Counterexample-Guided Learning of Monotonic Neural Networks

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Abstract

The widespread adoption of deep learning is often attributed to its automatic feature construction with minimal inductive bias. However, in many real-world tasks, the learned function is intended to satisfy domain-specific constraints. We focus on monotonicity constraints, which are common and require that the function’s output increases with increasing values of specific input features. We develop a counterexample-guided technique to provably enforce monotonicity constraints at prediction time. Additionally, we propose a technique to use monotonicity as an inductive bias for deep learning. It works by iteratively incorporating monotonicity counterexamples in the learning process. Contrary to prior work in monotonic learning, we target general ReLU neural networks and do not further restrict the hypothesis space. We have implemented these techniques in a tool called COMET. Experiments on real-world datasets demonstrate that our approach achieves state-of-the-art results compared to existing monotonic learners, and can improve the model quality compared to those that were trained without taking monotonicity constraints into account.

1 Introduction

Deep neural networks are increasingly used to make sensitive decisions, including financial decisions such as whether to give a loan to an applicant [26] and as controllers for safety critical systems such as autonomous vehicles [7]. In these settings, for safety, ethical, and legal reasons, it is of utmost importance that some of the decisions made are monotonic. For example, one would expect an individual with a higher salary to have a higher loan amount approved, all else equal, and the speed of a drone to decrease with its proximity to the ground. Learning problems in medicine, revenue-maximizing auctions [18], bankruptcy prediction, credit rating, house pricing, etc., all have monotonicity as a natural property to which a model should adhere. Guaranteeing monotonicity helps users to better trust and understand the learned model [25]. Furthermore, prior knowledge about monotonic relationships can also be an effective regularizer to avoid overfitting [15].

Unfortunately, there is no easy way to specify that a trained neural network should be monotonic in one or more of its features. Existing approaches to this problem, such as min-max networks [40], monotonic lattices [17], and deep lattice networks [53], guarantee monotonicity by construction but do so at the cost of significantly restricting the hypothesis class. Other solutions, such as learning a linear function with positive coefficients, are even more restrictive. Furthermore, techniques that

https://github.com/AishwaryaSivaraman/COMET

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enforce monotonicity as a soft constraint in neural networks \[41\] [24] suffer from not being able to provide any provable monotonicity guarantee at prediction time. Finally, the well-known framework of isotonic regression \[4\] [37] is effective only when the training data can be partially ordered, which is rarely the case in high dimensions.

This paper develops techniques to incorporate monotonicity constraints for standard ReLU neural networks without imposing further restrictions on the hypothesis space. These techniques leverage recent work that employs automated theorem provers to formally verify robustness and safety properties of neural networks \[49\] [50] [19] [29]. First, we present a counterexample-guided algorithm that provably guarantees monotonicity at prediction time, given an arbitrary ReLU neural network. Our approach works by constructing a monotonic envelope of the given model on-the-fly via verification counterexamples. Empirically we show that we guarantee monotonicity with little to no loss in model quality at a computational cost on the order of a few seconds on standard datasets. Second, we propose a new counterexample-guided algorithm to incorporate monotonicity as an inductive bias during training. We identify monotonicity counterexamples on the training data, inducing additional supervision for training the network, and perform this process iteratively. We also show that monotonicity is an effective regularizer: our counterexample-guided learning algorithm improves both generalization while guaranteeing monotonicity for both regression and classification tasks. We have implemented our algorithms in a tool called “C\text{ounterexample-guided Monotonicity Enforced Training}” (C\text{OMET}). Finally, we demonstrate that C\text{OMET} outperforms min-max and deep lattice networks \[53\] on four real-world benchmarks.

\textbf{Organization.} Section 2 introduces our problem statement and notation. Sections 3 and 4 respectively describe our proposed algorithms: counterexample-guided monotonic prediction and counterexample-guided monotonic training. Experimental results in Section 5.2 and 4.2 demonstrate the potential of C\text{OMET} on real-world benchmark datasets. Section 5 reviews related work in learning monotonic functions. We conclude and provide future directions in Section 6.

\section{Preliminaries: Finding Monotonicity Counterexamples}

We begin by introducing some common notation. Let \(\mathcal{X}\) be the input space consisting of \(d\) features, and suppose that it is a compact finite subset \(\mathcal{X} = [L, U]^d\) of \(\mathbb{R}^d\). Let \(\mathcal{Y}\) be the output space. We consider regression and (probabilistic) binary classification tasks where \(\mathcal{Y}\) is totally ordered.

Our goal will be to learn functions that are monotonic in some of their input features.

\textbf{Definition 1.} A function \(f : \mathcal{X} \to \mathcal{Y}\) is \textit{monotonically increasing} in features \(S\) iff each feature in \(S\) is totally ordered and for any two inputs \(x, x' \in \mathcal{X}\) that are (i) non-decreasing in features \(S\), \(\forall i \in S, x_i \leq x'_i\), and (ii) holding all else equal, \(\forall k \notin S, x[k] = x'[k]\), the output of the function is non-decreasing: \(f(x) \leq f(x')\).

Formal properties of functions are often characterized in terms of their counterexamples. Counterexample-guided algorithms are prevalent in the field of formal methods, for example to verify \[10\] and synthesize programs \[24\]. The techniques proposed in this paper will be centered around using counterexamples to the monotonicity specification.

\textbf{Definition 2.} A pair of inputs \(x, x' \in \mathcal{X}\) is a \textit{monotonicity counterexample pair} for the \(i\)th feature of function \(f : \mathcal{X} \to \mathcal{Y}\) iff the points are (i) non-decreasing in feature \(i\), that is, \(x[i] \leq x'[i]\), (ii) holding all else equal, that is, \(\forall k \neq i, x[k] = x'[k]\), and (iii) the function is decreasing: \(f(x) > f(x')\).

Notably, for a function to be (jointly) monotonic in features \(S\), it is both necessary and sufficient that there does not exist a monotonicity counterexample pair for any of the individual features in \(S\).

ReLU neural networks generalize well and are widely used \[21\] [51] [14], particularly in the context of verification and robustness. Hence, we will assume that \(f\) is a ReLU neural network.

