On Guaranteed Optimal Robust Explanations for NLP Models

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Abstract

We build on abduction-based explanations for machine learning and develop a method for computing local explanations for neural network models in natural language processing (NLP). Our explanations comprise a subset of the words of the input text that satisfies two key features: optimality w.r.t. a user-defined cost function, such as the length of explanation, and robustness, in that they ensure prediction invariance for any bounded perturbation in the embedding space of the left-out words. We present two solution algorithms, respectively based on implicit hitting sets and maximum universal subsets, introducing a number of algorithmic improvements to speed up convergence of hard instances. We show how our method can be configured with different perturbation sets in the embedded space and used to detect bias in predictions by enforcing include/exclude constraints on biased terms, as well as to enhance existing heuristic-based NLP explanation frameworks such as Anchors. We evaluate our framework on three widely used sentiment analysis tasks and texts of up to 100 words from SST, Twitter and IMDB datasets, demonstrating the effectiveness of the derived explanations\textsuperscript{1}.

1 Introduction

The increasing prevalence of deep learning models in real-world decision-making systems has made AI explainability a central problem, as we seek to complement such highly-accurate but opaque models with comprehensible explanations as to why the model produced a particular prediction [Samek and others, 2017; Ribeiro and others, 2016; Zhang and others, 2019; Liu and others, 2018; Letham and others, 2015]. Amongst existing techniques, local explanations explain the individual prediction in terms of a subset of the input features that justify the prediction. State-of-the-art explainers such as LIME and Anchors [Ribeiro and others, 2016; Ribeiro and others, 2018] use heuristics to obtain short explanations, which may generalise better beyond the given input and are more easily interpretable to human experts, but lack robustness to adversarial perturbations. The abduction-based method of [Ignatiev and others, 2019a], on the other hand, ensures minimality and robustness of the prediction by requiring its invariance w.r.t. any perturbation of the left-out features, meaning that the explanation is sufficient to imply the prediction. However, since perturbations are potentially unbounded, this notion of robustness may not be appropriate for certain applications.

In this paper, we focus on natural language processing (NLP) neural network models and, working in the embedding space with words as features, introduce optimal robust explanations (OREs). OREs are provably guaranteed to be both robust, in the sense that the prediction is invariant for any (reasonable) replacement of the features outside the explanation, and minimal for a given user defined cost function, such as the length of the explanation. Our core idea shares similarities with abduction-based explanations (ABE) of [Ignatiev and others, 2019a], but is better suited to NLP models, where the unbounded nature of ABE perturbations may result in trivial explanations equal to the entire input. We show that OREs can be formulated as a particular kind of ABE or, equivalently, minimal satisfying assignment (MSA). We develop two methods to compute OREs by extending existing algorithms for ABES and MSAs [Ignatiev and others, 2019a; Dillig and others, 2012]. In particular, we incorporate state-of-the-art robustness verification methods [Katz and others, 2019; Wang and others, 2018] to solve entailment/robustness queries and improve convergence by including sparse adversarial attacks and search tree reductions. By adding suitable constraints, we show that our approach allows one to detect biased decisions [Darwiche and Hirth, 2020] and enhance heuristic explainers with robustness guarantees [Ignatiev and others, 2019d].

To the best of our knowledge, this is the first method to derive local explanations for NLP models with provable robustness and optimality guarantees. We empirically demonstrate that our approach can provide useful explanations for non-trivial fully-connected and convolutional networks on three widely used sentiment analysis benchmarks (SST, Twitter and IMDB). We compare OREs with the popular Anchors method, showing that Anchors often lack prediction robustness in our benchmarks, and demonstrate the usefulness of

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\textsuperscript{2}Code available at https://github.com/EmanueleLM/OREs
our framework on model debugging, bias evaluation, and repair of non-formal explainers like Anchors.

