simple index shift so that it holds

$$\delta_{0,i+1} = \delta_{1,i} = \delta_{2,i-1}, \quad i = 0, \dots, N.$$
(31)

²⁰⁸ Finally, we obtain the flux approximations in the same way as in classical

²⁰⁹ WENO schemes, but using the new smoothness indicators (30):

$$\hat{f}_{i-\frac{1}{2}}^{p}$$
 and $\hat{f}_{i+\frac{1}{2}}^{n}$, (32)

which are used for approximating of a solution in a point x_i . Superscripts pand n indicate the difference between the values at the same location $x_{i+\frac{1}{2}}$ when we approximate the solution in points x_i and x_{i+1} (resp. at the same location $x_{i-\frac{1}{2}}$ when we approximate the solution in points x_{i-1} and x_i). We present the whole algorithm of the method in the Figure 1.



Figure 1: The structure of the WENO method combined with the neural network algorithm. The white parts of the graph correspond to the original WENO method. The grey parts are added to this method so that the whole graph corresponds to the new method WENO-DS. 2k + 1 is the size of the receptive field of the whole CNN, × denotes the element-wise multiplication.

As we mentioned before, the flux splitting technique (6) is used. Each

215

part of a flux, f^+ and f^- represents different type of input data to the neu-216 ral network. Therefore we use two neural networks, for the positive and 217 negative part of a flux with the input values $f^+(x_i)$ to the first neural net-218 work and $f^{-}(x_i)$ to the second neural network, $i = 0, \ldots, N$. Each of the 219 neural networks produces different outputs, multipliers corresponding to the 220 positive and negative part of a flux. For simplicity we further drop the 221 superscripts \pm and when we talk about the inputs to the neural network 222 we always mean both $f^+(x_i)$ and $f^-(x_i)$. We denote by f(x) the vector 223 $(f(x_0), f(x_1), \ldots, f(x_N))$ and formulate the neural network as a function 224 F(f(x)).225

To ensure consistency we propose the use of a *convolutional neural net*-226 work (CNN). Firstly, this type of neural network is computationally efficient 227 and secondly, it makes the multipliers independent of their position in the 228 spatial grid so that the final numerical scheme is spatially invariant. To 220 ensure the accuracy of the method, we use the differentiable activation func-230 tions like the exponential linear unit (ELU) and the sigmoid function. If the 231 layers of the neural network are differentiable functions, then their composi-232 tion, the neural network function $F(\cdot)$, is also a differentiable function. The 233 ELU activation function has the advantage that it does not cause the dying 234 gradient problem, the sigmoid activation function ensures that the output of 235 the neural network is between 0 and 1. 236

Let us note that we use for the implementation Python with the deep learning library PyTorch [44] (https://pytorch.org/), which is capable of GPU acceleration.

²⁴⁰ 4. Accuracy analysis of the new WENO scheme (WENO-DS)

²⁴¹ 4.1. Accuracy analysis of WENO-JS scheme with new smoothness indicators $\beta_{m,i\pm\frac{1}{2}}^{DS}$

Let us express the multipliers $\delta_{m,i}$ for the smoothness indicators $\beta_{m,i\pm\frac{1}{2}}$, m = 0, 1, 2 used in the node x_i as the outputs of a neural network function. Following (31) and using the fact, that the layers of the CNN are spatially invariant differentiable functions, we can write

$$\delta_{0,i} = F(f(\bar{x}_{i-1})) = \Phi(\bar{x}_i - \Delta x) = \Phi(\bar{x}_i) - O(\Delta x),$$

$$\delta_{1,i} = F(\bar{f}(\bar{x}_i)) = \Phi(\bar{x}_i),$$

$$\delta_{2,i} = F(\bar{f}(\bar{x}_{i+1})) = \Phi(\bar{x}_i + \Delta x) = \Phi(\bar{x}_i) + O(\Delta x),$$

(33)

247 where

$$\bar{x}_i = (x_{i-k}, x_{i-k+1}, \dots, x_{i+k}), \bar{f}(\bar{x}_i) = (f(x_{i-k}), f(x_{i-k+1}), \dots, f(x_{i+k})),$$
(34)

where 2k + 1 is the size of the receptive field of the whole CNN and Φ is the function composition $F \circ \overline{f}$. Then using (25) it holds

$$\beta_{m,i\pm\frac{1}{2}}^{DS} = \beta_{m,i\pm\frac{1}{2}} (\delta_{m,i} + C) = D \left(1 + O(\Delta x^2) \right) \left(\Phi(\bar{x}_i) + O(\Delta x) + C \right), \quad (35)$$

with *D* being some non-zero constant independent of *m*. We denote $P(\bar{x}_i) = \Phi(\bar{x}_i) + C$ and we set *C* such that $\Phi(\bar{x}_i) + C > \kappa > 0$ with κ fixed. Then we ensure that $P(\bar{x}_i) = O(1)$. Performing the multiplication in (35) we obtain

$$\beta_{m,i\pm\frac{1}{2}}^{DS} = D(P(\bar{x}_i) + P(\bar{x}_i)O(\Delta x^2) + O(\Delta x) + O(\Delta x^3))$$

= $DP(\bar{x}_i)(1 + O(\Delta x)) = \tilde{D}(1 + O(\Delta x)).$ (36)

