Discontinuity Identification in Numerical solutions of Differential equations

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Introduction

There is a need for identification of discontinuities that can form in finite time in the solutions of conservation laws. Without proper treatment of the discontinuities the solutions generated using a numerical scheme generates spurious Gibbs oscillations and may even converge to an entropy violating solution. The cells in which the discontinuity is present are known as ”troubled cells” and identification of these cells is crucial for simulations. Methods which help in identification of these cells are known as **troubled cell indicators** or shock detectors.
There has been recent development of using artificial neural networks as troubled cell indicators. The advantage of using ANNs for troubled cell identification is that they are problem independent.

Problem Description

Consider a function $f : D \to \mathbb{R}$ where $D \subset \mathbb{R}^d, d \geq 1$ is a compact set.
Without loss of generality let D is a $d-$ dimensional rectangle given by $D = I_1 \times I_2 \times \ldots \times I_d$ where $I_i = [a_i, b_i], b_i = a_i + n_i\delta$ where $n_i \in \mathbb{N}, \delta > 0$.
Consider a uniform grid over D of $\prod_{i=1}^{d}(n_i + 1)$ grid points

$$S = \{(a_1 + i_1\delta, a_2 + i_2\delta, \ldots, a_d + i_d\delta), i_k \in \{0, 1, 2, \ldots, n_k\}\forall k = 1, 2, \ldots, d\}$$

Given the value of f at each of the points in S, the problem is to find the grid cells which contain points of discontinuity of f. These cells are known as *troubled cells*

Polynomial Annihilation Detection

The goal of polynomial annihilation is to construct a function $L_m f(x), m \in \mathbb{N}$, such that for x away from discontinuity points of $f(\cdot), L_m f(x) \approx 0$.
Hence the detection of discontinuities is based on $|L_m f(x)| > t$ where t is some threshold.
Suppose that f is known only on the discrete set S. Let Π_m be the space of all polynomials of degree $\leq m$ in d variables.
xThe value of $L_m f(x)$ at $x \in D$ is determined by the function values of f on a local set $S_x \subset S$ of $m_d = \binom{m+d}{d}$ points around x.
Let $S_x = x_1, x_2, \ldots, x_{m_d}$, be the set of m_d nearest points to x.
For polynomial annihilation up to degree $m - 1$, one solves the linear system for coefficients $\{c_j(x) : j = 1, 2, \ldots, m_d\}$

$$\sum_{x_j \in S_x} c_j(x)p_i(x_j) = \sum_{|\alpha|_1 = m} p_i^{\alpha}(x)$$

wher $\alpha = (\alpha_1, \alpha_2, \ldots, \alpha_d), \alpha_i \in \mathbb{N}\bigcup\{0\}, p_1, p_2, \ldots, p_{m_d}$ is a basis of Π_m
Since the solution of the above system exists and is unique, one can define

$$L_m f(x) = \frac{1}{q_{m,d}(x)} \sum_{x_j \in S_x} c_j(x)f(x_j)$$

where $q_{m,d}(x)$ is a normalization factor.

Construction of Discontinuity Detector

1-D Detector

Here $D = [a, b]$ and $S = \{x_i = a + (i-1)\delta, i = 1, 2, \ldots, N+1\}$
This forms a uniform grid with N cells denoted by intervals $[x_i, x_{i+1}), i = 1, 2, \ldots, N$.
Let

$$y = (y_1, y_2, \ldots, y_n) \in \{0, 1\}^N$$

be a binary vector indicating the ground truth values for each $i = 1, 2, \ldots, N$ where $y_i = 1$ indicates that the i^{th} cell is a trouble cell and $y_i = 0$ otherwise.
Let $v_f = f(x) : x \in S$ be the set of observed function values on S.
We first standardize the observed function values and the feed them into a CNN to obtain an output vector of N real values.

$$\hat{y} = (\hat{y}_1, \hat{y}_2, \ldots, \hat{y}_N) = \mathcal{N}(\tilde{v}_f)$$

as an estimate of the ground truth y.
Here

$$\tilde{v}_f = \{\frac{f(x) - \mu_f}{\sigma_f} : x \in S\}$$

where μ_f, σ_f are the mean and standard-deviation of v_f respectively.
Then for a chosen threshold t, detector labels each of the i^{th} cell a trouble cell if $\hat{y}_i > t$

1D- Data generation

The CNN detector is trained on a synthetic dataset of $n = 1,000,00$ piecewise smooth function on Domain D.

1. Randomly select an integer N_d from the set $\{0, 1, \ldots, M\}$. In the experiments of the paper $M = 3$(i.e. at most 3 discontinuities).

2. Using uniform distribution on D, generate N_d random numbers as the locations of the discontinuities. This partitions D into $N_d + 1$ subdomains.