2 Related Work

Interpretability of machine learning models is receiving increasing attention [Chakraborty and others, 2017]. Existing methods broadly fall in two categories: explanations via globally interpretable models (e.g., [Wang and Rudin, 2015; Zhang and others, 2018]), and local explanations for a given input and prediction (to which our work belongs). Two prominent examples of the latter category are LIME [Ribeiro and others, 2016], which learns a linear model around the neighbourhood of an input using random local perturbations, and Anchors [Ribeiro and others, 2018] (introduced in Section 3). These methods, however, do not consider robustness, making them fragile to adversarial attacks and thus insufficient to imply the prediction. Repair of non-formal explainers has been studied in [Ignatiev and others, 2019d] but only for boosted trees predictors. [Narodytska and others, 2019] assesses the quality of Anchors’ explanations by encoding the has been studied in [Ignatiev and others, 2019d] but only for robust w.r.t. bounded perturbations in the embedding space [Baroni and others, 2014], which is considered a good proxy for semantic similarity with respect to the target task compared to count-based embeddings [Alzantot and others, 2018]. For classification we consider a neural network $M : \mathbb{R}^{d} \rightarrow \mathcal{Y}$ that operates on the text embedding.

Robust Explanations In this paper, we seek to provide local explanations for the predictions of a neural network NLP model. For a text embedding $x = \mathcal{E}(t)$ and a prediction $M(x)$, a local explanation $E$ is a subset of the features of $t$, i.e., $E \subseteq F$ where $F = \{w_{1}, \ldots, w_{t}\}$, that is sufficient to imply the prediction. We focus on deriving robust explanations, i.e., on extracting a subset $E$ of the text features $F$ which ensure that the neural network prediction remains invariant for any perturbation of the other features $F \setminus E$. Thus, the features in a robust explanation are sufficient to imply the prediction that we aim to explain, a clearly desirable feature for a local explanation. In particular, we focus on explanations that are robust w.r.t. bounded perturbations in the embedding space of the input text. We extract word-level explanations by means of word embeddings: we note that OREs work, without further extensions, with diverse representations (e.g., sentence-level, characters-level, etc.). For a word $w \in W$, with embedding $x_{w} = \mathcal{E}(w)$ we denote with $B(w) \subseteq \mathbb{R}^{d}$ a generic set of word-level perturbations. We consider the following kinds of perturbation sets, depicted also in Fig. 1.

$k$-NN box closure: $B(w) = B(\mathcal{E}(NN_{k}(w)))$, where $BB(X)$ is the minimum bounding box for set $X$; for a set $W' \subseteq W$, $\mathcal{E}(W') = \bigcup_{w' \in W'}\mathcal{E}(w')$; and $NN_{k}(w)$ is the set of the $k$ closest words to $w$ in the embedding space, i.e., words $w'$ with smallest $d(x_{w}, \mathcal{E}(w'))$, where $d$ is a valid notion of distance between embedded vectors, such as $p$-norms or cosine similarity. This provides an over-approximation of the $k$-NN convex closure, for which constraint propagation (and thus robustness checking) is more efficient [Jia and others, 2019; Huang and others, 2019].

For some word-level perturbation $B$, set of features $E \subseteq F$, and input text $t$ with embedding $(x_{1}, \ldots, x_{t})$, we denote

$$w_{i} \in \mathbb{W} \text{ with } W$$

2 even though the box closure can be calculated for any set of embedded words.
with \( B_E(t) \) the set of text-level perturbations obtained from \( t \) by keeping constant the features in \( E \) and perturbing the others according to \( B \):
\[
B_E(t) = \{ (x'_1, \ldots, x'_l) \in \mathbb{R}^{|d|} \mid x'_w = x_w \text{ if } w \in E; \quad x'_w \in B(w) \text{ otherwise} \}. \quad (1)
\]

A robust explanation \( E \subseteq F \) ensures prediction invariance for any point in \( B_E(t) \), i.e., any perturbation (within \( B \)) of the features in \( F \setminus E \).

**Def. 1 (Robust Explanation).** For a text \( t = (w_1, \ldots, w_l) \) with embedding \( x = E(t) \), word-level perturbation \( B \), and classifier \( M \), a subset \( E \subseteq F \) of the features of \( t \) is a robust explanation if
\[
\forall x' \in B_E(t). \quad M(x') = M(x). \quad (2)
\]
We denote (2) with predicate \( \text{Rob}_{M,x}(E) \).