Here we can proceed as in [19], but for the reader's convenience we repeat the steps of the proof: insert (36) into (15) and take $\epsilon = 0$

$$\alpha_{m,i\pm\frac{1}{2}}^{DS} = \frac{d_m}{\left(\tilde{D}(1+O(\Delta x))\right)^2} = \frac{d_m}{\tilde{D}^2} (1+O(\Delta x)).$$
(37)

²⁵⁵ This implies that

$$\sum_{m=0}^{2} \alpha_{m,i\pm\frac{1}{2}}^{DS} = \frac{1}{\tilde{D}^{2}} (1 + O(\Delta x)), \qquad (38)$$

where we used the fact that $\sum_{m=0}^{2} d_m = 1$. Finally, substituting into (15) we obtain

$$\omega_{m,i\pm\frac{1}{2}}^{DS} = d_m + O(\Delta x),\tag{39}$$

where the superscript *DS* denotes the enhancement of the nonlinear weights (15) using our novel method. We see, that neither the condition (21), nor (24) is satisfied. However, as (39) holds, we can still guarantee that for the WENO-JS scheme with the smoothness indicators (29) we have a formal order of accuracy degraded to the third order, cf. Borges et al. [13]. 4.2. Accuracy analysis of WENO-Z scheme with new smoothness indicators $\beta^{DS}_{m,i\pm\frac{1}{2}}$

Let us now analyse the formal order of accuracy (of the reconstruction) of the scheme (28) with the new smoothness indicators (29). From (19) we see that the smoothness indicators $\beta_{m,i\pm\frac{1}{2}}$ are of the form

$$\beta_{m,i\pm\frac{1}{2}} = f_x^2 \Delta x^2 + O(\Delta x^4),$$
(40)

²⁶⁸ and the global smoothness indicator (26)

$$\tau_5 = O(\Delta x^5). \tag{41}$$

269 Then it holds

$$\beta_{m,i\pm\frac{1}{2}}^{DS} = \beta_{m,i\pm\frac{1}{2}} (\delta_{m,i} + C) = (f_x^2 \Delta x^2 + O(\Delta x^4)) (P(\bar{x}_i) + O(\Delta x))$$

= $f_x^2 P(\bar{x}_i) \Delta x^2 + O(\Delta x^3).$ (42)

We take $\epsilon = 0$ and choose C such that $\Phi(\bar{x}_i) + C > \kappa > 0$, with κ fixed. Then we see that in the non-critical points where $f_x \neq 0$

$$\frac{\tau_5}{\beta_{m,i\pm\frac{1}{2}}^{DS}} = \hat{D}\Delta x^3 + O(\Delta x^4),$$
(43)

where $\hat{D} = \frac{\left|-\frac{13}{3}f_{xx}f_{xxx} + f_x f_{xxxx}\right|}{f_x^2 P(\bar{x}_i)}$. Substituting this into (28) we obtain

$$\alpha_{m,i\pm\frac{1}{2}}^{DS} = d_m \left(1 + O(\Delta x^6) \right) \quad \text{and} \quad \sum_{m=0}^2 \alpha_{m,i\pm\frac{1}{2}}^{DS} = \left(1 + O(\Delta x^6) \right), \quad (44)$$

273 so it follows directly

$$\omega_{m,i\pm\frac{1}{2}}^{DS} = d_m + O(\Delta x^6) \tag{45}$$

and the condition (21) is satisfied. Here we use the superscript DS denoting the enhancement of the nonlinear weights (28) using our novel method. Since we ensure $P(\bar{x}_i) > C > \kappa > 0$, the multipliers $P(\bar{x}_i)$ do not introduce any further critical points. Therefore the analysis of the critical points with $f_x = 0$ remains the same as in [13]. Thus we can guarantee the fifth order accuracy of the scheme (28) with the smoothness indicators (29) also in the critical points.

281 5. Numerical Results

For the system of ODEs resulting from (2) we use a third-order total variation diminishing (TVD) Runge-Kutta method [45] given by

$$u^{(1)} = u^{n} + \Delta t L(u^{n}),$$

$$u^{(2)} = \frac{3}{4}u^{n} + \frac{1}{4}u^{(1)} + \frac{1}{4}\Delta t L(u^{(1)}),$$

$$u^{n+1} = \frac{1}{3}u^{n} + \frac{2}{3}u^{(2)} + \frac{2}{3}\Delta t L(u^{(2)}),$$

(46)

where $L = -\frac{1}{\Delta x} (\hat{f}_{i+\frac{1}{2}} - \hat{f}_{i-\frac{1}{2}})$ and u^n is the solution at the time step n. For (6) we consider in our examples the Lax-Friedrichs flux splitting

$$f^{\pm}(u) = \frac{1}{2} \big(f(u) \pm \alpha u \big), \tag{47}$$

where $\alpha = \max_{u} |f'(u)|.$

287 The Neural Network Structure

The proposed neural network algorithm can be generally applied to any type of conservation laws. For the equations where discontinuities or shocks are present, we propose to train a neural network separately for each equation class. Then we can better adjust the size of a neural network and its structure as well as the loss function, which leads to better results.

As we mentioned earlier, the inputs to the CNN are the values $f^+(x_i)$ and $f^-(x_i)$, i = 0, ..., N and we train two neural networks for a positive and negative part of a flux. (The superscripts \pm will be further dropped.)