3. Inside each subdomain create fourier series

$$\tilde{a}_0 + \sum_{n=1}^{N_F} \left(\tilde{a}_n \cos nx + \tilde{b}_n \sin nx\right)$$

, where $\tilde{a}_n, b_n \sim N(0, 1)$ are i.i.d Gaussian random variables and $N_F = 15$

2D Detector

Let $D = [a, b]^2$ with uniform grid points $S = \{x_{ij} : 1 \leq i, j \leq N+1\}$
where $x_{ij} = (a + (i-1)\delta, a + (j-1)\delta)$
This creates N^2 cells C_{ij}
Let $y = (y_{ij}) \in \{0, 1\}^{N \times N}$ be a binary matrix indicating the ground truth values corresponding to the cells.
Let $v_f = \{f(x) : x \in S\}$ be the set of observed function values on S.
Similar to 1D, we construct a detector that takes in v_f and outputs a binary matrix to predict y

2D-Data generation

1. Domain D is divided into two sub-regions by a *random curve*

2. Inside each sub-region a smooth function is generated given by

$$f_i(x,y) = \sum_{m+n \leq N_p} a^{(i)}_{m,n} P_m(x) P_n(y) \ i = 1,2$$

   where $P_n's$ are the standard Legendre polynomials and $a_{m,n}$ are randomly sampled from $N(0,10)$, $N_p = 4$

3. For the random curve serving as an interface between the two sub-regions and is also the location of the discontinuity curve, following two cases are employed.

   - Line Cut: Defined by random straight line

$$\cos\theta(x - x_0) + \sin\theta(y - y_0) = 0$$

     where $\theta \sim U(0, 2\pi), (x_0, y_0) \sim U(D)$

   - Circular Cut: Defined as

$$(x - x_0)^2 + (y - y_0)^2 = r$$

     where $r \sim U(0,3), (x_0, y_0) \sim U(D)$

One-Level Detection method

We standardize input as done in 1D-Detector
Prediction is done on the standardized input using CNNs.
Then for a chosen threshold t, detector labels each of the $^{\text{th}}$ cell a trouble cell if $\hat{y}_{ij} > t$

Two-Level Detection Method

The issue with the one level detection method is the drastic increase in the number of parameters when dimension is increased by 1. To account for that, we can use two level detection method in which we first view the entire grid as a coarse grid and find the troubled cells in the coarse grid.
Now inside each cell of coarse grid is a sub-grid on which another detector is run if the grid cell was indicated as a troubled cell by level 1 detector.