**Optimal Robust Explanations (OREs)** While robustness is a desirable property, it is not enough alone to produce useful explanations. Indeed, we can see that an explanation \( E \) including all the features, i.e., \( E = F \), trivially satisfies Definition 1. Typically, one seeks short explanations, because these can generalise to several instances beyond the input \( x \) and are easier for human decision makers to interpret. We thus introduce optimal robust explanations (OREs), that is, explanations that are both robust and optimal w.r.t. an arbitrary cost function that assign a penalty to each word.

**Def. 2 (Optimal Robust Explanation).** Given a cost function \( C : W \rightarrow \mathbb{R}^+ \), and for \( t = (w_1, \ldots, w_l) \), \( x \), \( B \), and \( M \) as in Def. 1, a subset \( E^* \subseteq F \) of the features of \( t \) is an ORE if
\[
E^* \in \arg \min_{E \subseteq F} \sum_{w \in E} C(w) \text{ s.t. } \text{Rob}_{M,x}(E). \quad (3)
\]

Note that (3) is always feasible, because its feasible set always includes at least the trivial explanation \( E = F \). A special case of our OREs is when \( C \) is uniform (it assigns the same cost to all words in \( t \)), in which case \( E^* \) is (one of) the robust explanations of smallest size, i.e., with the least number of words.

**Relation with Abductive Explanations** Our OREs have similarities with the abduction-based explanations (ABEs) of [Ignatiev and others, 2019a] in that they also derive minimal-cost explanations with robustness guarantees. For an input text \( t = (w_1, \ldots, w_l) \), let \( C = \bigwedge_{i=1}^{l} \chi_i = x_{w_i} \) be the cube representing the embedding of \( t \), where \( \chi_i \) is a variable denoting the \( i \)-th feature of \( x \). Let \( N \) represent the logical encoding of the classifier \( M \), and \( \bar{y} \) be the formula representing the output of \( N \) given \( \chi_1, \ldots, \chi_l \).

**Def. 3 ([Ignatiev and others, 2019a])** An abduction-based explanation (ABE) is a minimal cost subset \( C^* \) of \( C \) such that \( C^* \wedge N \models \bar{y} \).

Note that the above entailment is equivalently expressed as \( C^* \models (N \rightarrow \bar{y}) \). Let \( B = \bigwedge_{i=1}^{l} \chi_i \in B(w_i) \) be the constraints encoding our perturbation space. Then, the following proposition shows that OREs can be defined in a similar abductive fashion and also in terms of minimum satisfying assignments (MSAs) [Dillig and others, 2012]. In this way, we can derive OREs via analogous algorithms to those used for ABEs [2019a] and MSAs [Dillig and others, 2012], as explained in Section 4. Moreover, we find that every ORE can be formulated as a prime implicant [Ignatiev and others, 2019a], a property that connects our OREs with the notion of sufficient reason introduced in [Darwiche and Hirth, 2020].

**Prop. 1.** Let \( E^* \) be an ORE and \( C^* \) its constraint encoding. Define \( \phi \equiv (B \wedge N) \rightarrow \bar{y} \). Then, all the following definitions apply to \( C^* \):
1. \( C^* \) is a minimal cost subset of \( C \) such that \( C^* \models \phi \).
2. \( C^* \) is a minimum satisfying assignment for \( \phi \).
3. \( C^* \) is a prime implicant of \( \phi \).

**Proof.** See supplement.

The key difference with ABEs is that our OREs are robust to bounded perturbations of the excluded features, while ABEs must be robust to any possible perturbation. This is an important difference because it is hard (often impossible) to guarantee prediction invariance w.r.t. the entire input space when this space is continuous and high-dimensional, like in our NLP embeddings. In other words, if for our NLP tasks we allowed any word-level perturbation as in ABEs, in most cases the resulting OREs will be of the trivial kind, \( E^* = F \) (or \( C^* = C \)), and thus of little use. For example, if we consider \( \epsilon \)-ball perturbations and the review “the gorgeously elaborate continuation of the lord of the rings”, the resulting smallest-size explanation is of the trivial kind (it contains the whole review) already at \( \epsilon = 0.1 \).