The first layer of the neural network is not learned, but represents a 296 preprocessing of the solution from the last time step into a set of features 297 that we assume to be suitable inputs for the following learned layers. Since 298 our goal is to improve the smoothness indicators, we first compute the first 299 and second central finite differences of $f(\bar{x}_i)$ as defined in (34), $i = 0, \ldots, N$. 300 These parameters give us information about the smoothness of the solution 301 and can facilitate and speed up the training of the CNN, and we can use 302 a rather small CNN that still remains powerful. So we have the following 303 values as input for the first learned hidden layer: 304

$$f_{\text{diff}1,i} = \bar{f}(\bar{x}_{i+1}) - \bar{f}(\bar{x}_{i-1}), \quad f_{\text{diff}2,i} = \bar{f}(\bar{x}_{i+1}) - 2\bar{f}(\bar{x}_i) + \bar{f}(\bar{x}_{i-1}).$$
(48)

The values $f_{\text{diff1,i}}$, $f_{\text{diff2,i}}$ computed from f^+ from (47) represent the input values for the first neural network and the values $f_{\text{diff1,i}}$, $f_{\text{diff2,i}}$ computed from f^- represent the input values for the second neural network.

Next, we use a fixed number of hidden layers, each with a specific kernel 308 size and number of channels. We set these CNN parameters separately for 309 each of the equation classes and experimentally find the best setting for each 310 equation, keeping the size of proposed CNN small. We move the kernel 311 by one space step so the stride is set to 1, and we use an ELU activation 312 function in all hidden layers except the last one where we use sigmoid. In all 313 our experiments, we set C = 0.1 in (29), which we experimentally found to 314 be efficient. Let us note, that due to subsequent normalization of β_m^{DS} during 315 the computation of nonlinear weights, using large value of C would decrease 316 the effect of the trained multipliers. On the other hand, for C close to zero 317 the experimental order of convergence could be smaller on coarse grids (but 318 still achieved for $\Delta x \to 0$). We use the nonlinear weights as defined in (28), 319 replacing β_m with β_m^{DS} . The value of ϵ is set to 10^{-13} . 320

As the first choice of the loss function we use the mean square error

$$LOSS_{\rm MSE}(u) = \frac{1}{N} \sum_{i=0}^{N} (u_i - u_i^{\rm ref})^2, \qquad (49)$$

where u_i is a numerical approximation of $u(x_i)$ and u_i^{ref} is the corresponding reference solution. An advantage of this L_2 -norm based loss function in contrast to the L_1 -norm based loss function is stronger gradients with respect to u_i resulting in faster training.

326 5.1. The Buckley-Leverett equation

In the first example, we apply our neural network algorithm to the Buckley-Leverett equation, which was also considered, for example, in [45, 46, 6]. It is a typical example with a non-convex flux function modeling a two-phase fluid flow in a porous medium [47]. The flux in (1) is given by

$$f(u) = \frac{u^2}{u^2 + a(1-u)^2}, \quad -1 \le x \le 1, \quad 0 \le t \le 0.4, \tag{50}$$

where a < 1 is a constant indicating the ratio of the viscosities of the two fluids. The initial condition is set as

$$u(x,0) = \begin{cases} 1, & \text{if } -0.5 \le x \le 0, \\ 0, & \text{elsewhere} \end{cases}$$
(51)

³³³ and we use periodic boundary condition.

In our implementation, we use the CNN with 3 hidden layers with the 334 structure described in the Figure 2. The inputs to the learned hidden layers 335 are the features (48). First, we create the dataset for which we compute 336 the reference solution for the equation (1) with the flux (50) and the initial 337 condition (51). We randomly generate the parameter a from a uniformly 338 distributed range [0.05, 0.95]. We divide the computational domain [-1, 1]339 into 1024 spatial steps and the solution is computed up to time T = 0.4, 340 where the time domain is divided into 8960 time steps. We use the WENO-Z 341 method to compute this reference solution. 342



Figure 2: A structure of the convolutional neural network used for the Buckley Leverett equation (the structure is same for both inputs $f^+(x_i)$ and $f^-(x_i)$, f_{diff1} and f_{diff2} are defined in (48) and are computed from both $f^+(x_i)$ and $f^-(x_i)$).

For the training, we proceed as follows. At the beginning, we randomly 343 choose a problem and its reference solution from our dataset. The weights 344 of the CNN are randomly initialized and we train our model on a solution 345 where our computational domain is divided into 128×140 steps and succes-346 sively compute the entire solution until the final time T. Using the solution 347 at the time step n, we compute the solution at the time step n+1 and 348 during this computation the CNN is used to predict the multipliers of the 349 smoothness indicators. After each of these time steps, we compute the loss 350 and its gradient with respect to the weights of the CNN using backpropa-351 gation algorithm. Then we use this gradient to update the weights, using 352 the well-known Adam optimizer [48] with learning rate 0.0001. After the last 353 time step at time T, we test a model on a validation set and repeat the above 354 steps. Then we select the model with the best performance on the validation 355 set as our final model. For both training and comparing the performance of 356 the models, we use the loss function defined as 357

$$LOSS(u) = LOSS_{MSE}(u) + LOSS_{OF}(u),$$
(52)

where $LOSS_{MSE}(u)$ is defined in (49) and

$$LOSS_{OF}(u) = \sum_{i=0}^{N} |\min(u_i, u_{\min}) - u_{\min}| + |\max(u_i, u_{\max}) - u_{\max}|$$
 (53)

represents the sum of the overflows of the solution above the maximum and below the minimum value of u, in our case $u_{\text{max}} = 1$ and $u_{\text{min}} = 0$. By adding this term to our loss function, we want to avoid the undesirable oscillations that occur especially in the first time steps of the solution.