\textbf{Definition 3.} A ReLU neural network consists of neurons that compute \(\text{ReLU}(\sum_i w_i x_i + b)\), where the activation function is a rectified linear unit \(\text{ReLU}(y) = \max(0, y)\), the weights \(w_i\) and bias \(b\) are parameters associated with each neuron, and neuron inputs \(x_i\) are either input features or values of other neurons. The value of a designated output neuron defines the value of a function \(f : \mathcal{X} \to \mathcal{Y}\).
Counterexample-guided algorithms rely on the ability to find counterexamples, usually by relegating the task to an off-the-shelf solver. This requires that both the counterexample specification and the object of interest – in this case the function $f$ – can be encoded in a formal language amenable to automated reasoning. We will use a *satisfiability modulo theories* (SMT) solver [5] for this purpose. Recall that satisfiability (SAT) is the problem of deciding the existence of assignments of truth values to variables such that a propositional logical formula is satisfied. SMT generalizes SAT to deciding satisfiability for formulas with respect to a decidable background theory [5]. We will use the background theory of linear real arithmetic (LRA), which allows for expressing Boolean combinations of linear inequalities between real number variables.

The encoding of ReLU neural networks into SMT(LRA) is well-known and readily available [29, 28]. Briefly, the relationship between any neuron value and its inputs is encoded in SMT(LRA) as follows. The linear sum over neuron inputs is already a linear constraint. Additionally, we encode the non-linearity of the ReLU activation function using logical implications in SMT. Concretely, for $z = \text{ReLU}(y) = \max(0, y)$, we add two SMT constraints: $y > 0 \rightarrow z = y$ and $y \leq 0 \rightarrow z = 0$.

We can now ask an SMT solver to find monotonicity counterexample pairs: we simply take the (linear) conditions in Definition 2 while encoding the function $f$ into SMT(LRA). Linear real arithmetic is a decidable theory [45]; hence we will always obtain a correct counterexample if one exists. In Section 3, we require the ability to obtain a counterexample that maximally violates the monotonicity specification. Hence, we use Optimization Modulo Theories (OMT) [38], which is an extension of SMT for finding models that optimize secondary linear objectives, which is again decidable. Note that our definitions consider monotonically increasing features, and we assume that form of monotonicity throughout. We can analogously define corresponding notions for monotonically decreasing features, and our algorithms can be applied straightforwardly to that setting as well.

While this setup allows us to verify monotonicity of a learned function, it is not at all clear how to guarantee monotonicity, or how to enforce monotonicity during training as an inductive bias. The next two sections present the counterexample-guided algorithms that address these challenges.

### 3 Counterexample-Guided Monotonic Prediction

A neural network trained using traditional approaches is not guaranteed to satisfy monotonicity constraints. In this section, we describe a technique to convert a non-monotonic model to a monotonic one. The technique leverages monotonicity counterexamples to construct a monotonic *envelope* (or *hull*) of the learned model. Further, our technique is online: the monotonic envelope is constructed on-the-fly at prediction time.

As an example, consider the regression task of predicting house prices, which monotonically increase with the number of rooms. Suppose that the solid line (---) in Figure 1 plots the learned model’s predictions. This function is not monotonic: for example $f(3) > f(4)$. The two dotted lines in Figure 1 show two monotonic envelopes that our technique produces: an upper envelope (----) that increases the output where necessary to ensure monotonicity, and a lower envelope (- - -) that decreases the output where necessary to ensure monotonicity. The rest of this section describes these envelopes formally and presents an empirical evaluation of the technique.

#### 3.1 Envelope Construction

We first describe the envelope construction for the single-dimensional case and then generalize the approach to handle multiple monotonic features.

##### 3.1.1 Envelope - Single-Dimensional Case

Recall that Definition 2 in the previous section defines when a pair of inputs constitutes a monotonicity counterexample. To construct the envelope we require a special form of such counterexamples, namely *maximal* ones in terms of the degree of monotonicity violation, while fixing a single input example.
We will prove that it is not necessary to construct the envelope function explicitly (even representing it compactly appears to be impossible). Rather, to ensure monotonicity, it suffices to construct the envelope incrementally at prediction time. Given an input $x'$, we make a single query to an SMT solver to find the input’s upper (lower) envelope counterexample or determine that no such counterexample exists. Note that this query is much simpler than would be required to verify that the original function is monotonic. Doing the latter would require searching for an arbitrary monotonicity counterexample pair (Definition 7), which is a pair of points. In contrast, our query is given the input $x'$ and hence only requires the SMT solver to search over the space of inputs that are identical to $x'$ except in the $i$th dimension. Concretely, for a feature $i$ in the bounded interval $[L, U]$, the upper envelope search is over the interval $[L, x'[i])$ and the lower envelope search is over the interval $(x'[i], U]$. Empirically we will later show that our envelope construction is faster than querying for an arbitrary counterexample pair (see Figure 3).

### 3.1.2 Envelope - Multi-Dimensional Case

We now generalize our envelope construction to the case where multiple dimensions are monotonic. For space reasons we present only the upper envelope construction; the lower envelope is analogous.

Recall from Section 2 that, to verify if a function is monotonic in more than one dimension, it is sufficient to verify that it is monotonic in each dimension separately. However, to construct the envelope, it is not sufficient to identify maximal counterexamples in each dimension and then take the maximum of these maxima. The envelopes produced using that approach are not guaranteed to be monotonic (see appendix for an example). To overcome this problem, we generalize to multiple dimensions by searching jointly in all monotonic dimensions and prove that this approach is correct.

**Definition 6.** Consider example $x \in X$, function $f : X \to Y$, and set of features $S$. Let set $B$ consist of all examples $x'$ such that $\forall i \in S, x'[i] \leq f[i]$ and $\forall i \notin S, x'[k] = x[k]$ and $f(x') > f(x)$. An upper envelope counterexample is an example $x' \in B$ that maximizes $f(x')$.

It is easy to show that this approach does not identify spurious counterexamples: if an upper envelope counterexample exists for $x$ and $f$ and set of features $S$, then there is a dimension $i \in S$ and points $x'$ and $x''$ such that $x'$ and $x''$ are a monotonicity counterexample for $f$ in the $i$th dimension.

We can now define the upper envelope function, analogous to the single-dimensional case:

**Definition 7.** The upper envelope $f^u_S$ of function $f : X \to Y$ for feature set $S$ is defined as follows:

$$f^u_S(x) = \begin{cases} f(x') & \text{where } x' \text{ is an upper envelope counterexample for } x, f, \text{ and } S \\ f(x) & \text{if no such counterexample exists} \end{cases}$$

Finally, we prove that the upper envelope is in fact monotonic, even when the function $f$ is not.