**Exclude and include constraints** We further consider OREs \( E^* \) derived under constraints that enforce specific features \( F' \) to be included/excluded from the explanation:
\[
E^* \in \arg \min_{E \subseteq F} \sum_{w \in E} C(w) \text{ s.t. } \text{Rob}_{M,x}(E) \wedge \phi(E), \quad (4)
\]
where \( \phi(E) \) is one of \( F' \cap E = \emptyset \) (exclude) and \( F' \subseteq E \) (include). Note that adding include constraints doesn’t affect the feasibility of our problem\(^3\). Conversely, exclude constraints

\(^3\)because the feasible region of (4) always contains at least the explanation \( E^* \cup F' \), where \( E^* \) is a solution of (3) and \( F' \) are the features to include. See Def. 1.
might make the problem infeasible when the features in $F'$ don’t admit perturbations, i.e., they are necessary for the prediction, and thus cannot be excluded. Such constraints can be easily accommodated by any solution algorithm for non-constrained OREs: for include ones, it is sufficient to restrict the feasible set of explanations to the supersets of $F'$; for exclude constraints, we can manipulate the cost function so as to make any explanation with features in $F'$ strictly sub-optimal w.r.t. explanations without it.

Constrained OREs enable two crucial use cases: detecting biased decisions, and enhancing non-formal explainability frameworks.

Detecting bias Following [Darwiche and Hirth, 2020], we deem a classifier decision biased if it depends on protected features, i.e., a set of input words that should not affect the decision (e.g., a movie review affected by the director’s name). In particular, a decision $M(x)$ is biased if we can find, within a given set of text-level perturbations, an input $x'$ that agrees with $x$ on all but protected features and such that $M(x) \neq M(x')$.

**Def. 4.** For classifier $M$, text $t$ with features $F$, protected features $F'$ and embedding $x = \mathcal{E}(t)$, decision $M(x)$ is biased w.r.t. some word-level perturbation $\mathcal{B}$, if

$$\exists x' \in \mathcal{B}_{F',F}(t). M(x) \neq M(x').$$

The proposition below allows us to use exclude constraints to detect bias.

**Prop. 2.** For $M, t, F, F', x$ and $\mathcal{B}$ as per Def. 4, decision $M(x)$ is biased iff (4) is infeasible under $F' \cap E = \emptyset$.

**Proof.** See supplement

Enhancing non-formal explainers The local explanations produced by heuristic approaches like LIME or Anchors do not enjoy the same robustness/invariance guarantees of our OREs. We can use our approach to minimally extend (w.r.t. the chosen cost function) any non-robust local explanation $F'$ in order to make it robust, by solving (4) under the exclude constraint $F' \subseteq E$. In particular, with a uniform $C$, our approach would identify the smallest set of extra words that make $F'$ robust. Being minimal/smallest, such an extension retains to a large extent the original explainability properties.

Relation with Anchors Anchors [Ribeiro and others, 2018] are a state-of-the-art method for ML explanations. Given a perturbation distribution $\mathcal{D}$, classifier $M$ and input $x$, an anchor $A$ is a predicate over the input features such that $A(x)$ holds and $A$ has high precision and coverage, defined next.

$$\text{prec}(A) = \frac{\Pr_{\mathcal{D}(x')} (M(x) = M(x'))}{\Pr_{\mathcal{D}(x')} (A(x'))}; \text{cov}(A) = \frac{\Pr_{\mathcal{D}(x')} (A(x'))}{\Pr_{\mathcal{D}(x')} (A(x'))}.$$ (5)

In other words, prec$(A)$ is the probability that the prediction is invariant for any perturbation $x'$ to which explanation $A$ applies. In this sense, precision can be intended as

4That is, we use cost $C'$ such that $\forall w \in F \setminus F', C'(w) = C(w)$ and $\forall w \in F\setminus F', C'(w') > \sum_{w \in F\setminus F', C(w)}$. The ORE obtained under cost $C'$ might still include features from $F'$, which implies that (4) is infeasible (i.e., no robust explanation without elements of $F'$ exists).

a robustness probability. cov$(A)$ is the probability that explanation $A$ applies to a perturbation. To discuss the relation between Anchors and OREs, for an input text $t$, consider an arbitrary distribution $\mathcal{D}$ with support in $\mathcal{B}_0(t)$ (the set of all possible text-level perturbations), see (1); and consider anchors $A$ defined as subsets $E$ of the input features $F$, i.e., $A_E(x) = \bigwedge_{w \in E} x_w = \mathcal{E}(w)$. Then, our OREs enjoy the following properties.