Figure 3: Loss values for different validation problems at different training cycles (x-axis).

The Figure 3 shows how the value of the loss function for the problems 363 from the validation set (which are not present in the training set) changes 364 with increasing number of training cycles. As training cycle we denote a 365 sequence of training steps performed on a solution for a single randomly 366 chosen parameter a until the final time T. The loss is then evaluated at this 367 final time T. We apparently see two optima for different values of a. If there 368 are more than 50 training cycles, the loss begins to increase significantly 360 for some problems, indicating that further training is not efficient. This is 370 caused by a fact, that the neural network structure is not complex enough 371 to represent multipliers suitable for the whole range of problems. Instead, 372 the optimization finds a compromise, which is suboptimal for some of the 373 problems (leading to loss increase). Since we want only one final numerical 374

scheme as output, we choose the model obtained after the 46th training cycle
as the final model and present the result computed with it.

We compare the L_{∞} - and L_2 -error in the Table 1 for the solution of the conservation law (1) with (50), $a \in \{0.25, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9\}$. Let us note that these parameters were neither in the training, nor in the validation set. We highlight the best performing WENO method in bold. In the 'ratio'

		L_{∞}		L_2				
a	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
0.25	0.429654	0.435090	0.183302	2.34	0.068405	0.067912	0.034065	1.99
0.4	0.408252	0.405047	0.340068	1.19	0.059344	0.058160	0.056051	1.04
0.5	0.317824	0.320094	0.179696	1.77	0.049913	0.049026	0.033758	1.45
0.6	0.459994	0.456687	0.297523	1.53	0.062155	0.061275	0.048766	1 26
0.7	0.476089	0.475015	0.310196	1.53	0.073021	0.072581	0.049836	1.46
0.8	0.207676	0.197021	0.250032	0.79	0.032560	0.030994	0.038974	0.80
0.9	0.375720	0.367802	0.181120	2.03	0.062257	0.061834	0.038510	1.61

Table 1: Comparison of L_{∞} and L_2 error of WENO-JS, WENO-Z and WENO-DS methods for the solution of the Buckley-Leverett equation with the initial condition (51). As 'ratio' we denote the minimum error of the methods WENO-JS and WENO-Z divided by the error of WENO-DS (rounded to 2 decimal points).

380

column, we divide the minimum error of WENO-JS and WENO-Z by the 381 error of WENO-DS to show how well our new method performs compared 382 to the better of the standard methods mentioned. WENO-DS outperforms 383 the standard WENO methods in most cases. Only for a = 0.8 is the error 384 of WENO-DS larger than the error of the other two methods. However, 385 this may be due to the fact that the standard WENO methods perform 386 disproportionately well for a = 0.8. a = 0.8 perform disproportionately well 387 compared to other values of the parameter a. 388

In the Figure 4, we show the solution of the Buckley-Leverett equation for the test problems with a = 0.25 and a = 0.5. It can be seen that the WENO-DS gives a better solution quality than the WENO-JS or WENO-Z.

We also analyze the computational cost of our method and present the comparison in Figure 5. For this purpose, we also retrained the neural network on 64 and 256 grid points in space. In the Figure 5a, we compare the computational cost of all discussed methods for solving the Buckley-Leverett equation with a = 0.25. We see that WENO-DS performs significantly better than WENO-JS and WENO-Z. In the second Figure 5b we compare the methods for a = 0.6. From the Table 1, we see that WENO-DS provides only



Figure 4: Comparison of the WENO-JS, WENO-Z and WENO-DS methods on the solution of the Buckley-Leverett equation with the initial condition (51), N = 128.

a moderate improvement in error rate, but even in this case it outperforms
the other two methods in efficiency. Furthermore, it should be noted that
the neural network implementation is not yet optimized. For example, the
speed could be further increased by GPU acceleration.



Figure 5: Comparison of computational cost against L_2 -error on the solution of the Buckley-Leverett equation with the initial condition (51).

A further improvement in the speed of our method could be achieved if the multipliers were updated only once per time step. More precisely, we can compute the multipliers only in the first Runge-Kutta stage and then, assuming that the smoothness of the solution does not change significantly within one time step, the same multipliers could be used in the following two Runge-Kutta stages. This means that the costly evaluation of the CNN is ⁴¹⁰ performed only once per time step instead of three times per time step, and ⁴¹¹ the corresponding additional time cost is reduced to only about 1/3. We ⁴¹² used this approach to test our method and examine how the error values ⁴¹³ change. Corresponding results can be found in Table 2. We see that very ⁴¹⁴ similar error values are obtained, which justifies this approach and makes it ⁴¹⁵ interesting for future research.