**Theorem 1.** For any function $f$ and set of features $S$, the upper envelope $f^u_S$ is monotonic in $S$.

**Proof.** Let $i_0 \in S$ and $x$ and $x'$ be any two inputs such that $x[i_0] \leq x'[i_0]$ and $\forall k \neq i_0, x[k] = x'[k]$. We will prove that $f^u_S(x) \leq f^u_S(x')$ and hence that $f^u_S$ is monotonic. There are two cases:
1. An input \( x' \) is the upper envelope counterexample for \( x' \), \( f \), and \( S \), so \( f_S^u(x') = f(x') \).

We have two subcases.

- An input \( x_e \) is the upper envelope counterexample for \( x \), \( f \), and \( S \), so \( f_S^u(x) = f(x_e) \). By Definition 6 we have that \( \forall i \in S, x_e[i] \leq x[i] \land \forall i \not{\in} S, x_e[k] = x[k] \), so also \( \forall i \in S, x_e[i] \leq x'[i] \land \forall i \not{\in} S, x_e[k] = x'[k] \). Therefore again by Definition 6 it must be the case that \( f(x_e) \leq f(x') \).

- There is no upper envelope counterexample for \( x \), \( f \), and \( S \), so \( f_S^u(x) = f(x) \). Since \( \forall i \in S, x[i] \leq x'[i] \land \forall i \not{\in} S, x[k] = x'[k] \), by Definition 6 it must be the case that \( f(x) \leq f(x') \).

2. There is no upper envelope counterexample for \( x' \), \( f \), and \( S \). The proof is similar (details in appendix).

Hence, our envelope construction algorithm guarantees monotonicity of the predictive function, regardless of where it is evaluated, and regardless of the underlying learned function.

3.2 Empirical Evaluation of Monotonic Envelopes

We report the experimental results on the quality and performance of the envelope construction algorithm. Experiments were implemented in Python using the Keras deep learning library [9], we use the ADAM optimizer [30] to perform stochastic optimization of the neural network models, and the Optimathsat [39] solver for counterexample generation. The code and data will be made available upon publication of this paper.

Data and experiment setup: We use four datasets: Auto MPG and Boston Housing are regression datasets used for predicting miles per gallon (monotonically decreasing with respect to features weight (\( W \)), displacement (\( D \)), and horsepower (\( HP \))) and housing prices (monotonically decreasing in crime rate and increasing in number of rooms) respectively and are obtained from the UCI machine learning repository [6]; Heart Disease [20] and Adult [6] are classification datasets used for predicting the presence of heart disease (monotonically increasing with \( \text{trestbps} \) (\( T \)), \( \text{cholesterol} \) (\( C \))) and income level (monotonically increasing with \( \text{capital-gain} \) and \( \text{hours per week} \)) respectively. For each dataset, we identify the best baseline architecture and parameters by conducting grid search and we learn the best ReLU neural network (\( \text{NN}_b \)) with 3-fold validation of 80/20 split, except for the Adult dataset, for which we did 1-fold validation (see appendix for more details).

Q1. Is a deep neural network trained on such data monotonic? Figure 2 shows that the best baseline model (\( \text{NN}_b \)) is not monotonic. The figure presents the percentage of counterexamples in test and train data that have an upper or lower envelope counterexample for the Auto MPG dataset.

![Figure 2: Empirically, the best learned baseline model is not monotonic. The figure presents the percentage of counterexamples in test and train data that have an upper or lower envelope counterexample for the Auto MPG dataset.](image)

| Dataset | Feature | \( \text{NN}_b \) | Envelope |
|---------|---------|----------------|----------|
| Auto-MPG | Weight | 9.33±3.22 | 9.19±3.41 |
|          | Displ.  | 9.33±3.22 | 9.63±2.61 |
|          | W,D     | 9.33±3.22 | 9.63±2.61 |
|          | W,D,HP  | 9.33±3.22 | 9.63±2.61 |
| Boston  | Rooms   | 14.37±2.4  | 14.19±2.28 |
|          | Crime   | 14.37±2.4  | 14.02±2.17 |

Q2. When enforcing monotonicity using an envelope, does it come at a cost in terms of prediction quality? In this experiment, we compare the quality of the original model (\( \text{NN}_b \)) with its
envelope on the test data. We select the envelope with the lowest train mean squared error (MSE) in case of regression and highest train accuracy in case of classification. Table 1 demonstrates that envelope can be used in both single and multi-dimensional cases, with little to no loss in prediction quality. In fact, in some cases (see rows in bold), the envelope has better average quality. This can be explained as follows: although the true data distribution is naturally monotonic, existing learning algorithms might be missing simpler monotonic models, or existing models might be overfitting to a non-monotonic function because of noise in the training data.

Q3. How scalable is on-the-fly envelope construction? In this experiment, we report the run times for the Auto MPG dataset. Recall that the envelope approach need only search for maximal counterexamples relative to a given input. Owing to the narrowed search space, we see that envelope prediction time is comparable to the baseline model’s prediction time in smaller models (see Figure 3). Overhead caused by envelope construction is only a few seconds. In contrast, the overhead to finding maximal counterexample pair (Definition 2) for a single monotonic feature is 48.29 minutes. This illustrates the computational advantage of our algorithm.

As a scalability study, in Figure 4, we plot the time taken to obtain a monotonic prediction for various model sizes. We can see that the envelope prediction time is comparable to the baseline prediction time in smaller models but grows with the model size. The growth is significantly less pronounced in the number of monotonic features.

4 Counterexample-Guided Monotonicity Enforced Training

In this section we propose an algorithm that uses monotonicity as an inductive bias during learning to improve model quality. This algorithm is orthogonal to the envelope prediction technique of the previous section; we evaluate the learning algorithm both on its own and in conjunction with the envelope technique.

4.1 Counterexample-guided Learning

The learning algorithm consists of two phases that iterate: the training phase and the verification phase. The training phase is given labeled input data and produces the best candidate model \( f \). The verification phase checks if a given model is monotonic; if not then generates one or more counterexamples, which are provided as additional data for the next iteration of the training phase.

The algorithm starts by training the best model for a given set of input data, and then re-training with counterexamples iterates for \( T \) epochs, which is a hyperparameter to the algorithm. The algorithm is universal in the sense that it is compatible with any training technique that produces ReLU models and does not further restrict the hypothesis class. This gives our approach an advantage over prior monotonic learners [40, 53].