**Prop. 3.** If $E$ is a robust explanation, then prec$(A_E) = 1$.

**Proof.** See supplement

Note that when $\mathcal{D}$ is continuous, cov$(A_E)$ is always zero unless $E = \emptyset$. We thus illustrate the next property assuming that $\mathcal{D}$ is discrete (when $\mathcal{D}$ is continuous, the following still applies to any empirical approximation of $\mathcal{D}$).

**Prop. 4.** If $E \subseteq E'$, then cov$(A_E) \geq$ cov$(A_{E'})$.

**Proof.** See supplement

The above proposition suggests that using a uniform $C$, i.e., minimizing the explanation’s length, is a sensible strategy to obtain high-coverage OREs.

4 Solution Algorithms

We present two solution algorithms to derive OREs, respectively based on the hitting-set (HS) paradigm of [Ignatiev and others, 2019a] and the MSA algorithm of [Dillig and others, 2012]. Albeit different, both algorithms rely on repeated entailment/robustness checks $B \land E \land N \models \tilde{y}$ for a candidate explanation $E \subset C$. For this check, we employ two state-of-the-art neural network verification tools, Marabou [Katz and others, 2019] and Neurify [Wang and others, 2018]: they both give provably correct answers and, when the entailment is not satisfied, produce a counter-example $x' \in B_{E}(t)$, i.e., a perturbation that agrees with $E$ and such that $B \land C' \land N \not\models \tilde{y}$, where $C'$ is the cube representing $x'$. We now briefly outline the two algorithms. A more detailed discussion (including the pseudo-code) is available in the supplement.

Minimum Hitting Set For a counterexample $C'$, let $I'$ be the set of feature variables where $C'$ does not agree with $C$ (the cube representing the input). Then, every explanation $E$ that satisfies the entailment must hit all such sets $I'$ built for any counter-examples $C'$ [Ignatiev and others, 2016]. Thus, the HS paradigm iteratively checks candidates $E$ built by selecting the subset of $C$ whose variables form a minimum HS (w.r.t. cost $C$) of said $I'$s. However, we found that this method often struggles to converge for our NLP models, especially with large perturbations spaces (i.e., large $\epsilon$ or $k$). We solved this problem by extending the HS approach with a sub-routine that generates batches of sparse adversarial attacks for the input $C$. This has a two-fold benefit: 1) we reduce the number of entailment queries required to produce counter-examples,

5In which case cov$(A_0) = 1$ (as $A_0 = \text{true}$). Indeed, for $E \neq \emptyset$, the set $\{x' \mid A_E(x')\}$ has $|E|$ fewer degrees of freedom than the support of $\mathcal{D}$, and thus has both measure and coverage equal to zero.
and 2) sparsity results in small $I'$ sets, which further improves convergence.

**Minimum Satisfying Assignment** This algorithm exploits the duality between MSAs and maximum universal subsets (MUSs): for cost $C$ and formula $\phi \equiv (B \land N) \rightarrow \hat{y}$, an MUS $X$ is a set of variables with maximum $C$ such that $\forall X, \phi$, which implies that $C \setminus X$ is an MSA for $\phi$ [Dillig and others, 2012] and, in turn, an ORE. Thus, the algorithm of [Dillig and others, 2012] focuses on deriving an MUS, and it does so in a recursive branch-and-bound manner, where each branch adds a feature to the candidate MUS. Such an algorithm is exponential in the worst-case, but we mitigated this by selecting a good ordering for feature exploration and performing entailment checks to rule out features that cannot be in the MUS (thus reducing the search tree).

