How to Incorporate Monotonicity in Deep Networks While Preserving Flexibility?

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Abstract

The importance of domain knowledge in enhancing model performance and making reliable predictions in the real-world is critical. This has led to an increased focus on specific model properties for interpretability. We focus on incorporating monotonic trends, and propose a novel gradient-based point-wise loss function for enforcing partial monotonicity with deep neural networks. While recent developments have relied on structural changes to the model, our approach aims at enhancing the learning process. Our model-agnostic point-wise loss function acts as a plug-in to the standard loss and penalizes non-monotonic gradients. We demonstrate that the point-wise loss produces comparable (and sometimes better) results on both AUC and monotonicity measure, as opposed to state-of-the-art deep lattice networks that guarantee monotonicity. Moreover, it is able to learn differentiated individual trends and produces smoother conditional curves which are important for personalized decisions, while preserving the flexibility of deep networks.

1 Introduction

Neural networks have recently demonstrated tremendous success in influencing decisions across mass-impact domains, such as finance [Nelson et al., 2017; Lee et al., 2018], pricing [Chiarazzo et al., 2014; Shukla et al., 2019a; Ye et al., 2018] and policy-making [Höchtl et al., 2016]. Because decisions in these domains have significant societal implications, questions about the models’ interpretability and learning behavior commonly arise. Trust in the system and associated applicability take center stage when analysts intend to validate their prior domain expertise about the data, vis-à-vis the learned statistical model. This a priori knowledge can relate to an attribute following a certain distribution in nature. In this work, we focus on one such intuitive trend, namely, monotonicity.

Even though real-world data encompasses high-dimensional inputs with multiple interactions [Hall and Xue, 2014], it is common to possess prior domain knowledge about the monotonic trend (non-increasing / non-decreasing) between a subset of input features and the output, giving rise to partial monotonicity [Daniels and Velikova, 2010]. For instance, economic theories in house pricing [Pottharst and Feelders, 2002] expect selling price to increase with total area. Monotonicity constraints act as a regularizer, and enhance generalization to test data, apart from facilitating human-in-the-loop adaptive learning. Such considerations demand specific attention in deep learning where prediction accuracy may be improved at the expense of interpretability [Chen et al., 2018].

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We present a point-wise loss (PWL) function that incorporates monotonic knowledge into neural networks. Without loss of generality, we use non-decreasing monotonicity for our study.

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To evaluate the performance of DNN trained with PWL, we compare it to DLN. DLN is geared towards providing structural monotonicity guarantees irrespective of the trends in data, while PWL leads to sub-optimal outputs. Pathak et al. [2015] show that alternative loss formulations can be equivalent to optimizing convolutional networks in a constrained manner. We contribute to this field by introducing a point-wise loss (PWL) function for enforcing partial monotonicity within any DNN, without any change in architecture.

Monotonicity can be incorporated within the learning process i.e. the backpropagation step by adding constraints, either as an additional cost with standard loss function ("soft" constraint); or as a "hard" constraint, similar to Lagrangian multipliers. Márquez-Neila et al. [2017] compare these two types of constraints and establish that soft constraints perform better because satisfying hard constraints leads to sub-optimal outputs. Pathak et al. [2015] show that alternative loss formulations can be equivalent to optimizing convolutional networks in a constrained manner. We contribute to this field of soft-constraint methods by introducing a point-wise loss (PWL) function for enforcing partial monotonicity within deep neural networks.

### 2 Related work

Monotonicity is enforced commonly with neural networks either by changing (i) model architecture or (ii) the learning process. Architecture alterations relate to connecting hidden nodes differently or imposing constraints on weights of certain input/hidden nodes. Most published work has focused on these structural changes - starting from positive weight constraints by Archer and Wang [1993], Sill et al. [1998] introduced those constraints into a three-layer neural network for full monotonicity, which was further extended by Daniels and Velikova [2010] to partial monotonic functions for low-dimensional spaces. Generalizing the approach, You et al. [2017] proposed deep lattice networks (DLN) using a combination of linear calibrators and lattices for learning monotonic functions. Though DLN outperforms previous methods, constructing a lattice with \( D \) features (\( 2^D \) simplex) is computationally expensive for large spaces. Moreover, lattices, being structurally rigid, use multi-linear interpolation for unseen data - leading to step-wise and non-intuitive relationship between the input and output.