		L_{∞}		L_2				
a	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
0.25	0.429654	0.435090	0.209345	2.05	0.068405	0.067912	0.036956	1.84
0.4	0.408252	0.405047	0.314087	1.29	0.059344	0.058160	0.054628	1.06
0.5	0.317824	0.320094	0.166484	1.91	0.049913	0.049026	0.033010	1.49
0.6	0.459994	0.456687	0.306510	1.49	0.062155	0.061275	0.047933	1.28
0.7	0.476089	0.475015	0.318173	1.49	0.073021	0.072581	0.050179	1.45
0.8	0.207676	0.197021	0.226666	0.87	0.032560	0.030994	0.036531	0.85
0.9	0.375720	0.367802	0.184700	1.99	0.062257	0.061834	0.038899	1.59

Table 2: Comparison of L_{∞} and L_2 error of WENO-JS, WENO-Z and WENO-DS methods for the solution of the Buckley-Leverett equation with the initial condition (51), when the evaluation of the CNN was done only in the first Runge-Kutta stage.

Finally, we verify the analytically proven fifth-order accuracy of the WENO-DS scheme for a transport equation with a smooth solution given as

$$\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x} = 0, \quad u(x,0) = \sin(\pi x), \quad 0 \le x \le 2, \quad 0 \le t \le 0.5, \tag{54}$$

with periodic boundary conditions. Let us note, that we use the same 418 WENO-DS method, which is an output of the training procedure for the 419 Buckley-Leverett equation and we also do not retrain the neural network 420 for different N. Here we demonstrate numerically, that our method can be 421 reliably used also for different class of equation with different initial condi-422 tion and remains convergent. The results can be found in Table 3. There 423 is a great improvement when we compare our scheme with the WENO-NN 424 scheme of Stevens and Colonius [38], where the resulting scheme exhibits 425 only first-order accuracy. 426

Although our scheme remains convergent for any type of equation and for arbitrary discretization, in examples with strong discontinuities we recommend to retrain the neural network for solving a new class of PDE. Doing so, we can improve the performance of the neural network and achieve the enhancement when compared to the existing methods. We refer to [38], where authors aim to use the neural network trained only once for any class

	WENG	D-Z	WENO	-DS	
N	L_{∞}	L_{∞} Order		Order	
20	9.369742e-03	-	9.402549e-03	-	
40	2.558719e-04	5.194516	2.558830e-04	5.199496	
80	9.466151e-06	4.756500	9.466165e-06	4.756560	
160	3.177833e-07	4.896663	3.177834e-07	4.896665	
320	9.957350e-09	4.996137	9.957351e-09	4.996138	
640	3.117835e-10	4.997145	3.117834e-10	4.997146	

Table 3: L_{∞} -norm error and convergence order of WENO-Z and WENO-DS on (54).

of PDE. However, no improvement e.g. in Burgers' equation is achieved and
as demonstrated on example with 1-D Euler equations, also no improvement
can be guaranteed when the discretization changes.

436 5.2. The inviscid Burgers' equation

⁴³⁷ In the next example we consider the inviscid Burgers' equation, where ⁴³⁸ the flux function in (1) is given by

$$f(u) = \frac{u^2}{2}, \quad 0 \le x \le 2, \quad 0 \le t \le 0.3.$$
 (55)

We consider following initial conditions

$$u(x,0) = \begin{cases} z_1, & \text{if } 1 \le x \le 2, \\ 0, & \text{elsewhere,} \end{cases}$$
(56)

$$u(x,0) = \exp(-z_2(x-1)^2),$$
 (57)

$$u(x,0) = z_3 \sin(\pi x),$$
 (58)

439 where

 $z_1 \in \mathcal{U}[1,2], \quad z_2 \in \mathcal{U}[10,30], \quad z_3 \in \mathcal{U}[1,2].$ (59)

⁴⁴⁰ Using these initial conditions, we cover problems with both continuous and
⁴⁴¹ discontinuous initial conditions, and we simulate the shocks and discontinu⁴⁴² ities very well. We train a single CNN on all mentioned classes of initial
⁴⁴³ conditions and use periodic boundary condition.

We first create the data set for training, in which we compute the reference solution of the Burgers' equation with the initial conditions (56)-(58). The



Figure 6: A structure of the convolutional neural network used for the Burgers' equation (the structure is the same for both inputs $f^+(x_i)$ and $f^-(x_i)$, f_{diff1} and f_{diff2} are defined in (48) and are computed from both $f^+(x_i)$ and $f^-(x_i)$).

computational domain is divided into 1024 space steps and 6400 time steps 446 and the solution is computed up to time T = 0.3 using the WENO-Z scheme. 447 We use the CNN with 3 hidden layers with the structure described in the 448 Figure 6. For the training, we proceed in the same way as in the previous 449 example. The only differences are that the computational domain is divided 450 into 128×100 steps and the learning rate used by the Adam optimizer is 451 0.001. In this example, we use the mean square error loss function (49) for 452 training and validation. As the training on Burgers' equation exhibits much 453 higher variance than in the Buckley-Leverett case, we performed 3 trainings 454 each with 90 training cycles and finally selected the model showing the best 455 performance on the validation set. 456

