Towards Formal XAI: Formally Approximate Minimal Explanations of Neural Networks

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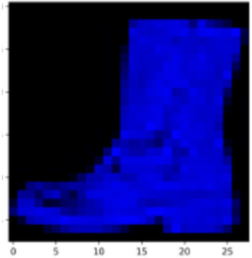
Motivation



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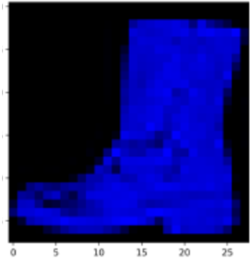

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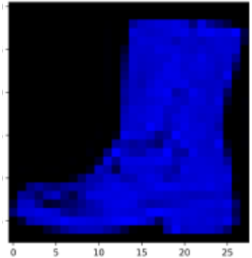

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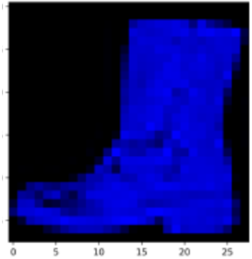

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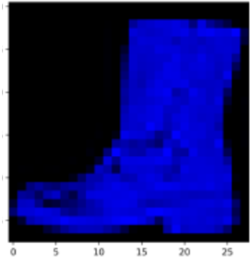
- DNNs can't provide a verbal explanation for the classification instance.



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- How to formalize the term ”Justify”?

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6. Future works.

DNN Verification

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- A DNN verifier checks whether there exists an input x_0 such that $P(x_0) \wedge Q(N(x_0))$ holds:
  - **SAT** case: Determines if there exists an input satisfying the condition (satisfiability).
  - **UNSAT** case: Verifies that no such input exists (validity).
- Just note that the DNN verification problem is known to be NP-Complete, we will use this information later.

Classification

Definition

A **classification problem** is a tuple (F, D, K, N) where

- $F = \{1, \ldots, m\}$ denotes the features;
- $D = \{D_1 \times D_2 \times \ldots \times D_m\}$ denotes the domains of each of the features;
- $K = \{c_1, c_2, \ldots, c_n\}$ is a set of classes, i.e., the possible labels;
- $\mathbb{F} = D_1 \times D_2 \times \ldots \times D_m$ is the entire input space
- $N : \mathbb{F} \to K$ is a (non-constant) classification function (in our case is a neural network).

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Definition

A **classification instance** is a pair (v, c) where $v \in \mathbb{F}, c \in K$ and $c = N(v)$. In other words, v is mapped by the neural network N to class c.

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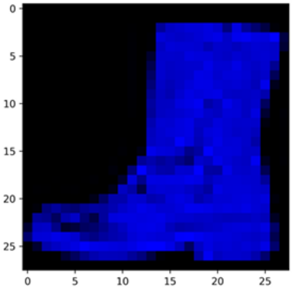
- If we set set the sky dark and draw a moon, it will always be a night time.
- Those pixels serve as an explanation because it will always be night, whether there is a river or a tree.
- In other words, even if the values to the features that are not in the explanation are changed arbitrarily, the classification remains the same.

Example



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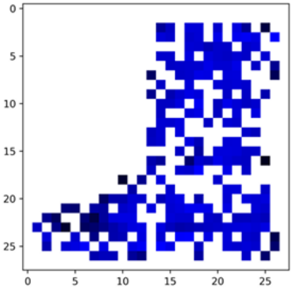

(b) Explanation

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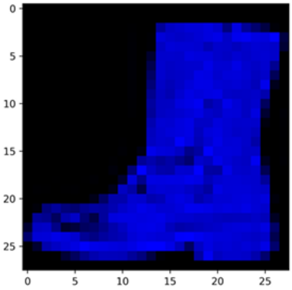

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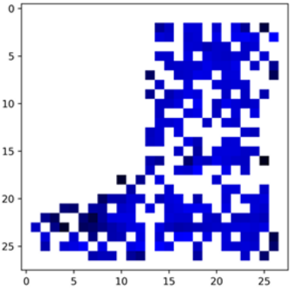

(b) Explanation

- F: All the pixels, i.e., *784 pixels*.
- D_i: Assume 2 possible colors, i.e., $\{Black, Blue\}$.
- Explanation: A subset that is enough for the class to be "Shoe".
- Even if we change the remaining pixels, still a "Shoe".