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### 3 Point-wise Loss (PWL)

Consider the general setting of a supervised learning problem with a training set of \( n \) examples \( \{(x_i, y_i)\}, i = 1, \ldots, n \). The label could either be real-valued \( (y_i \in \mathbb{R}) \), or binary \( (y_i \in \{0, 1\}) \) such as classification labels. The objective of the methods presented below is to determine an estimator \( f(x) \) which is monotonic with respect to \( x[M] \), where \( M \) is a subset of features defined by \( M \subseteq D \) in \( x \in \mathbb{R}^D \). A function \( f \) is said to be monotonically increasing in \( M \) if \( f(x_i) \geq f(x_j) \) for any two feature vectors \( x_i, x_j \in x \), such that \( x_i[M] \geq x_j[M] \) and \( x_i[p] = x_j[p] \), for all \( p \in D \setminus M \).

Without loss of generality, we use non-decreasing monotonicity for our study. We present a point-wise loss (PWL) function that incorporates monotonic knowledge into neural networks by altering the learning process. The objective function with point-wise derivatives which embeds a priori knowledge about monotonicity is inspired from finite element analysis as approximation [Strang 1972, Wilmott et al. 1995] and classes of functions presented by Dugas et al. [2009]. We formulate the following minimax objective function \( \mathcal{L}_{\text{mono}} \) computed over \( x_i, \forall i \in [1, n] \):

\[
\min \mathcal{L}_{\text{mono}} = \min \left\{ \max_{i=1}^{n} \left\{ 0, -\nabla \cdot_M f(x_i; \theta) + \mathcal{L}_{\text{NN}} \right\} \right\}
\]

where \( \nabla \cdot_M \) is divergence with respect to feature set \( x[M] \), i.e., \( \sum_j \frac{\partial f(x; \theta)}{\partial x_j[M]} \) \( \forall j \in M \), \( \theta \) are the trainable parameters, and \( \mathcal{L}_{\text{NN}} \) refers to the empirical risk minimization for neural networks.

#### 3.1 Evaluation Strategy

To evaluate the performance of DNN trained with PWL, we compare it to DLN. DLN is geared towards providing structural monotonicity guarantees irrespective of the trends in data, while PWL
focuses on learning monotonicity from the data. We use two metrics: (i) area under the ROC curve (AUC) and (ii) our monotonicity metric $M_k$ (defined in (2) and (3)) for this analysis.

$$M_k = \frac{1}{n} \sum_{i=1}^{n} \mathbb{1}(\delta_i),$$

$$\delta_i = \begin{cases} 
1 & \text{if } \Delta_+ f(x_j; \theta) \geq 0 \ \forall \ j \ni \{x_j[k] \in [\kappa_{\text{min}}, \kappa_{\text{max}}], x_j[p] = x_i[p] \ \forall \ p \neq k\} \\
0 & \text{otherwise.} 
\end{cases}$$

Here, the latent variable $\delta$ is an indicator that measures the degree of monotonicity $M_k$ for the $k^{th}$ feature across the entire dataset. $\Delta_+$ refers to the forward difference operator for non-decreasing monotonicity [Wilmott et al., 1995]. The range for evaluating monotonicity of feature $k$ is set to $[\kappa_{\text{min}}, \kappa_{\text{max}})$, i.e. the lowest and highest values of the $k^{th}$ feature present in the training data.

4 Experiments

We compare the performance of PWL and DLN across three data sources: (1) an artificial dataset, (2) UCI - Adult dataset and (3) Airline Ancillary dataset, summarized in Appendix (Table 2). Our models are trained on cross-entropy loss for classification problems, and mean squared loss for regression. PWL uses Stochastic Gradient Descent (SGD) for optimization of the objective loss function. DLN implementation is similar to the one proposed by [You et al., 2017].

4.1 Artificial dataset

We synthesize an artificial dataset (sinusoidal in $x$ and exponential in $y$; Fig. 1a) to visualize learning on the 2-D functional space. We observe that standard DNN with squared loss and moderate batch size detects the overall trend, but there are regions of non-monotonicity (Fig. 1b). Monotonicity is ensured along $y$ after incorporating PWL with same DNN architecture, however, the curves appear to be marginally sharper than the target function (Fig. 1c). Contour lines for DLN are closest to the target function (Fig. 1d). Although DLN learns better than PWL, our alternative PWL formulation is able to bring DNN closer to monotonicity without a complete overhaul in architecture, unlike DLN.