### 5 Experimental Results

**Settings** We have trained fully connected (FC) and convolutional neural networks (CNN) models on sentiment analysis datasets that differ in the input length and difficulty of the learning task.\(^{4}\) We considered 3 well-established benchmarks for sentiment analysis, namely SST [Socher and others, 2013], Twitter [Go and others, 2009] and IMDB [Maas and others, 2011] datasets. From these, we have chosen 40 representative input texts, balancing positive and negative examples. Embeddings are pre-trained on the same datasets used for classification [Chollet and others, 2015]. Both the HS and MSA algorithms have been implemented in Python and use Marabou [Katz and others, 2019] and Neurify [Wang and others, 2018] to answer robustness queries.\(^{5}\) In the experiments below, we opted for the kNN-box perturbation space, as we found that the $k$ parameter was easier to interpret and tune than the $\epsilon$ parameter for the $\epsilon$-ball space, and improved verification time. Further details on the experimental settings, including a selection of $\epsilon$-ball results, are given in the supplement.

**Effect of classifier’s accuracy and robustness.** We find that our approach generally results in meaningful and compact explanations for NLP. In Figure 2, we show a few OREs for negative and positive texts, where the returned OREs are both concise and semantically consistent with the predicted sentiment. However, the quality of our OREs depends on that of the underlying classifier. Indeed, enhanced models with better accuracy and/or trained on longer inputs tend to produce higher quality OREs. We show this in Figures 3 and 4, where we observe that enhanced models tend to result in more semantically consistent explanations. For lower-quality models, some OREs include seemingly irrelevant terms (e.g., “film”, “and”), thus exhibiting shortcomings of the classifier.

**Detecting biases** As per Prop. 2, we applied exclude constraints to detect biased decisions. In Figure 5, we provide a few example instances exhibiting such a bias, i.e., where any robust explanation contains at least one protected feature. These OREs include proper names that shouldn’t constitute a sufficient reason for the model’s classification. When we try to exclude proper names, no robust explanation exists, indicating that a decision bias exists.

**Debugging prediction errors** An important use-case for OREs is when a model commits a *misclassification*. Misclassifications in sentiment analysis tasks usually depend on over-sensitivity of the model to polarized terms. In this sense, knowing a minimal, sufficient reason behind the model’s prediction can be useful to debug it. As shown in the first example in Figure 6, the model cannot recognize the double negation constituted by the terms not and dreadful as a syntax construct, hence it exploits the negation term not to classify the review as negative.

### 6 Conclusions

We have introduced optimal robust explanations (OREs) and applied them to enhance interpretability of NLP models. OREs provide concise and sufficient reasons for a particular prediction, as they are guaranteed to be both minimal w.r.t. a given cost function and robust, in that the prediction is invariant for any bounded replacement of the left-out features. We have presented two solution algorithms that build

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\(^{4}\)Experiments were parallelized on a server with two 24-core Intel Xeon 6252 processors and 256GB of RAM, but each instance is single-threaded and can be executed on a low-end laptop.

\(^{5}\)Marabou is fast at verifying ReLU FC networks, but it becomes memory intensive with CNNs. On the other hand, the symbolic interval analysis of Neurify is more efficient for CNNs. A downside of Neurify is that it is less flexible in the constraint definition (inputs have to be represented as squared bi-dimensional grids, thus posing problems for NLP inputs which are usually specified as 3-d tensors).

\(^{8}\)Accuracies are 0.89 for FC+SST, 0.82 for FC+Twitter, 0.89 for CNN+SST, and 0.77 for CNN+Twitter.
Figure 2: OREs for IMDB, SST and Twitter datasets (all the texts are correctly classified). Models employed are FC with 50 input words each with accuracies respectively 0.89, 0.77 and 0.75. OREs are highlighted in blue. Technique used is kNN boxes with k=15.

Figure 3: Comparison of OREs for SST and Twitter texts on FC (red) vs CNN (blue) models (common words in magenta). The first two are positive reviews, the third is negative (all correctly classified). Accuracies of FC and CNN models are, respectively, 0.88 and 0.89 on SST, 0.77 on Twitter. Models have input length of 25 words, OREs are extracted with kNN boxes (k=25).