The verification phase could use Definition 2 to identify monotonicity counterexamples, but this has two major drawbacks: (1) it is computationally expensive as the size of the pre-trained model grows; (2) an arbitrary counterexample might include out-of-distribution examples, which are therefore not representative. Hence, we instead appeal to Definition 6 to generate maximal counterexamples relative to each training point. In each epoch, for each train point we generate and use both upper and lower envelope counterexamples as additional data for the next round of training.

At this point, we are almost done with the algorithm, with the following detail to address. Counterexamples generated by the verification procedure do not have a known ground-truth label. There are different heuristics that one could adopt to label these points and encourage the learned function to become more monotonic. In our algorithm, for regression tasks we calculate the average prediction values of upper and lower counterexamples and the given training point and assign this average as the label for these counterexamples and the training point. The hypothesis is that using the average value will result in a smoother loss with respect to monotonicity. For classification tasks, we assign
We will now evaluate our iterative algorithm for training with monotonicity counterexamples, as well as the entire COMET pipeline, which also includes the envelope technique from the previous section. We use the same datasets and hardware as in Section 3.2.

Table 2: Counterexample-guided Learning (CGL) improves the quality of the baseline model in regression (MSE, Left Table) and classification (Accuracy, Right Table) datasets

| Dataset | Feature | NNb | CGL |
|---------|---------|-----|-----|
| Auto-MPG | Weight | 9.33±3.22 | 9.04±2.76 |
|         | Displ. | 9.33±3.22 | 9.08±2.87 |
|         | W,D   | 9.33±3.22 | 8.86±2.67 |
|         | W,D,HP| 9.33±3.22 | 8.63±2.21 |
| Boston  | Rooms | 14.37±2.4 | 12.24±2.87 |
|         | Crime | 14.37±2.4 | 11.66±2.89 |

| Dataset | Feature | NNb | CGL |
|---------|---------|-----|-----|
|         | Trestbps| 0.85±0.04 | 0.86±0.02 |
|         | Chol.   | 0.85±0.04 | 0.85±0.05 |
|         | T,C     | 0.85±0.04 | 0.86±0.06 |
| Adult   | Cap. Gain| 0.84     | 0.84   |
|         | Hours   | 0.84     | 0.84   |

Q4. Is the stronger inductive bias of our learning algorithm able to improve the overall quality of the original non-monotonic model? In this experiment we compare the test quality of the model learned with monotonicity counterexamples with the original model (NNb). From Table 2 we can see that monotonicity is indeed an effective inductive bias that helps improve the model quality. It is able to reduce the error on all regression datasets, with the biggest decrease from 14.37 to 11.66 for the Boston Housing dataset when employing monotonicity counterexamples based on the Crime Rate feature. Although the algorithm improves the quality, it does not guarantee monotonic predictions.

Q5. Does our learning algorithm make the original non-monotonic model more monotonic? To quantify if a function is more monotonic, we calculate the reduction in the number of counterexamples. On average, our algorithm reduces the number of test counterexamples by 62%. Although in some cases, we can remove all counterexamples, in general, this is not the case (see Table 3 in Appendix for detailed results). This motivates the need for using monotonic envelopes (described in Section 4) in conjunction with the counterexample-guided learning algorithm, to guarantee monotonic predictions.

Table 3: For regression (MSE, Left Table) and classification (Accuracy, Right Table) datasets, counterexample-guided learning improves the envelope quality

| Dataset | Features | NNb, Env. | COMET |
|---------|----------|-----------|-------|
| Auto-MPG | Weight | 9.19±3.41 | 8.92±2.93 |
|         | Displ. | 9.63±2.61 | 9.11±2.25 |
|         | W,D   | 9.63±2.61 | 8.89±2.29 |
|         | W,D,HP| 9.33±2.61 | 8.81±1.81 |
| Boston  | Rooms | 14.19±2.28 | 11.54±2.55 |
|         | Crime | 14.02±2.17 | 11.07±2.99 |

| Dataset | Features | NNb, Env. | COMET |
|---------|----------|-----------|-------|
|         | Trestbps| 0.85±0.04 | 0.86±0.03 |
|         | Chol.   | 0.85±0.05 | 0.87±0.03 |
|         | T,C     | 0.85±0.05 | 0.86±0.03 |
| Adult   | Cap. Gain| 0.84     | 0.84   |
|         | Hours   | 0.84     | 0.84   |

Q6. Does counterexample-guided learning help improve the quality of the original model’s envelope? In Section 3.2 Q2, (Table 1), we showed that envelope has similar model quality compared to the baseline model. By additionally enforcing monotonicity constraints through counterexample-guided re-training, we further improve the envelope quality (Table 3). In this experiment we re-train NNb with counterexamples for 40 epochs, model selection is based on train quality, and we report the change in the quality of the test envelope (see Appendix for additional model selection experiments). Thus, we get both a monotonicity guarantee, as well as better generalization performance.

Q7. How does the performance of COMET compare to existing work? Table 4 reports MSE and accuracy of COMET, compared to two existing methods that guarantee monotonicity: min-max network [12] and deep lattice networks (DLN) [5]. For DLN, we report the results based on the six-layer DLN architecture, as proposed by the authors. We tune the Adam stepsize, learning rate, number of epochs, batch size, and number of keypoints. Similarly, for min-max network, we tune the Adam stepsize, learning rate, number of epochs, and batch size. The results in Table 4 indicate
that COMET outperforms both of these existing approaches in all datasets except the Adult dataset, where we achieve similar results.

## 5 Related Work

**Monotonic Networks.** Related work in this area can be categorized into algorithms that (1) guarantee monotonicity, or (2) incorporate monotonicity during learning without any guarantees. In the first category, monotonicity is guaranteed by restricting the hypothesis space. Archer and Wang [3] propose a monotone model by constraining the neural net weights to be positive. Other methods enforce constraints on model weights [11, 46, 33, 16, 2], and force the derivative of the output to be strictly positive [47]. Monotonic networks [40] guarantee monotonicity by constructing a three-layer network using monotonic linear embedding and max-min-pooling. Daniels and Velikova [13] generalized this approach to handle functions that are partially monotonic. Deep lattice networks (DLN) [63] proposed a combination of linear calibrators and lattices for learning monotonic functions. Lattices are structurally rigid thereby restricting the hypothesis space significantly. Our envelope technique is similar to these works in that it guarantees monotonicity. However, it does so at prediction time and can do so for any ReLU neural networks, without needing to restrict the hypothesis space further. Finally, isotonic regression [4, 37] requires the training data to be partially ordered, which is unlikely to happen: it requires that non-monotonic features are identical between examples.