			L_{∞}		L_2				
initial condition	z_j	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
(56)	1.19	0.632213	0.632788	0.303060	2.09	0.082373	0.082141	0.046932	1.75
	1.53	0.594943	0.58678	0.485714	1.21	0.080341	0.07877	0.067175	1.17
	1.84	0.704680	0.694358	0.542599	1.28	0.094967	0.093019	0.076102	1.22
(57)	14.94	0.113498	0.104374	0.100061	1.04	0.016926	0.015137	0.015164	1.00
	21.65	0.236125	0.229290	0.196110	1.17	0.032979	0.031680	0.029141	1.09
	29.08	0.312595	0.310937	0.388739	0.80	0.040632	0.040199	0.049385	0.81
(58)	1.46	0.059072	0.056751	0.051553	1.10	0.010443	0.010032	0.007307	1.37
	1.6	0.063780	0.061391	0.037165	1.65	0.011275	0.010853	0.005552	1.95
	1.9	0.072586	0.069995	0.023841	2.94	0.012831	0.012373	0.003396	3.64

Table 4: Comparison of L_{∞} and L_2 error of WENO-JS, WENO-Z and WENO-DS methods for the solution of the Burgers' equation with the initial condition parameters inside of training set intervals (59). As 'ratio' we denote the minimum error of the methods WENO-JS and WENO-Z divided by the error of WENO-DS (rounded to 2 decimal points).

We compare the errors on the problems from the test set in Table 4 and 5. These were not in the training or validation set and the parameters were randomly generated. We observe rather small or no improvement for problems with the initial condition (57), but the improvement is significant for the solution with the discontinuous initial condition (56) as well as with

			L_{∞}		L ₂				
initial condition	z_j	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
(56)	0.71	0.204162	0.199246	0.150400	1.32	0.031740	0.030740	0.028178	1.09
	2.41	1.541714	1.554201	1.004904	1.53	0.199285	0.200194	0.129223	1.54
	2.57	1.063823	1.055948	0.755908	1.40	0.140068	0.138411	0.102963	1.34
	3.13	0.622858	0.600619	0.287540	2.09	0.087067	0.084495	0.054477	1.55
(57)	33.9	0.351086	0.345278	0.266422	1.30	0.045665	0.044691	0.036426	1.23
	34.67	0.285791	0.283237	0.194424	1.46	0.037350	0.036815	0.027150	1.36
(58)	0.94	0.009524	0.007189	0.007898	0.91	0.001737	0.001509	0.001491	1.01
	2.12	0.077503	0.074744	0.012296	6.08	0.013701	0.013213	0.001712	7.72
	2.44	0.083010	0.080022	0.003978	20.12	0.014675	0.014147	0.000537	26.35

Table 5: Comparison of L_{∞} and L_2 error of WENO-JS, WENO-Z and WENO-DS methods for the solution of the Burgers' equation with the initial condition parameters outside of training set intervals (59). As 'ratio' we denote the minimum error of the methods WENO-JS and WENO-Z divided by the error of WENO-DS (rounded to 2 decimal points).



Figure 7: Comparison of the WENO-JS, WENO-Z and WENO-DS methods for the solution of the Burgers' equation with various initial conditions, N = 128.

 $_{462}$ the initial condition (58).

We conclude that the WENO-DS significantly outperforms the classical WENO methods. It should be noted that although our training set was created with the parameters sampled from uniform distribution as specified in (59), the method can also generalise for parameter values outside of these intervals, as can be seen in Table 5. Especially, we highlight the last two problems from Table 5, where we see a great improvement.

In the Figure 7 we show the solution of the Burgers' equation with the initial condition (56) for $z_1 = 2.41$, (57) for $z_2 = 29.08$, (58) for $z_3 = 1.6$ and (58) for $z_3 = 2.12$. We observe that WENO-DS captures shocks and discontinuities very well and gives us a better solution compared to WENO-JS and WENO-Z.

Next, we test our method on two examples, where the Burgers' equation with the flux function (55) and following initial conditions will be solved:

$$u(x,0) = 1 + \sin(4\pi x), \quad 0 \le x \le 2,$$
(60)

$$u(x,0) = -x\sin\left(\frac{3}{2}\pi x\right), \quad -1 \le x \le 1.$$
 (61)



Figure 8: Comparison of the WENO-JS, WENO-Z and WENO-DS methods for the solution of the Burgers' equation with various initial conditions, N = 128.

We compute the solution up to time T = 0.3. Let us note, that the method was not retrained on these initial conditions and still performs well. Figure 8 illustrates the solution.

Finally, we test our method on the equation (1) with another flux func-

⁴⁷⁸ tion, according to [37]

$$f(u) = \frac{u^4}{16}, \quad 0 \le x \le 2, \quad 0 \le t \le 0.3.$$
 (62)

For this purpose, we use the initial condition (56) with $z_1 = 1.5$ and $z_1 = 2$. We illustrate the solution in Figure 9 computed up to the final time T = 0.3and see that WENO-DS performs very well in both cases.



Figure 9: Comparison of the WENO-JS, WENO-Z and WENO-DS methods for the solution of the equation (1) with the flux function (62), N = 128.

482 5.3. The two-dimensional Burgers' equation

To demonstrate the performance of WENO-DS in two dimensional space we apply the method trained on one-dimensional data for the 1D Burgers' equation (55) to the two-dimensional Burgers' equation of the form

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} + \frac{\partial f(u)}{\partial y} = 0, \qquad f(u) = \frac{u^2}{2}$$
(63)

on the spatial domain $[-1, 1] \times [-1, 1]$ divided into 128×128 uniform cells. As considered by Cao, Xu and Zheng [49] we use the initial condition

$$u(x, y, 0) = (x^2 - 1)^2 (y^2 - 1)^2, \qquad -1 \le x \le 1, \quad -1 \le y \le 1.$$
 (64)

We present the solution at time T = 0.8 in the Figure 10. We compare the error values in Table 6, where the reference solution was computed on the spatial discretization with 256×256 cells. Let us note, that no additional retraining was needed, as we apply the method using dimension-by-dimension principle.