![Figure 1: Function $f(x, y) = \sin(x) + e^y$; $x \in [0, 1]$ and $y \in [0, 1]$ are the principal axis along horizontal and vertical dimensions respectively. Contours: (a) Target (b) DNN estimated (c) PWL estimated (d) DLN estimated](image)

Table 1: Model performance on the two datasets. ($M_k$: monotonicity metric (2); $T$: run-time in $10^3$ seconds)

| Models   | UCI - Adult | Airline Ancillary |
|----------|-------------|-------------------|
|          | AUC | $M_k$ | $T$      | AUC | $M_k$ | $T$      |
| DLN      | 0.917 | 1.000 | 5.586 | 0.708 | 1.000 | 7.770 |
| PWL      | 0.908 | 0.856 | 0.338 | 0.722 | 0.985 | 1.375 |

4.2 UCI - Adult dataset

Similar to [You et al., 2017], census data from the UCI repository [Dua and Graff, 2017] is used to predict whether a person’s income exceeds $50,000 or not. Monotonicity is enforced with respect to education level, hours per week, and capital gain. Considering education level for illustration, we note that DLN marginally edges out PWL on AUC and monotonicity measure $M_k$ (See Table 1). However, analysis of conditioned trends on education level (Fig. 2a) suggests that the DLN is learning similar (consistent step-wise slope) patterns for each person. PWL results demonstrate varying trajectories for each person, i.e. it differentiates between individuals after considering non-linear interactions. We
found the actual correlation between education level and income to be 0.33, indicating that the data may not be completely positive monotonic. Hence, the DLN does guarantee monotonicity but at the cost of sometimes ignoring real signals from data, which are detected by PWL (red lines in Fig. 2b).

![Figure 2: UCI - Adult dataset: Conditioned trends for Education Level](image)

![Figure 3: Airline Ancillary dataset: Conditioned trends for Ancillary Price](image)

### 4.3 Airline Ancillary dataset

Ancillary pricing [Shukla et al., 2019a,b] is a sub-field within airline pricing where ancillaries are priced in association with partner airlines using an A/B testing framework. Domain knowledge suggests that the ancillary purchase probability should follow a non-increasing monotonic trend with respect to price. Upon experimenting with different iterations of the DLN i.e. increasing lattice size and number of lattices, we find that DLN’s training time increases significantly without noticeable improvement in AUC (Appendix: Table 3). On the other hand, PWL model is more tractable and solves faster (Table 1). In addition, we find that PWL outperforms DLN in terms of AUC and has similar $M_k$ score (Table 1). DLN makes predictions in a step-wise fashion with linearly interpolated segments (Fig. 3a), thereby missing out on customer dynamics for unobserved regions. However, PWL produces curves with smoother derivatives - suggesting the possibility of greater personalization for customers, and establishing continuity of trend on either side of the price horizon (as expected).

### 5 Conclusion

In this work, we explored one way of incorporating a priori knowledge - monotonicity, to leverage domain expertise into data-driven approaches. We tested a point-wise loss (PWL) function that penalizes non-monotonicity, against deep lattice networks (DLN) which enforce monotonicity via calibrated look-up tables. We discussed how DLN guarantees monotonicity at the cost of learning from data, whereas PWL strives to achieve a compromise between minimizing empirical risk and enforcing monotonicity. DLN is unable to differentiate between individual data points, a model characteristic desired in the real-world to drive personalized decisions. In contrast, varying trajectories learned by PWL provide more power for customized decision-making. In addition, PWL can be used as a plug-in for enforcing soft monotonicity, while retaining the flexibility and power of deep networks. However, PWL demands a wise choice of the relative importance of different terms in the loss function - an open problem in the deep learning community. In future work, we aim to facilitate transfer learning between different PWL model iterations to regularize the loss weight proportions.
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Appendices

A Additional Information

Table 2 provides additional details on the experimental setup mentioned in Section 4. Function approximation on artificial dataset presented in Section 4.1 has been formulated as a regression task. Hence, we used mean squared error as loss function for simplicity. Cross-entropy loss was used as the primary loss function for UCI - Adult and Airline Ancillary datasets. Here, loss function refers to $L_{NN}$ defined in Equation [1].