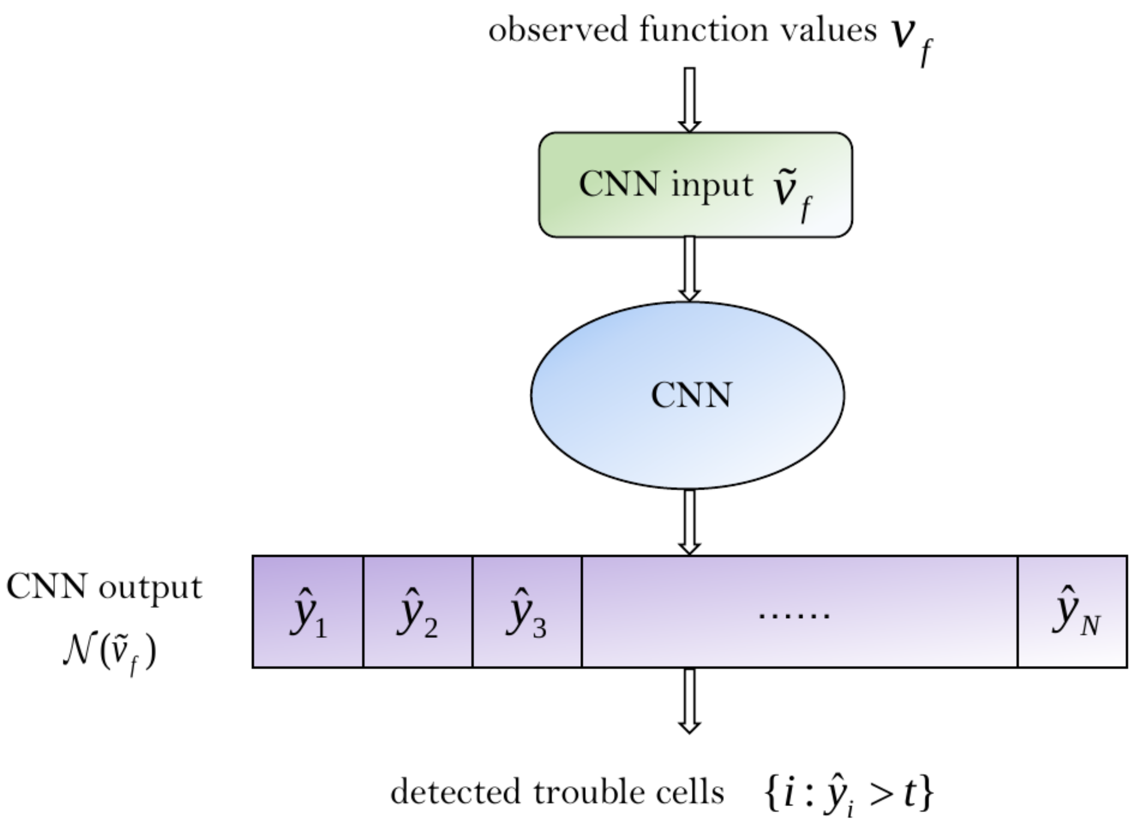

Figure 1: 1D - One Level Detector

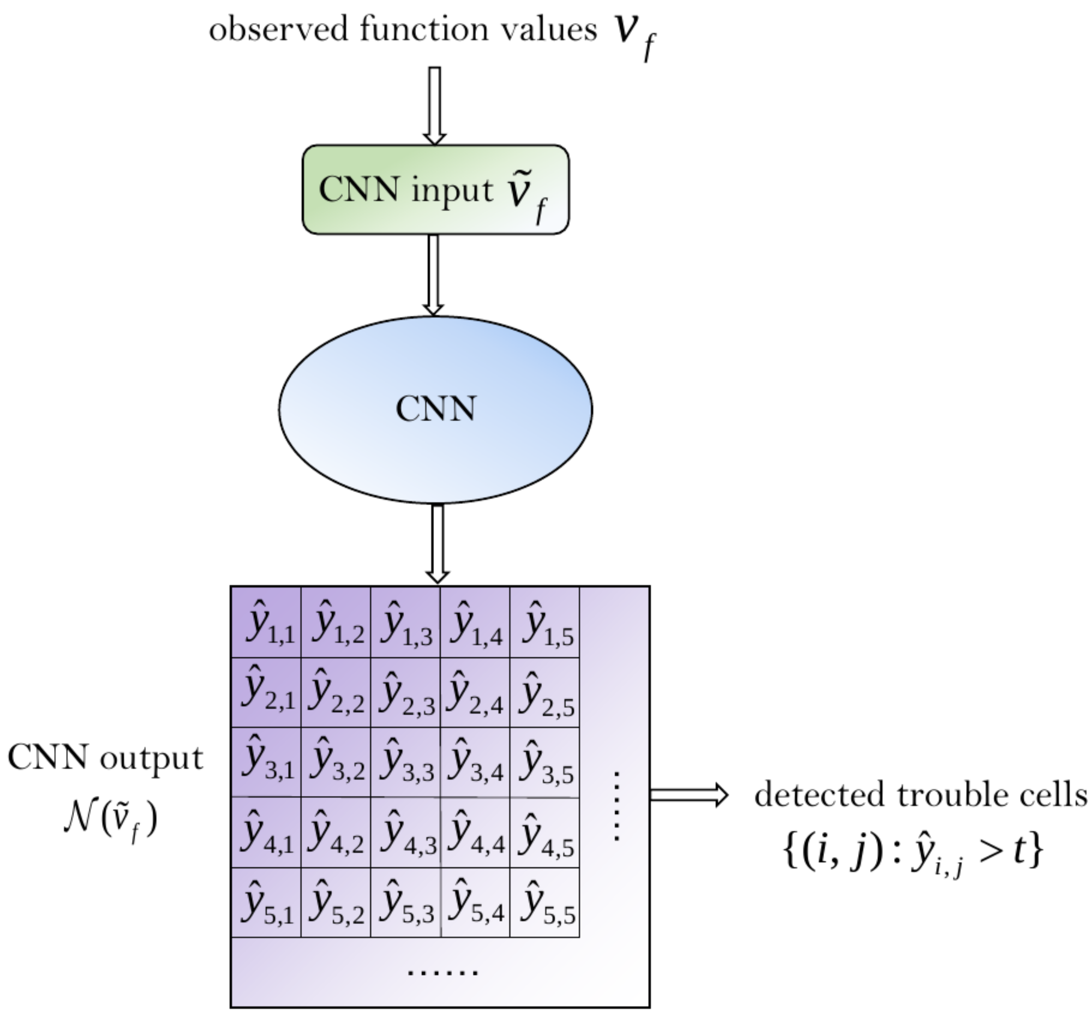

Figure 2: 2D- One Level Detector