In the second category, monotonicity can be incorporated in the learning process by modifying the loss function or by adding additional data. Monotonicity Hints [41] proposes a modified loss function that penalizes non-monotonicity of the model. The algorithm models the input distribution as a joint Gaussian estimated from the training data and samples random pairs of monotonic points that are added to the training data. Gupta et. al. [24] introduce a point-wise loss function that acts as soft monotonicity constraints. Our approach is similar to these works in that it adds additional data to enforce monotonicity. However, COMET’s counterexample-guided learning and envelope technique together guarantee monotonicity, while these works provide no such guarantees. In addition, unlike prior work, since we look for maximum violations, we look beyond the neighborhood of a training point. Other works enforce monotonicity to accelerate learning of probabilistic models in data-scarce and knowledge-rich domains [34, 1, 52]. Similarly, these works fail to provide any formal guarantee for the learned model.

**Verification of Neural Networks and Adversarial Learning.** Reluplex [29], an augmented SMT solver, verifies properties of networks with ReLU activation functions. Huang et. al. [28] leverage SMT by discretizing the continuous region around an input and show that there are no counterexamples. Our approach leverages the SMT encodings of neural networks from this prior work but uses them only to obtain counterexamples rather than for verification. Recently, many approaches propose adversarially robust algorithms which can be divided into empirical [31, 32, 22, 23] and certified defenses [48, 43, 35, 27, 36, 42, 19]. We are closely related to these works, in that we carry out adversarial training using counterexamples. However, we differ in two ways. First, to the best of our knowledge, there is no related work in adversarial robustness literature for ensuring monotonicity. Second, related work in adversarial training only ensures correctness in the neighborhood of a training point, while we globally search for a counterexample and are able to discover long-range monotonicity violations. Counterexample-driven learning has also been used to enforce fairness constraints on Bayesian classifiers [8].
6 Conclusion

We presented two algorithms that incorporate monotonicity constraints into neural networks: counterexample-guided prediction that guarantees monotonicity and counterexample-guided training that enforces monotonicity as an inductive bias. We demonstrate the effectiveness of these techniques on regression and classification tasks. In future, we plan to further increase the scalability of COMET, and study how to modify learning in order to enable that scalability. Another interesting direction for future work is to study other types of inductive bias, such as algorithmic fairness. We plan to explore new strategies that use counterexamples to learn with and enforce these desirable properties.

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Broader Impact In scenarios where monotonicity is a natural and fair requirement on the learned function, it is clear that eliminating errors or noise coming from monotonicity violations can increase the fairness of the predictions, and eliminate some frustration with receiving arbitrary outcomes. At the same time, one can imagine someone requiring monotonicity of certain features that should not be monotonic, and the work in this paper can enable such undesirable behavior. By incorporating correct and ethical domain knowledge using our algorithms, we make a learned model more robust. We acknowledge that the counterexamples generated based on data can be used in ways other than the mentioned ways in the paper. Although our approach can produce monotonic predictions, it is still based on a model produced by a machine learning algorithm. Therefore, it becomes essential to understand that the monotonic model could also suffer from the same disadvantages as the original model, and reinforce the same biases. Hence, the user must be aware of such a system’s limitations, especially when using these models to replace people in decision making.

References

[1] Eric E Altendorf, Angelo C Restificar, and Thomas G Dietterich. Learning from sparse data by exploiting monotonicity constraints. arXiv preprint arXiv:1207.1364, 2012.

[2] Brandon Amos, Lei Xu, and J Zico Kolter. Input convex neural networks. In Proceedings of the 34th International Conference on Machine Learning-Volume 70, pages 146–155. JMLR. org, 2017.

[3] Norman P. Archer and Shouhong Wang. Learning bias in neural networks and an approach to controlling its effect in monotonic classification. IEEE transactions on pattern analysis and machine intelligence, 15(9):962–966, 1993.

[4] Richard E Barlow and Hugh D Brunk. The isotonic regression problem and its dual. Journal of the American Statistical Association, 67(337):140–147, 1972.

[5] Clark Barrett and Cesare Tinelli. Satisfiability modulo theories. In Handbook of Model Checking, pages 305–343. Springer, 2018.

[6] Catherine L Blake and Christopher J Merz. Uci repository of machine learning databases, 1998, 1998.

[7] Mariusz Bojarski, Davide Del Testa, Daniel Dworakowski, Bernhard Firner, Beat Flepp, Prasoon Goyal, Lawrence D Jackel, Mathew Monfort, Urs Muller, Jiakai Zhang, et al. End to end learning for self-driving cars. arXiv preprint arXiv:1604.07316, 2016.

[8] YooJung Choi, Golnoosh Farnadi, Behrouz Babaki, and Guy Van den Broeck. Learning fair naive bayes classifiers by discovering and eliminating discrimination patterns. In Proceedings of the 34th AAAI Conference on Artificial Intelligence, 2020.

[9] François Chollet et al. Keras. https://github.com/keras-team/keras, 2015.
[10] Edmund Clarke, Orna Grumberg, Somesh Jha, Yuan Lu, and Helmut Veith. Counterexample-guided abstraction refinement. In *International Conference on Computer Aided Verification*, pages 154–169. Springer, 2000.

[11] Hennie Daniels and B Kamp. Application of mlp networks to bond rating and house pricing. *Neural Computing & Applications*, 8(3):226–234, 1999.

[12] Hennie Daniels and Marina Velikova. Monotone and partially monotone neural networks. *IEEE Trans. Neural Networks*, 21(6):906–917, 2010.

[13] Hennie Daniels and Marina Velikova. Monotone and partially monotone neural networks. *IEEE Transactions on Neural Networks*, 21(6):906–917, 2010.

[14] Marcelo Carvalho dos Santos, Victor Henrique Cabral Pinheiro, Filipe Santana Moreira do Desterro, Renato Koga de Avellar, Roberto Schirru, Andressa dos Santos Nicolau, and Alan Miranda Monteiro de Lima. Deep rectifier neural network applied to the accident identification problem in a pwr nuclear power plant. *Annals of Nuclear Energy*, 133:400–408, 2019.