Table 2: Data Summary

| Dataset          | Type       | # Training | # Test  | # Features (Monotonic) |
|------------------|------------|------------|---------|------------------------|
| Artificial       | Regression | 10,000     | -       | 2 (1)                  |
| UCI - Adult      | Classification | 26,048   | 16,281  | 90 (3)                |
| Airline Ancillary| Classification | 106,003 | 26,513  | 32 (1)                |

In Table 3 parameter $\theta_1$ refers to number of monotonic lattices and $\theta_2$ refers to the lattice size/rank for DLN. For DNN based models trained with PWL, these parameters are the hidden units in the 2-layer neural network. Performance has been evaluated on a machine with NVIDIA Tesla K80 GPU.

Table 3: Comparison of various experiments on PWL and DLN.

| Dataset           | Model | Parameters $[\theta_1, \theta_2]$ | AUC  | $M_k$  | $T_{10^3}$ |
|-------------------|-------|----------------------------------|------|--------|------------|
| UCI - Adult       | DLN   | [70, 5]                          | 0.917| 1.000  | 5.586      |
| UCI - Adult       | PWL   | [32, 11]                         | 0.908| 0.856  | 0.338      |
| Airline Ancillary | DLN   | [20, 3]                          | 0.709| 1.000  | 0.277      |
| Airline Ancillary | DLN   | [30, 3]                          | 0.706| 1.000  | 0.373      |
| Airline Ancillary | DLN   | [70, 3]                          | 0.708| 1.000  | 0.738      |
| Airline Ancillary | DLN   | [70, 4]                          | 0.709| 1.000  | 1.451      |
| Airline Ancillary | DLN   | [70, 5]                          | 0.708| 1.000  | 7.770      |
| Airline Ancillary | PWL   | [32, 11]                         | 0.722| 0.985  | 1.375      |

B Additional Observations

Various iterations of DLN on airline ancillary dataset (Section 4.3) show that an increase in lattice size/rank ($\theta_2$) for enhanced model learning leads to an exponential increase in the run-time, without any improvement in AUC (Table 3). On the other hand, PWL converges faster and outperforms DLN on the AUC. Even though $M_k$ for PWL is marginally lower than 1 (DLN), PWL is picking the real signal from the data when sample behavior is not monotonic in practice.

Figure 4: UCI - Adult dataset: Conditioned trends for Capital Gain
Model results for PWL and DLN on the UCI - Adult dataset (capital gain feature) are presented in Figure 4. For this feature, DLN shows more variance in learning curves than PWL which generates similar trajectory for a group of data points. Reason can be attributed to the interdependence of different loss terms in the PWL function, necessitating the importance of balancing trade-off. For instance, $(\mathcal{L}_{\text{mono}} - \mathcal{L}_{\text{NN}})$ i.e. the monotonicity loss could be decreasing with respect to one of the monotonic feature but not getting equally minimized for the other monotonic feature. One way of countering this limitation is transfer of model weights between various PWL iterations for optimization of the custom loss coefficients (weights of $\mathcal{L}_{\text{mono}}$ as defined in Equation 1 - kept same for this work).

![Figure 5](image-url)

**Figure 5**: Artificial dataset analysis. (a) Illustration of contour plots for two competing loss functions: loss 1 and loss 2 with respective normal vectors as $N_1$ and $N_2$. (b) PWL estimated contour plot for different hyperparameters: horizontally increasing frequency for $(\mathcal{L}_{\text{mono}} - \mathcal{L}_{\text{NN}})$ from left to right, vertically increasing frequency for $\mathcal{L}_{\text{NN}}$ from bottom to top.

The weighted loss method or the loss term switching method can be used to train PWL-based model. Figure 5b shows the estimated contour plots for different frequencies (hyperparameter) when switching between two objective functions. As we move from left to right, $(\mathcal{L}_{\text{mono}} - \mathcal{L}_{\text{NN}})$ has an overpowering effect and flat lines are observed. Hence, hyperparameter is crucial for maintaining equilibrium between losses. Figure 5a shows a graphical illustration for two different loss contour planes which are mutually inclined at an angle $\theta$ with respect to each other. If the contours are not perpendicular ($\theta \neq 90^\circ$), the SGD steps for each of the loss values could be sub-optimal. This may result in instability while training PWL and can be considered as one of the limitations. We plan to study the loss trade-off and sub-optimality analysis in future.