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Given an input $v = (v_1, \ldots, v_m)$, with the classification $N(v) = c$, for some $c \in K$, an explanation (sometimes, referred to as abductive explanation or AXP) is a subset of the features $E \subseteq F$, such that

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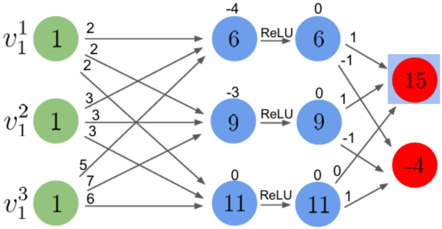
- We will see an example in the next slide.

Example

Consider the following DNN with 3 input nodes and 2 output nodes:



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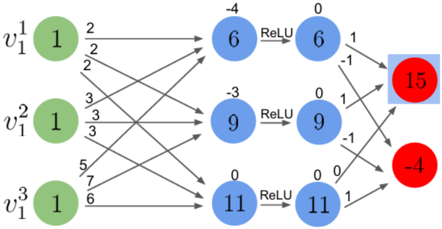

- Here the feature space is the set of nodes $\{v_1^1, v_1^2, v_1^3\}$ and each of the node can take values from the set $\{0, 1\}$, so the value space will be $\{0, 1\}^3$.
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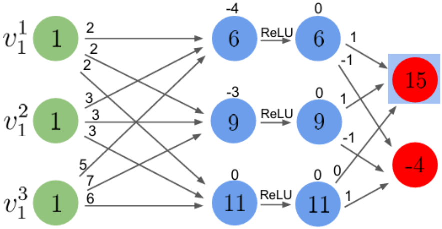

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- For input $v_1 = [1, 1, 1]^T$, the output class is predicted to be c_1 because the value 15 of the output node corresponding to c_1 is higher compared to the other -4. So, we have a classification instance (v_1, c_1) where $c_1 = N(v_1)$

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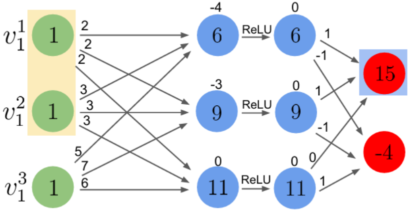

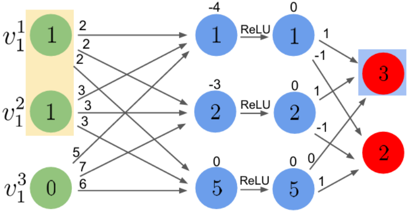

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- The example from the previous slide can be encoded as: $UNSAT\langle x_1 = 1 \wedge x_2 = 1 \wedge N(x) \neq c_1 \rangle$, where x_is a binary variable.

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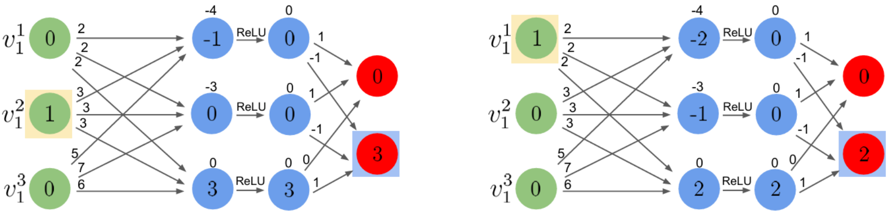
Definition

A minimum explanation is *minimal explanation* of the smallest size.

Examples



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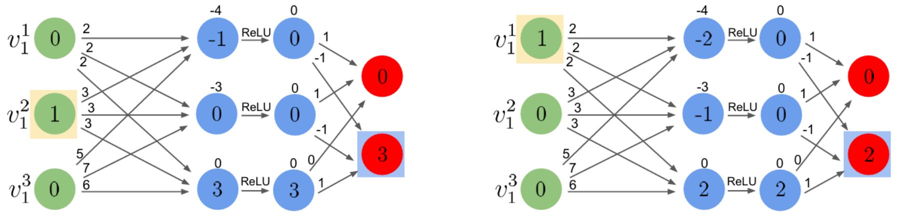

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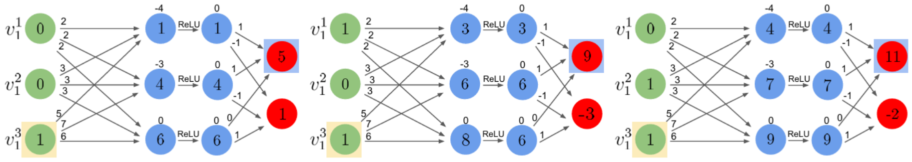