[15] Charles Dugas, Yoshua Bengio, François Bélisle, Claude Nadeau, and René Garcia. Incorporating second-order functional knowledge for better option pricing. In *Advances in neural information processing systems*, pages 472–478, 2001.

[16] Charles Dugas, Yoshua Bengio, François Bélisle, Claude Nadeau, and René Garcia. Incorporating functional knowledge in neural networks. *Journal of Machine Learning Research*, 10(Jun):1239–1262, 2009.

[17] Mahdi Milani Fard, Kevin Canini, Andrew Cotter, Jan Pfeifer, and Maya Gupta. Fast and flexible monotonic functions with ensembles of lattices. In *Advances in Neural Information Processing Systems*, pages 2919–2927, 2016.

[18] Zhe Feng, Harikrishna Narasimhan, and David C Parkes. Deep learning for revenue-optimal auctions with budgets. In *Proceedings of the 17th International Conference on Autonomous Agents and Multiagent Systems*, pages 354–362. International Foundation for Autonomous Agents and Multiagent Systems, 2018.

[19] Timon Gehr, Matthew Mirman, Dana Drachsler-Cohen, Petar Tsankov, Swarat Chaudhuri, and Martin Vechev. Ai2: Safety and robustness certification of neural networks with abstract interpretation. In *2018 IEEE Symposium on Security and Privacy (SP)*, pages 3–18. IEEE, 2018.

[20] John H. Gennari, Pat Langley, and Douglas H. Fisher. Models of incremental concept formation. *Artif. Intell.*, 40(1-3):11–61, 1989.

[21] Xavier Glorot, Antoine Bordes, and Yoshua Bengio. Deep sparse rectifier neural networks. In *Proceedings of the fourteenth international conference on artificial intelligence and statistics*, pages 315–323, 2011.

[22] Ian J Goodfellow, Jonathon Shlens, and Christian Szegedy. Explaining and harnessing adversarial examples. *arXiv preprint arXiv:1412.6572*, 2014.

[23] Shixiang Gu and Luca Rigazio. Towards deep neural network architectures robust to adversarial examples. *arXiv preprint arXiv:1412.5068*, 2014.

[24] Akhil Gupta, Naman Shukla, LLC Deepair, Lavanya Marla, Arinbjörn Kolbeinsson, and Kartik Yellepeddi. How to incorporate monotonicity in deep networks while preserving flexibility? In *Advances in Neural Information Processing Systems 32*. Curran Associates, Inc., 2019.

[25] Maya Gupta, Andrew Cotter, Jan Pfeifer, Konstantin Voevodski, Kevin Canini, Alexander Mangylov, Wojciech Moczylowski, and Alexander Van Esbroeck. Monotonic calibrated interpolated look-up tables. *The Journal of Machine Learning Research*, 17(1):3790–3836, 2016.

[26] Moritz Hardt, Eric Price, and Nati Srebro. Equality of opportunity in supervised learning. In *Advances in neural information processing systems*, pages 3315–3323, 2016.

[27] Matthias Hein and Maksym Andriushchenko. Formal guarantees on the robustness of a classifier against adversarial manipulation. In *Advances in Neural Information Processing Systems*, pages 2266–2276, 2017.

[28] Xiaowei Huang, Marta Kwiatkowska, Sen Wang, and Min Wu. Safety verification of deep neural networks. In *International Conference on Computer Aided Verification*, pages 3–29. Springer, 2017.
[29] Guy Katz, Clark Barrett, David L Dill, Kyle Julian, and Mykel J Kochenderfer. Reluplex: An efficient smt solver for verifying deep neural networks. In International Conference on Computer Aided Verification, pages 97–117. Springer, 2017.

[30] Diederik P Kingma and Jimmy Ba. Adam: A method for stochastic optimization. arXiv preprint arXiv:1412.6980, 2014.

[31] Alexey Kurakin, Ian Goodfellow, and Samy Bengio. Adversarial machine learning at scale. arXiv preprint arXiv:1610.02246, 2016.

[32] Aleksander Madry, Aleksandar Makelov, Ludwig Schmidt, Dimitris Tsipras, and Adrian Vladu. Towards deep learning models resistant to adversarial attacks. arXiv preprint arXiv:1706.06083, 2017.

[33] Alexey Minin, Marina Velikova, Bernhard Lang, and Hennie Daniels. Comparison of universal approximators incorporating partial monotonicity by structure. Neural Networks, 23(4):471–475, 2010.

[34] Phillip Odom and Sriraam Natarajan. Human-guided learning for probabilistic logic models. Frontiers in Robotics and AI, 5:56, 2018.

[35] Aditi Raghunathan, Jacob Steinhardt, and Percy Liang. Certified defenses against adversarial examples. arXiv preprint arXiv:1801.09344, 2018.

[36] Hadi Salman, Jerry Li, Ilya Razenshteyn, Pengchuan Zhang, Huan Zhang, Sebastien Bubeck, and Greg Yang. Provably robust deep learning via adversarially trained smoothed classifiers. In Advances in Neural Information Processing Systems, pages 11289–11300, 2019.

[37] Michael J Schell and Bahadur Singh. The reduced monotonic regression method. Journal of the American Statistical Association, 92(437):128–135, 1997.

[38] Roberto Sebastiani and Silvia Tomasi. Optimization modulo theories with linear rational costs. ACM Transactions on Computational Logic (TOCL), 16(2):1–43, 2015.

[39] Roberto Sebastiani and Patrick Trentin. Optimathsat: A tool for optimization modulo theories. Journal of Automated Reasoning, Dec 2018.

[40] Joseph Sill. Monotonic networks. In Advances in neural information processing systems, pages 661–667, 1998.

[41] Joseph Sill and Yaser S Abu-Mostafa. Monotonicity hints. In Advances in neural information processing systems, pages 634–640, 1997.

[42] Gagandeep Singh, Timon Gehr, Matthew Mirman, Markus Püschel, and Martin Vechev. Fast and effective robustness certification. In Advances in Neural Information Processing Systems, pages 10802–10813, 2018.

[43] Aman Sinha, Hongseok Namkoong, and John Duchi. Certifiable distributional robustness with principled adversarial training. arXiv preprint arXiv:1710.10571, 2, 2017.

[44] Armando Solar-Lezama, Liviu Tancau, Rastislav Bodik, Sanjit Seshia, and Vijay Saraswat. Combinatorial sketching for finite programs. In Proceedings of the 12th international conference on Architectural support for programming languages and operating systems, pages 404–415, 2006.