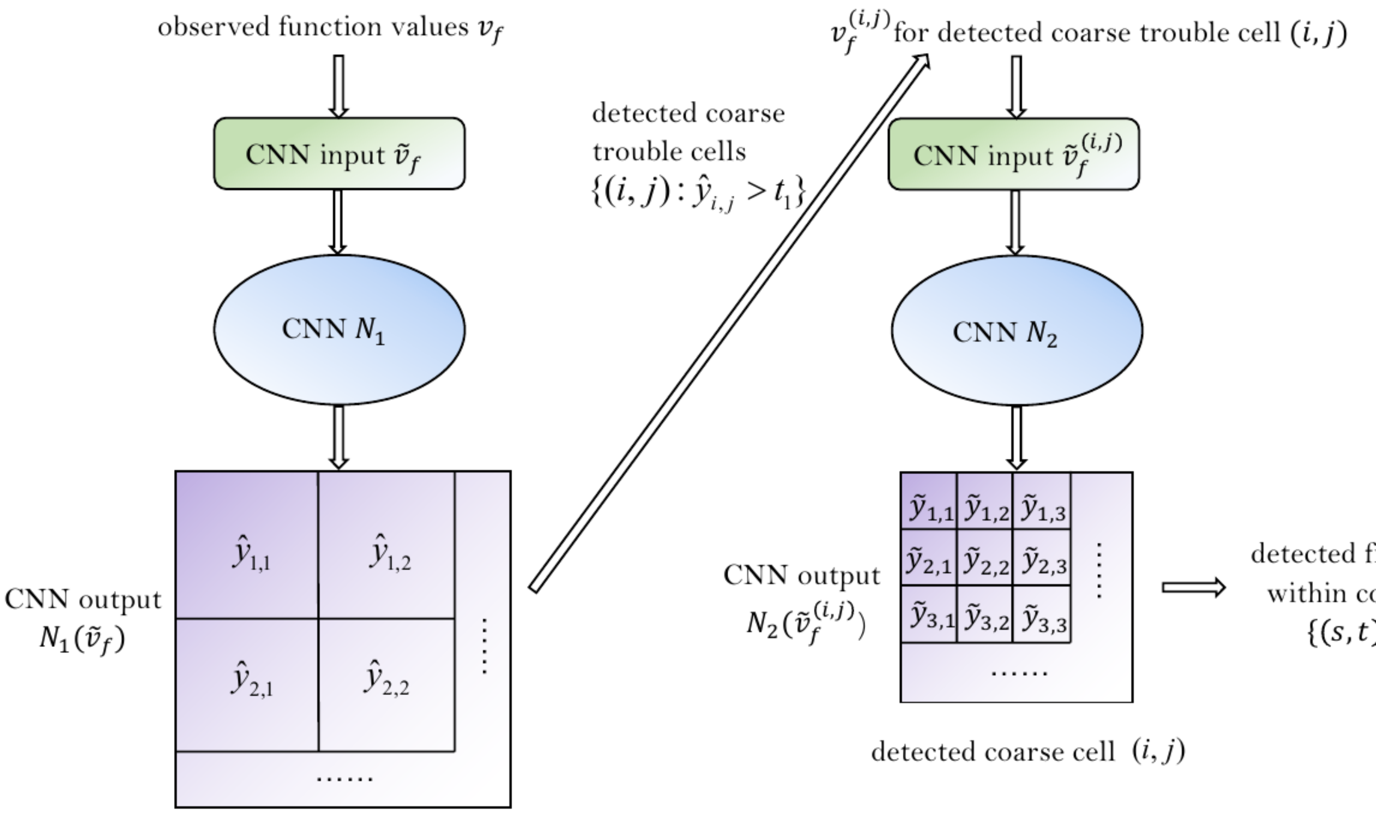

Figure 3: 2D- Two Level Detector

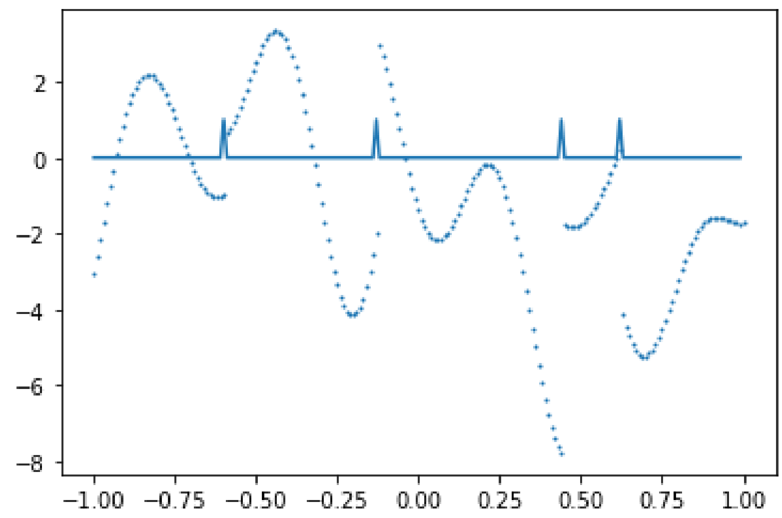

Figure 4: Model predictions for 1D Data