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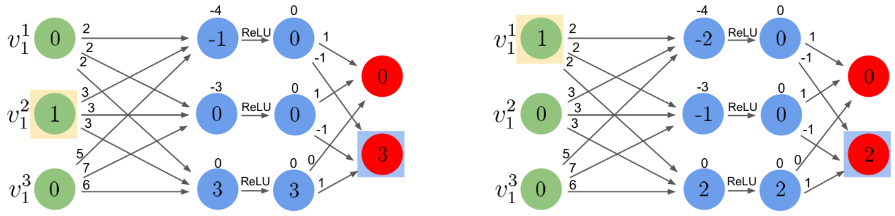

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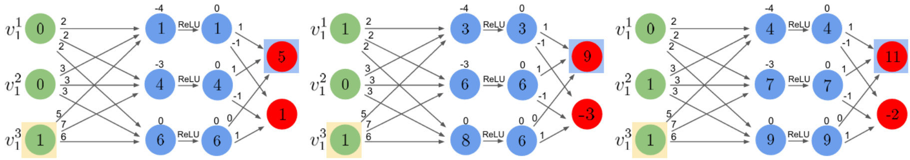

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What will be a trivial algorithm to find a minimum explanation?

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Algorithm 2 T_{UB}: Upper Bounding Thread

Use a heuristic model to sort F's features by ascending relevance
for each $f \in F$ **do**
    Explanation $\leftarrow$ F$\setminus$Free
    if Verify((Explanation$\setminus$\{f\})=v,N,$Q_{\neg c}$) is `UNSAT` **then**
        Free $\leftarrow$ Free $\cup$ \{f\}
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    end if
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4. How far are we from a minimum explanation?

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3. Can we get a lower bound (under-approximation) for the minimum explanation size to get an idea how far we are?
4. Also, are there some features which will always be in every explanation?

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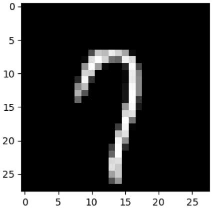
1. Both of the naive algorithms were not efficient, linear number of queries still bad for zillion features.
2. Moreover, we don't even know how far we are from the minimum explanation in case of the latter algorithm.
3. Can we get a lower bound (under-approximation) for the minimum explanation size to get an idea how far we are?
4. Also, are there some features which will always be in every explanation?
5. Both the answers are Yes, thanks to the dual concept of Contrastive Example which will help us calculate the lower bound of the minimum explanation as well as speed up the algorithms we have already seen.

One Pixel Attack



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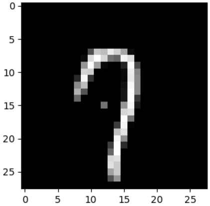

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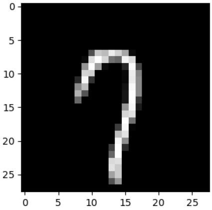

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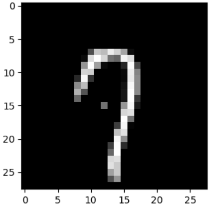

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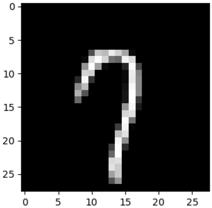

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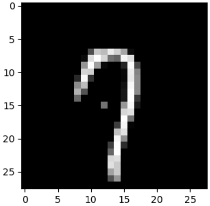

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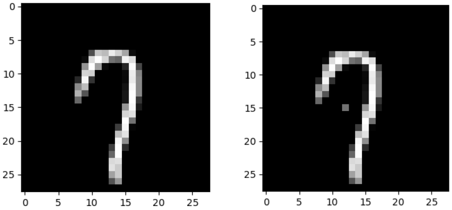

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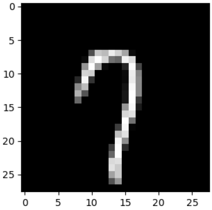

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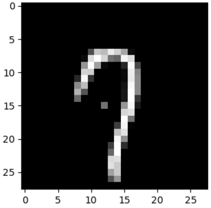

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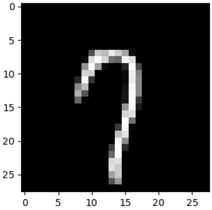

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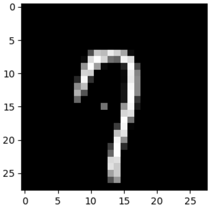

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- In the above picture, the original image was classified as 1.
- However, after flipping a single pixel, the image was classified as 9.
- Now, we will formally introduce Contrastive Examples.