[45] Alfred Tarski. A decision method for elementary algebra and geometry. In Quantifier elimination and cylindrical algebraic decomposition, pages 24–84. Springer, 1998.

[46] Shouhong Wang. A neural network method of density estimation for univariate unimodal data. Neural Computing & Applications, 2(3):160–167, 1994.

[47] Antoine Wehenkel and Gilles Louppe. Unconstrained monotonic neural networks. In Advances in Neural Information Processing Systems, pages 1543–1553, 2019.

[48] Eric Wong and J Zico Kolter. Provable defenses against adversarial examples via the convex outer adversarial polytope. arXiv preprint arXiv:1711.00851, 2017.

[49] Weiming Xiang, Hoang-Dung Tran, and Taylor T Johnson. Reachable set computation and safety verification for neural networks with relu activations. arXiv preprint arXiv:1712.08163, 2017.
Theorem 1. For any function $f$ and set of features $S$, the upper envelope $f^u_S$ is monotonic in $S$.

Proof. Let $i_0 \in S$ and $x$ and $x'$ be any two inputs such that $x[i_0] \leq x'[i_0]$ and $\forall k \neq i_0, x[k] = x'[k]$. We will prove that $f^u_S(x) \leq f^u_S(x')$ and hence that $f^u_S$ is monotonic. There are two cases:

- An input $x'_e$ is the upper envelope counterexample for $x'$, $f$, and $S$, so $f^u_S(x') = f(x'_e)$ and by Definition 6 $f(x') < f(x'_e)$. We have two subcases.
  - An input $x_e$ is the upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x_e)$. By Definition 6 we have that $\forall i \in S, x_e[i] \leq x[i] \land \forall i \not\in S, x_e[k] = x[k]$, so also $\forall i \in S, x_e[i] \leq x'[i] \land \forall i \not\in S, x_e[k] = x'[k]$. Therefore again by Definition 6 either $f(x_e) \leq f(x')$ or $f(x_e) \leq f(x'_e)$. Since $f(x') < f(x'_e)$, either way we have that $f(x_e) \leq f(x'_e)$.
  - There is no upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x)$. Since $\forall i \in S, x[i] \leq x'[i] \land \forall i \not\in S, x[k] = x'[k]$, by Definition 6 either $f(x) \leq f(x')$ or $f(x) \leq f(x'_e)$. Since $f(x') < f(x'_e)$, either way we have that $f(x) \leq f(x'_e)$.

- There is no upper envelope counterexample for $x'$, $f$, and $S$, so $f^u_S(x') = f(x')$. We have two subcases.
  - An input $x_e$ is the upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x_e)$. By Definition 6 we have that $\forall i \in S, x_e[i] \leq x[i] \land \forall i \not\in S, x_e[k] = x[k]$, so also $\forall i \in S, x_e[i] \leq x'[i] \land \forall i \not\in S, x_e[k] = x'[k]$. Therefore again by Definition 6 it must be the case that $f(x_e) \leq f(x')$, or else $x'$ would have an upper envelope counterexample.
  - There is no upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x)$. Then again by Definition 6 it must be the case that $f(x) \leq f(x')$, or else $x'$ would have an upper envelope counterexample. 

A Appendix

A.1 Envelope - Multi-Dimensional Case

Recall from Section 3.1.2 that to construct an envelope for a function $f$ and $S$ set of features, it is not sufficient to identify maximal counterexamples in each dimension and then take the maximum of these maxima. The envelopes produced using this approach are not guaranteed to be monotonic, which we now demonstrate with an example. Consider a function $f$ that is intended to be monotonically increasing in its two input features. Now, consider the point $(3, 5)$, suppose that $(1, 5)$ and $(3, 3)$ are the upper envelope counterexamples in each dimension (Definition 4), and suppose that $f(3, 5) > f(1, 5)$ so we set $f^u_{(1, 1)}(3, 5) = f(3, 3)$. Now consider a second point $(7, 5)$, suppose that $(1, 5)$ and $(7, 2)$ are the upper envelope counterexamples in each dimension, and suppose that $f(1, 5) > f(7, 2)$ so we set $f^u_{(1, 1)}(7, 5) = f(1, 5)$. Since $f(3, 3) > f(1, 5)$ we have that $f^u_{(1, 1)}(3, 5) > f^u_{(1, 1)}(7, 5)$, which violates monotonicity.

Therefore in the multi-dimensional case we search for counterexamples jointly over all monotonic dimensions (Definition 6). We now prove the correctness of this approach.

Theorem 1. Therefore in the multi-dimensional case we search for countereXamples that are the upper envelope counterexamples in each dimension (Definition 4), and suppose $\forall i \in S, x_e[i] \leq x[i] \land \forall i \not\in S, x_e[k] = x[k]$, so also $\forall i \in S, x_e[i] \leq x'[i] \land \forall i \not\in S, x_e[k] = x'[k]$. Therefore again by Definition 6 it must be the case that $f(x_e) \leq f(x')$, or else $x'$ would have an upper envelope counterexample.

We have

$$\forall x, f, S, \ f^u_S(x) \leq f^u_S(x').$$

We prove that $f^u_S(x) \leq f^u_S(x')$ and hence that $f^u_S$ is monotonic. There are two cases:

- An input $x'_e$ is the upper envelope counterexample for $x'$, $f$, and $S$, so $f^u_S(x') = f(x'_e)$ and by Definition 6 $f(x') < f(x'_e)$. We have two subcases.
  - An input $x_e$ is the upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x_e)$. By Definition 6 we have that $\forall i \in S, x_e[i] \leq x[i] \land \forall i \not\in S, x_e[k] = x[k]$, so also $\forall i \in S, x_e[i] \leq x'[i] \land \forall i \not\in S, x_e[k] = x'[k]$. Therefore again by Definition 6 either $f(x_e) \leq f(x')$ or $f(x_e) \leq f(x'_e)$. Since $f(x') < f(x'_e)$, either way we have that $f(x_e) \leq f(x'_e)$.
  - There is no upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x)$. Since $\forall i \in S, x[i] \leq x'[i] \land \forall i \not\in S, x[k] = x'[k]$, by Definition 6 either $f(x) \leq f(x')$ or $f(x) \leq f(x'_e)$. Since $f(x') < f(x'_e)$, either way we have that $f(x) \leq f(x'_e)$.