Figure 4: Comparison of OREs on negative IMDB and Twitter inputs for FC models. The first and third examples are trained with 25 (red) VS 50 (blue) input words (words in common to both OREs are in magenta). The second example further uses an FC model trained with 100 input words (words in common to all three OREs are in orange). Accuracy is respectively 0.7 and 0.77 and 0.81 for IMDB, and 0.77 for both Twitter models. All the examples are classified correctly. OREs are extracted with kNN boxes (k=25).

Figure 5: Two examples of decision bias from an FC model with an accuracy of 0.80.

Figure 6: Two examples of over-sensitivity to polarized terms (in red). Other words in the OREs are highlighted in green. Models used are FC with 25 input words (accuracy 0.82 and 0.74). Method used is kNN with k respectively equal to 8 and 10.

Figure 7: Examples of Anchors explanations (in blue) along with the minimal extension required to make them robust (in red). Examples are classified (without errors) with a 25-input-word CNN (accuracy 0.89). OREs are extracted for kNN boxes and k=25.
on the relation between our OREs, abduction-based explanations and minimum satisfying assignments. We have demonstrated the usefulness of our approach on widely-adopted sentiment analysis tasks, providing explanations for neural network models beyond reach for existing formal explainers. Detecting biased decisions, debugging misclassifications, and repairing non-robust explanations are some of key use cases that our OREs enable. Future research plans include exploring more general classes of perturbations beyond the embedding space.

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7 Appendix

We structure the Appendix in the following way. We first provide proofs of the propositions in Section 3. Second, we give details (through the pseudo-code) of the Algorithms and sub-routines that were used to find Optimal Robust Explanations; in particular we describe the shrink (used to improve MSA) and the Adversarial Attacks procedures (used to improve HS). We then provide details on the datasets and the architectures that we have used in the Experimental Evaluation, and finally we report many examples of interesting OREs that we were able to extract with our methods, along side with tables that complete the comparison between MSA and HS as described in the Experimental Evaluation Section.

7.1 Proofs

Proof of Prop. 2 Call \( A = "M(x) is biased" \) and \( B = "(4) is infeasible under F' \cap E = \emptyset".\) Let us prove first that \( B \rightarrow A. \) Note that \( B \) can be equivalently expressed as

\[ \forall x \in F. (E \cap F' \neq \emptyset \lor \exists x' \in B_E(t), M(x) \neq M(x')) \]

If the above holds for all \( E \) then it also holds for \( E = F \setminus F' \), and so it must be that \( \exists x' \in B_{F \setminus F'}(t), M(x) \neq M(x') \) because the first disjunct is clearly false for \( E = F \setminus F' \).

We now prove \( A \rightarrow B \) by showing that \( \neg B \rightarrow \neg A. \) Note that \( \neg B \) can be expressed as

\[ \exists x \in F. (E \cap F' = \emptyset \land \forall x' \in B_E(t), M(x) = M(x')) \]

and \( \neg A \) can be expressed as

\[ \forall x \in B_{F \setminus F'}(t), M(x) = M(x') \].

To see that (6) implies (7), note that any \( E \) that satisfies (6) must be such that \( E \cap F' = \emptyset \), which implies that \( E \subseteq F \setminus F' \), which in turn implies that \( B_{F \setminus F'}(t) \subseteq B_E(t) \). By (6), the prediction is invariant for any \( x' \in B_E(t) \), and so is for any \( x' \in B_{F \setminus F'}(t) \).

Proof of Prop. 3 A robust explanation \( E \subseteq F \) guarantees prediction invariance for any \( x' \in B_E(t) \), i.e., for any \( x' \) (in the support of \( D \)) to which \( A_E \) applies.