Contrastive Examples

Definition

A subset of features $C \subseteq F$ is a contrastive example (CXP), if altering one or more of the features in C causes a misclassification of given classification instance (v, c). Formally:

$$\exists x \in \mathbb{F}.[\wedge_{i \in F \setminus C}(x_i = v_i) \wedge (N(x) \neq c)]$$

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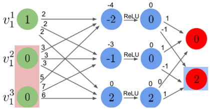

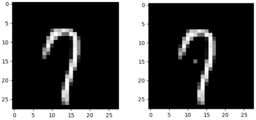

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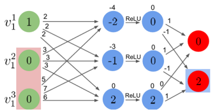

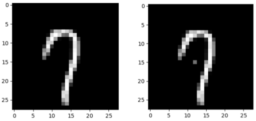

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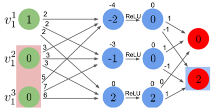

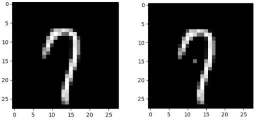

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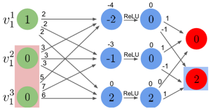

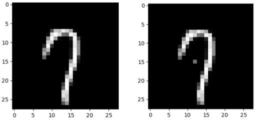

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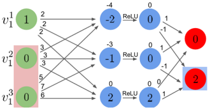

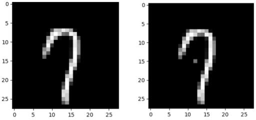

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- Then, we will prove that such E can't be an explanation.

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- So, E can't be an explanation.

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Given a collection $\mathcal{S}$ of sets from a universe U, a set $h \subseteq U$ is called a *hitting set* for $\mathcal{S}$ if

$$\forall s \in \mathcal{S}, \quad h \cap s \neq \emptyset.$$

A hitting set h is said to be:

- **Minimal** if no proper subset of h is also a hitting set.
- **Minimum** if it has the smallest possible cardinality among all hitting sets.

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- Further, enumerating all contrastive examples may in itself take exponential time.
- Finally, DNN verification is itself an NP-Complete problem which may slow down the AXP and CXP queries.

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5. Using this methods, the authors proposed a novel approach to provably approximate the Minimal Explanation we will get.
6. We will first explain the naive version and then we will try to optimize the approach to speed up the algorithm.

Provable Approximations for Minimal Explanations

Algorithm 1 Minimal Explanation Search

Input N (Neural network), F (features), v (input values), c (class prediction)

1: Singletons, Pairs, Free $\leftarrow \varnothing$, UB $\leftarrow |F|$, LB $\leftarrow 0$ $\triangleright$ Global variables
2: Launch thread T_{UB}
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- T_{UB} computes a minimal explanation by reducing the feature space, providing an upper bound (over-approximation) on the minimum explanation size.
- T_{LB} constructs contrastive sets to compute a lower bound (under-approximation) on the same, and the UB and LB together enable estimating the approximation ratio.

The Upper Bounding Thread

Algorithm 2 T_{UB}: Upper Bounding Thread

```
1: Use a heuristic model to sort F's features by ascending relevance
2: for each f ∈ F do
3:     Explanation ← F∖Free
4:     if Verify((Explanation∖{f})=v,N,Q_¬c) is UNSAT then
5:         Free ← Free ∪ {f}
6:         UB ← UB − 1
7:     end if
8: end for
```

The Lower Bounding Thread

Algorithm 3 T_{LB}: Lower Bounding Thread

for each $f \in F$ **do** ▷ Find all singletons
  if Verify((F∖{f}=v,N,$Q_{\neg c}$) is `SAT` **then**
    Singletons ← Singletons ∪ $\{f\}$
    LB ← LB +1
  end if
end for

AllPairs ← Distinct pairs of F∖Singletons
for each (a,b) ∈ AllPairs **do** ▷ Find all pairs
  if Verify((F∖{a,b}=v,N,$Q_{\neg c}$) is `SAT` **then**
    Pairs ←Pairs ∪ $\{(a, b)\}$
  end if
end for
LB ← LB + MVC(Pairs)