Figure 10: Numerical solution of the two-dimensional Burgers' equation using WENO-DS at T = 0.8. 128×128 cells.

	L_{∞}				L_2			
$N \times N$	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
64×64	0.411625	0.409869	0.323205	1.27	0.023487	0.022837	0.020863	1.09

Table 6: Comparison of L_{∞} and L_2 error of WENO-JS, WENO-Z and WENO-DS methods for the solution of the two-dimensional Burgers equation with the initial condition (64). As 'ratio' we denote the minimum error of the methods WENO-JS and WENO-Z divided by the error of WENO-DS (rounded to 2 decimal points).

493 5.4. The one-dimensional Euler equations

We now investigate how WENO-DS behaves when applied to the onedimensional Euler system, which is considered a classical benchmark problem for methods for conservation laws. It has the form

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0,$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial (\rho u^2 + p)}{\partial x} = 0,$$

$$\frac{\partial E}{\partial t} + \frac{\partial (uE + up)}{\partial x} = 0,$$

(65)

⁴⁹⁷ where ρ is the density, u is the velocity, p is the pressure and E is a total ⁴⁹⁸ energy given by

$$E = \frac{p}{\gamma - 1} + \frac{1}{2}\rho u^2.$$
 (66)

We take $\gamma = 1.4$, which is the ratio of the specific heats. To compute the fluxes, we use the characteristic decomposition of the system according to the steps in [5]. We use the Roe scheme to obtain the eigenvectors and eigenvalues [50] and the Lax-Friedrichs flux splitting to obtain the corresponding component of the flux. We take the solution based on [51] as the reference solution.

The most common benchmark problems are the Sod problem [52], where the initial condition is specified as

$$(\rho, u, p) = \begin{cases} (1, 0.75, 1) & 0 \le x < 0.5, \\ (0.125, 0, 0.1) & 0.5 \le x \le 1 \end{cases}$$
(67)

⁵⁰⁷ and the Lax problem [53] with an initial condition

$$(\rho, u, p) = \begin{cases} (0.445, 0.698, 3.528) & 0 \le x < 0.5, \\ (0.5, 0, 0.571) & 0.5 \le x \le 1. \end{cases}$$
(68)

⁵⁰⁸ We use an adaptive step size

$$\Delta t = \frac{0.9\Delta x}{\max(c_i + |u_i|)}, \quad c^2 = \frac{\gamma p}{\rho},\tag{69}$$

⁵⁰⁹ where u_i is the local velocity and c_i the local speed of sound.

The solution consists of the left rarefaction wave, the right travelling contact wave and the right shock wave. We want to imitate this behavior of the solution, so we construct our data set as described in Appendix A.

We use the CNN with 3 hidden layers with the structure described in Figure 11. After projecting the flux and the solution on the characteristic fields using the left eigenvectors, we use Lax-Friedrichs flux splitting for each component of characteristic variables. From these values we compute the features (48), which are the inputs to the learned hidden layers.

In this example we repeat the training procedure of the previous exam-518 ples with some small modifications described below. To begin, we randomly 519 generate the initial state from the dataset described earlier. We divide the 520 spatial domain into 100 steps and compute the solution for the given initial 521 state up to the time T = 0.05. After each time step we compute loss using 522 the reference solution from [51]. We use the gradient to update the weights. 523 using Adam optimizer with learning rate 0.001. At the last time step we test 524 the model on the validation problems, which are the problems with randomly 525



Figure 11: A structure of the convolutional neural network used for the Euler system (the structure is same for both inputs $f^+(x_i)$ and $f^-(x_i)$, f_{diff1} and f_{diff2} are defined in (48) and are computed from both $f^+(x_i)$ and $f^-(x_i)$).

generated initial conditions according to algorithm described in Appendix A and repeat the procedure with the new initial parameters (ρ, u, p) . We use the loss function

$$LOSS(\rho, u, p) = LOSS_{MSE}(\rho) + LOSS_{MSE}(u) + LOSS_{MSE}(p)$$
(70)

⁵²⁹ for training and validation.

⁵³⁰ Based on the validation problems, we choose the final model and present ⁵³¹ the solution of the Sod problem (67) for ρ , u and p using 100, 200 and 300 ⁵³² space points. We compute the solution up to time T = 0.2. We illustrate the ⁵³³ solution in Figure 12 and compare the corresponding error values in Table 7. ⁵³⁴ Next, we also present the solution of the Lax problem (68) with the final

time T = 0.13 in the Figure 13.



Figure 12: Solution of Sod problem (67), using the WENO-JS, WENO-Z and WENO-DS methods, T = 0.2, N = 100.

