

# Incorporating Prior Domain Knowledge into Deep Neural Networks

<http://people.cs.vt.edu/ramakris/papers/PID5657885.pdf>

## Abstract

- domain adapted neural network (DANN)
  - knowledge is incorporated in loss terms
    - monotonicity constraints
    - approximation constraints
  - tested on synthetic and real world data
    - noisy data
    - limited data

## Problem Formulation and Solution Approach

### Problem Statement

leverage domain knowledge to train a robust accurate learning model that yields good model performance even with sparse, noisy training data

### Approximation Constraints

$$g(\hat{Y}) = \begin{cases} 0 & \text{if } \hat{Y} \in [y_l, y_u] \\ |y_l - \hat{Y}| & \text{if } \hat{Y} < y_l \\ |y_u - \hat{Y}| & \text{if } \hat{Y} > y_u \end{cases}$$

$$\text{Loss}_D(\hat{Y}) = \sum_{i=1}^m \text{ReLU}(y_l - y^i) + \text{ReLU}(y^i - y_u)$$

$$\text{ReLU}(z) = z^+ = \max(0, z)$$

- constraints that specify a quantitative range of operation of the target variable
  - ReLU term ensures that the output is non-zero if the input is positive

## Monotonicity Constraints

$$\text{Loss}_D(\hat{Y}_1, \hat{Y}_2) = \sum_{i=1}^m \mathbb{I}\left((x_1^i < x_2^i) \wedge (\hat{y}_1^i > \hat{y}_2^i)\right) \cdot \text{ReLU}(\hat{y}_1^i - \hat{y}_2^i)$$

- $h(x) = y$  such that  $x_1 > x_2 \rightarrow h(x_1) > h(x_2)$  then  $x_1, x_2$  and  $h(x_1), h(x_2)$  share a monotonic relationship
- $\mathbb{I}$  represents the identity function  $\rightarrow$  true if the boolean statement is true, else false
  - serves as a boolean mask which captures errors only of the instances where the domain constraint is violated

## Synthetic Datasets

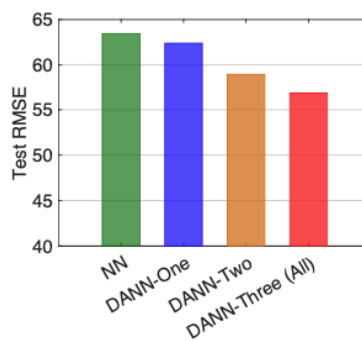
- use Bohachevsky function as the basis for generating synthetic datasets
  - **approximation constraints:** dataset  $X = [x_{i,1}, x_{i,2}]$ ,  $Y$ 
    - randomly select a subset of rows in  $X$  and interchange the values of  $x_1$  and  $x_2$  in those rows  $\rightarrow$  value of  $f(x_1, x_2)$  in  $Y$  for those rows is outside of the approximate range
  - **monotonicity constraints:**  $X', X'', X'''$  such that  $x_{i,1} < x'_{i,1} < x''_{i,1}$

- randomly sample a subset of rows and switch the values of  $y$  and  $y'$  to create data where the monotonicity constraints are violated

## Real Datasets

- prediction of oxygen solubility in water
  - influenced by water temperature, salinity, pressure

## Experimental Findings



- DANN and vanilla NN are compared with respect to noise and amount of training data
- see paper for details