The Lower Bounding Thread

Algorithm 3 T_{LB}: Lower Bounding Thread

for each $f \in F$ **do** ▷ Find all singletons
    if Verify((F∖{f}=v,N,$Q_{\neg c}$) is SAT **then**
        Singletons ← Singletons ∪ $\{f\}$
        LB ← LB +1
    end if
end for

AllPairs ← Distinct pairs of F∖Singletons
for each (a,b) ∈ AllPairs **do** ▷ Find all pairs
    if Verify((F∖{a,b}=v,N,$Q_{\neg c}$) is SAT **then**
        Pairs ←Pairs ∪ $\{(a, b)\}$
    end if
end for
LB ← LB + MVC(Pairs)

- Note that, finding the MHS of all contrastive pairs is the 2-MHS problem, which is the Minimum Vertex Cover problem.

The Lower Bounding Thread

We can constrain LB by the following inequality,

$$
\begin{aligned}
\mathrm{LB} &= |\mathrm{Singletons}| + |\mathrm{MVC}(\mathrm{Pairs})| \\
&\leq \sum_{\mathrm{k=1}}^{\mathrm{k=maxk}} |\mathrm{K\text{-}MHS(k\text{-}Cxps)}| \\
&= \mathrm{MHS(Cxps)} = E_M
\end{aligned}
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where, E_M denotes the size of the Minimum Explanation.

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where, E_M denotes the size of the Minimum Explanation.

- Unfortunately, the MVC problem is NP-Complete.
- However, the problem has a linear 2-approximating greedy algorithm, which can be used for finding a lower bound in cases of large feature spaces.

Towards the Optimization

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5. The second method uses binary search to discover the minimal explanation in fewer calls.
6. The third method is a heuristic to remove those features from the search space that are very likely to be in the explanation.