⁵³⁶ Finally, we also applied the trained method to the shock entropy wave ⁵³⁷ interaction problem [46] with an initial condition

$$(\rho, u, p) = \begin{cases} (3.857143, 2.629369, 10.33333) & -5 \le x < -4, \\ (1+0.2\sin(5x), 0, 1) & -4 \le x \le 5. \end{cases}$$
(71)

		I		La				
		L_{∞}						
N = 100	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
ρ	0.150172	0.152604	0.151802	0.99	0.024930	0.024381	0.023882	1.02
p	0.225413	0.228468	0.211217	1.07	0.026963	0.026894	0.025194	1.07
u	0.628438	0.643351	0.577795	1.09	0.069043	0.069791	0.064271	1.07
N = 200	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
ρ	0.136956	0.138225	0.136976	1.00	0.016462	0.015903	0.015272	1.04
p	0.215353	0.217666	0.186693	1.15	0.017538	0.017530	0.015451	1.13
u	0.591525	0.603275	0.495718	1.19	0.046245	0.046542	0.042207	1.10
N = 300	WENO-JS	WENO-Z	WENO-DS	ratio	WENO-JS	WENO-Z	WENO-DS	ratio
ρ	0.126180	0.125691	0.124829	1.01	0.012834	0.012254	0.011701	1.05
p	0.204582	0.208307	0.165333	1.24	0.013423	0.013479	0.011468	1.17
u	0.553209	0.570251	0.430247	1.29	0.035888	0.036231	0.035287	1.02

Table 7: Comparison of L_{∞} and L_2 error of WENO-JS, WENO-Z and WENO-DS methods for the solution of the Euler equations of gas dynamics for the Sod problem (67) with N = 100, N = 200 and N = 300. As 'ratio' we denote the minimum error of the methods WENO-JS and WENO-Z divided by the error of WENO-DS (rounded to 2 decimal points).



Figure 13: Solution of Lax problem (68), using the WENO-JS, WENO-Z and WENO-DS methods, T = 0.13, N = 100.

In the Figure 14 we show the solution using WENO-Z and WENO-DS me-538 thods, when the computational domain is divided into 512 uniform cells up 539 to final time T = 1.8. As a reference solution we used the solution computed 540 using WENO-Z method with 2048 space points. This is an example, which 541 has a moving Mach = 3 shock interacting with sine waves in density, so the 542 numerical method needs to deal with the physical oscillations contained in a 543 flow. Finally, let us note, that although we have not trained the presented 544 model on the parameters that would lead to such a solution, the method is 545 robust enough and can detect the shocks present in the solution. 546



Figure 14: Solution of shock entropy wave interaction problem (71), N = 512.

547 6. Conclusion

In this work, we have improved the fifth-order WENO shock-capturing scheme by using deep learning techniques. To do this, we trained a relatively small neural network to obtain modified smoothness indicators of the WENO scheme. This was done in a way that avoided post-processing of the coefficients to ensure consistency. We applied our enhancement to the WENO-Z scheme, where the (formal) fifth-order accuracy on the smooth solutions can be proven analytically.

Our new method, the WENO-DS scheme, is quite easy to use and significantly improves the numerical results, especially in the presence of discontinuities, even for cases that have not been trained before. We have demonstrated our results with the inviscid Burgers' equation, the Buckley-Leverett equation, and the 1-D Euler equations of gas dynamics. We showed, that the method can efficiently solve the problems in more dimensional space without additional retraining.

Finally, let us note, that this paper can be seen as a proof of concept, that neural networks can be efficiently combined with an existing numerical scheme, preserving its formal accuracy order. As part of our future work we will extend our numerical scheme to more applications in 2D and 3D and also study more efficient variants of our approach using GPU computing.

Appendix A. Parameters used for generating the data set for 1-D Euler equations of gas dynamics

The problem samples representing different versions of the Euler equations of gas dynamics (67) were defined using parameters generated by the following algorithm.

Choose randomly $s \in \{0, 2\}$ 572 if s = 0 then 573 $a \in \mathcal{U}[0.5, 10], \quad b \in \mathcal{U}[-0.05, 0.05],$ $p_l = a + b,$ 574 $p_r = 1/c, \quad c \in \mathcal{U}[5, 10],$ 575 $\rho_l = p_l,$ 576 $\rho_r = p_r + d, \quad d \in \mathcal{U}[-0.05, 0.05],$ 577 $u_l = e, \quad e \in \mathcal{U}[0, 1],$ 578 $u_r = 0,$ 579 else if s = 1 then 580 $p_l = 1$, 581 $p_r = 0.1,$ 582 $\rho_l = k, \quad k \in \mathcal{U}[1,3],$ 583 $\rho_r = \frac{1}{10}\rho_l + l, \quad l \in \mathcal{U}[-0.05, 0.05],$ 584 $u_l = m, \quad m \in \mathcal{U}[0,1],$ 585 $u_r = 0,$ 586 else 587 $p_l = n, \quad n \in \mathcal{U}[3, 4],$ 588 $p_r = \frac{1}{7}p_l + q, \quad q \in \mathcal{U}[-0.05, 0.05]$ 589 $\rho_l = r, \quad r \in \mathcal{U}[0.3, 0.6],$ 590 $\rho_r = \rho_l + s, \quad s \in \mathcal{U}[-0.05, 0.05],$ 591 $u_l = t, \quad t \in \mathcal{U}[0,1],$ 592 $u_r = 0,$ 593 end if 594 where 595 1

$$(\rho, u, p) = \begin{cases} (\rho_l, u_l, p_l) & 0 \le x < 0.5, \\ (\rho_r, u_r, p_r) & 0.5 \le x \le 1. \end{cases}$$
(A.1)

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