- There is no upper envelope counterexample for $x'$, $f$, and $S$, so $f^u_S(x') = f(x')$. We have two subcases.
  - An input $x_e$ is the upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x_e)$. By Definition 6 we have that $\forall i \in S, x_e[i] \leq x[i] \land \forall i \not\in S, x_e[k] = x[k]$, so also $\forall i \in S, x_e[i] \leq x'[i] \land \forall i \not\in S, x_e[k] = x'[k]$. Therefore again by Definition 6 it must be the case that $f(x_e) \leq f(x')$, or else $x'$ would have an upper envelope counterexample.
  - There is no upper envelope counterexample for $x$, $f$, and $S$, so $f^u_S(x) = f(x)$. Then again by Definition 6 it must be the case that $f(x) \leq f(x')$, or else $x'$ would have an upper envelope counterexample.

\[ \square \]
A.2 Empirical Evaluation

In this section we provide additional experiment setup details and results from Section 3.2 and Section 4.2.

**System Specifications and experiment Setup:** All experiments were run on an Intel(R) Xeon(R) Gold 5220 CPU @ 2.20GHz CPU with 512GB of DDR3 RAM running Ubuntu 18.04.3 LTS with kernel 5.3.0-28-generic. Experiments were implemented in Python using the Keras deep learning library [9]. We use the ADAM optimizer [30] to perform stochastic optimization of the neural network models, and the Optimathsat [39] solver for counterexample generation. For each dataset, we train five baseline architectures from a set of configurations and choose the best architecture based on train error. For *Boston Housing*, *Heart Diseases*, and *Adult* dataset, best baseline architecture includes three layers and 16 hidden neurons per layer. For *Auto MPG* dataset, best baseline architecture includes three layers and 12 hidden neurons per layer (see Table 7 for best baseline neural network parameters).

**Min-Max and Deep Lattice Network setup:** Min-Max network [12] proposes a fixed, feedforward three-layer (two hidden layer) architecture. The first layer computes different linear combinations of input that are partitioned into different groups. If increasing monotonicity is desired, then all weights connected to that input are constrained to be positive. Corresponding to each group, the second layer computes the maximum, and the final layer computes the minimum over all groups. For monotone features that are decreasing, we negate the feature to use the same architecture. The Deep Lattice Network [53] architecture consists of six layers as proposed by the authors: calibrators, linear embedding, calibrators, ensemble of lattices, calibrators, and linear embedding. Note that for these approaches, for each dataset, we tune parameters separately for each combination of monotone features at each fold using grid search; hence it is optimized for each monotone prediction task. However, for COMET it is sufficient to tune parameters for the original neural network (NNb) once per fold per dataset.

Table 5: Here we present the results referred to in Q1. Empirically, the best baseline neural network model (NNb) trained on data is not monotonic. The table presents the percentage of counterexamples found in test and train data that have an upper or lower envelope counterexample.

| Dataset     | Feature | Train % CG | Test % CG |
|-------------|---------|------------|-----------|
| Auto-MPG    | Weight  | 1.11       | 0.91      |
|             | Displ.  | 48.62      | 52.99     |
|             | W,D     | 50.85      | 54.7      |
|             | W,D,HP  | 50.96      | 54.7      |
| Boston Housing | Rooms  | 1.59       | 1.39      |
|             | Crime   | 16.75      | 16.5      |
| Heart       | Trestbps| 73.14      | 74.86     |
|             | Chol.   | 86.91      | 87.98     |
|             | T.C     | 97.38      | 98.91     |
| Adult       | Cap. Gain| 18.93      | 19.58     |
|             | Hours   | 1.57       | 1.39      |
Table 6: Here we present the results referred to in Q5. Counterexample-guided learning (CGL) is able to make a model more monotonic by reducing the number of test and train counterexamples compared to the baseline model (NNb). However, the algorithm is unable to guarantee monotonicity, motivating the need for monotonic envelopes.

| Dataset   | Features | Train          | Test          |
|-----------|----------|----------------|---------------|
|           |          | NNb  | CGL | NNb  | CGL |
| Auto-MPG  | Weight   | 22.33| 11.33| 5    | 2   |
|           | Displ.   | 139.67| 37  | 37   | 10.33|
|           | W,D      | 159.67| 85.67| 42.67| 22.67|
|           | W,D,HP   | 149.67| 61.33| 39.33| 15   |
| Boston    | Rooms    | 30   | 15.67| 8    | 6.33 |
|           | Crime    | 80   | 38.67| 19   | 8   |
| Heart     | Trestbps | 188.67| 31  | 49   | 7   |
|           | Chol.    | 212.67| 45.33| 53  | 10.67|
|           | T.C      | 235.67| 169.67| 60.33| 40.33|
| Adult     | Cap. Gain| 7407 | 2755 | 1903 | 700  |
|           | Hours    | 379  | 0   | 84   | 0   |

Table 7: Best parameter configurations on each dataset for each data fold found using Gridsearch for baseline neural networks (NNb).

| Auto-MPG          | Batch Size | # Epochs | LR  | Boston   | Batch Size | # Epochs | LR  | Heart     | Batch Size | # Epochs | LR  | Adult     | Batch Size | # Epochs | LR  |
|-------------------|------------|----------|-----|----------|------------|----------|-----|-----------|------------|----------|-----|-----------|------------|----------|-----|
|                   | 4          | 2000     | 0.01| 64       | 1000       | 0.01     |     | 32        | 400        | 0.01     |     | 1024      | 500        | 0.01     |     |
|                   | 1          | 32       | 1500| 0.01     | 64         | 1000     | 0.001| 32        | 400        | 0.01     |     | -         | -          | -        |     |
|                   | 2          | 32       | 2000| 0.01     | 32         | 500      | 0.01 | 32        | 400        | 0.001    |     | -         | -          | -        |     |

Q6. Additional model selection experiment.
In Section 4.2 model selection was based on minimum train error. In this experiment, we carry out model selection based on the least number of counterexamples. Overall, we find that monotonicity counterexamples act as a good inductive bias and improve model quality. However, there is a tradeoff on how much one could enforce monotonicity as a bias. Figure 5 plots test envelope MSE of Auto MPG and Boston Housing datasets. We can see that envelope construction on a function with minimum counterexamples has a higher error than the original model’s envelope.

Figure 5: Monotonicity is a good inductive bias and helps in improving model accuracy. However, there is a tradeoff between performance and reducing counterexamples.