Method 1: Information from T_{LB}

Algorithm 4 T_{UB} using information from T_{LB}

```
Use a heuristic model to sort F by ascending relevance
RemainingFeatures ← F∖Singletons
for each f ∈ RemainingFeatures do
    Explanation ← F∖Free
    if Verify((Explanation∖{f})=v,N,Q_¬c) is UNSAT then
        Free ← Free ∪ {f}
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2. Contrastive Singletons must be a part of any minimal explanation.
3. Same goes for one of the elements of every Contrastive Pair.

Method 2: Binary Search

Algorithm 6 T_{UB} using binary-search

Use a heuristic model to sort F by ascending relevance
$L = 0$
$R = |F| - 1$
while $L \leq |F| - 1$ **do**
    while $L \leq R$ **do** ▷ The inner loop is a single binary search
        Mid $\leftarrow \frac{L-R}{2}$
        Explanation $\leftarrow$F$\setminus$Free
        if Verify((Explanation$\setminus\{$L,L+1,...,Mid$\})$=v,N,$Q_{\neg c}$) is `UNSAT` **then**
            Free $\leftarrow$ Free $\cup$ $\{$L,L+1,...,Mid$\}$
            UB $\leftarrow$ UB $-|\{L, L+1, ...,\mathrm{Mid}\}|$
            $L \leftarrow$ Mid+1
        else
            $R \leftarrow$ Mid$-$1
        end if
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Use a heuristic model to sort F by ascending relevance
L = 0
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        Mid ← (L−R)/2
        Explanation ←F∖Free
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            Free ← Free ∪ {L,L+1,...,Mid}
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            L ← Mid+1
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            R ← Mid−1
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- A heuristic model to sort the features based on ”importance”.

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```

- A heuristic model to sort the features based on "importance".
- Ideally, features in Minimum Explanation get highest weights.
- Utilize the structure, use binary search to find the pivot.

Method 3: Local Singleton Search

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5. If there is such a feature then it's likely a contrastive singleton based on the hypothesis and can be exempted from checking.
6. Trade-off between the size of the explanation and the time complexity.

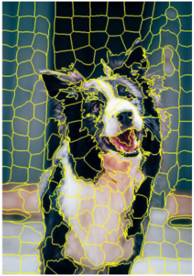
Algorithm for method 3: Local-Singleton Search

Algorithm 5 T_{UB} using local-singleton search

Use a heuristic model to sort F by ascending relevance
RemainingFeatures $\leftarrow$ F$\setminus$Singletons
for each f $\in$ RemainingFeatures **do**
    Explanation $\leftarrow$ F$\setminus$Free
    if Verify((Explanation$\setminus$\{f\})=v,N,$Q_{\neg c}$) is `UNSAT` **then**
        Free $\leftarrow$ Free $\cup$ \{f\}
        UB $\leftarrow$ UB $-$ 1
    else
        Extract counter example C
        LocalSingletons $\leftarrow \varnothing$
        for each f' $\in$ RemainingFeatures **do**
            if Verify(Explanation$\setminus\{f'\}$ = C,N,$Q_{\neg c}$) is `SAT` **then**
                LocalSingletons $\leftarrow$ LocalSingletons $\cup$ $\{f'\}$
            end if
        end for
        RemainingFeatures $\leftarrow$ RemainingFeatures $\setminus$ LocalSingletons
    end if
end for

Bundles

- Mainly to tackle the challenge ”low-level” explanations for certain users.
- Intuitively, bundles are a partitioning of the features into disjoint sets.
- Explanations in terms of bundles are often easier to comprehend.
- Also curtails the search space traversed by the verifier hence speeds up the process further.



Definition

A **bundle** is a subset $b \subseteq F$. The set of all bundles $B = \{b_1, \ldots, b_n\}$ forms a partitioning of F, i.e., $F = \coprod b_i$.

Bundle Explanations

Definition

A ***bundle explanation*** E_B for a classification instance (v, c) is a subset of bundles, $E_B \subseteq B$, such that

$$\forall x \in \mathbb{F}.[\wedge_{i \in \cup E_B}(x_i = v_i) \implies (N(x) = c)]$$

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The union of features in a bundle explanation is an explanation.

- Can develop similar notions like minimum bundle explanations, contrastive bundle examples, etc.
- Algorithmic methods can be extended to the case of bundles to perhaps get more comprehensible explanations.

Experimental Setup

- They implemented a Python framework using the Marabou DNN verifier, supporting proofs, abstraction, and optimization.

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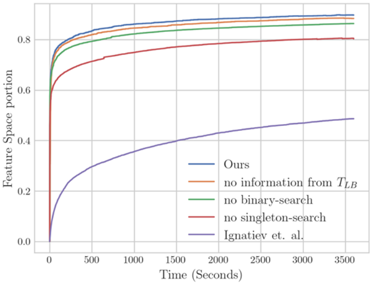
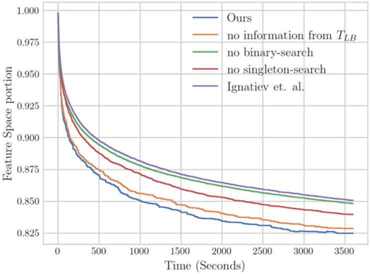
- Such low-confidence inputs yield more meaningful and larger explanations, aiding thorough experimentation.

Experimental results



(a) Average portion of features verified to participate in the explanation.



(b) Average explanation size.

Fig. 7: Our full and ablation-based results, compared to the state of the art for finding minimal explanations on the MNIST dataset.

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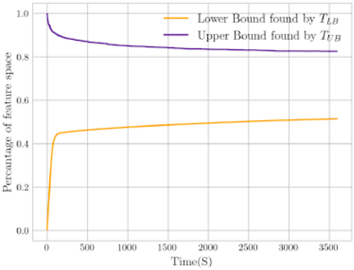

Fig. 8: Average approximation of *minimum* explanation over time.

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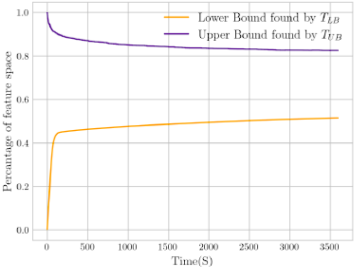

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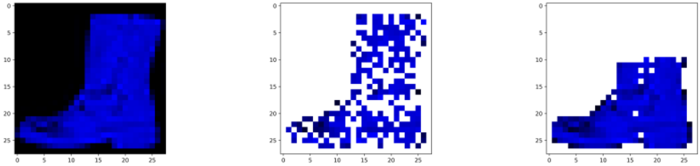

(a) Original Image (b) Explanation (c) Bundle explanation

Future Work

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3. Can we get some approximate algorithms that can find the explanation up to size k of the minimum explanation in linear (or polynomial) time?
4. The authors used LIME to sort the input features by relevance. Yu et. al. also proposed an algorithm to approximate FFA (Formal Feature Attribution) in an anytime fashion. We can use that algorithm instead of LIME.

Thank You