Proof of Prop. 4 For discrete \( D \) with pmf \( f_D \), we can express \( \text{cov}(A_E) \) as

\[ \text{cov}(A_E) = \sum_{x' \in \text{supp}(D)} f_D(x') \cdot 1_{A_E(x')} = \sum_{x' \in \text{supp}(D)} f_D(x') \cdot \prod_{w \in E} 1_{x'_w \in \mathcal{E}(w)} \]

To see that, for \( E' \supseteq E \), \( \text{cov}(A_{E'}) \leq \text{cov}(A_E) \), observe that \( \text{cov}(A_{E'}) \) can be expressed as

\[ \text{cov}(A_{E'}) = \sum_{x' \in \text{supp}(D)} f_D(x') \cdot \prod_{w \in E'} 1_{x'_w \in \mathcal{E}(w)} = \sum_{x' \in \text{supp}(D)} f_D(x') \cdot \prod_{w \in E} 1_{x'_w \in \mathcal{E}(w)} \prod_{w \in E \setminus E'} 1_{x'_w \in \mathcal{E}(w)} \]

and that for any \( x' \), \( \prod_{w \in E \setminus E'} 1_{x'_w \in \mathcal{E}(w)} \leq 1. \)

Proof of Prop. 1 With abuse of notation, in the following we use \( C^* \) to denote both an ORE and its logical encoding.

1. If \( C^* \) is an ORE, then \( \phi \equiv (B \land \mathcal{N}) \rightarrow \hat{y} \) is true for any assignment \( x' \) of the features not in \( C^* \). In particular, \( \phi \) is trivially satisfied for any \( x' \) outside the perturbation space \( \hat{B} \), and, by Definition 1, is satisfied for any \( x' \) within the perturbation space.

2. As also explained in [Dillig and others, 2012], finding an optimal \( C^* \) such that \( C^* \models \phi \) is equivalent to finding an MSA \( C^* \) for \( \phi \). We should note that \( C^* \) is a special case of an MSA, because the possible assignments for the variables in \( C^* \) are restricted to the subsets of the cube \( C \).

3. \( C^* \) is said a prime implicant of \( \phi \) if \( C^* \models \phi \) and there are no proper subsets \( C' \subset C^* \) such that \( C' \models \phi \). This holds regardless of the choice of the cost \( C \), as long as it is additive and assigns a positive cost to each feature as per Definition 2. Indeed, for such a cost function, any proper subset \( C' \subset C^* \) would have cost strictly below that of \( C^* \), meaning that \( C' \not= \phi \) (i.e., is not robust) because otherwise, \( C' \) (and not \( C^* \)) would have been (one of) the robust explanations with minimal cost.

7.2 Optimal Cost Algorithms and Sub-Routines

In this Section we provide a full description and the pseudo-code of the algorithms that for reason of space we were not able to insert in the main paper. We report a line-by-line description of the HS procedure (Algorithm 1): we further describe how the adversaril attacks procedure is used to generate candidates that help the HS approach converge on hard instances, as reported in Section 4. We then describe the algorithm to compute Smallest Cost Explanations (Algorithm 4). In Algorithm 5, we finally detail the shrink procedure as sketched in Section 3.

Minimal Hitting-Set and Explanations

One way to compute optimal explanations against a cost function \( C \), is through the hitting set paradigm \( [\text{Ignatiev and others, 2019}] \), that exploits the relationship between diagnoses and conflicts \( [\text{Reiter, 1987}] \): the idea is to collect perturbations and to calculate on their indices a minimum hitting set (MHS) i.e., a minimum-cost explanation whose features are in common with all the others. We extend this framework to find a word-level explanation for non-trivial NLP models. At each iteration of Algorithm 1, a minimum hitting set \( E \) is extracted (line 3) from the (initially empty, line 1) set \( \Gamma \). If function \( \text{Entails} \) evaluates to \( \text{False} \) (i.e., the neural network \( \mathcal{N} \) is provably safe against perturbations on the set of features identified by \( F \setminus F' \)) the procedure terminates and \( E \) is returned as an ORE. Otherwise, (at least) one feasible attack is computed on \( F \setminus E \) and added to \( \Gamma \) (lines 7-8): the routine then re-starts. Differently from \( [\text{Ignatiev and others, 2019}] \), as we have experienced that many OREs whose a large perturbation space - i.e. when \( \epsilon \) or \( k \) are large - do not terminate in a reasonable amount of time, we have extended the vanilla hitting set approach by introducing \( \text{SparseAttacks} \) function (line 7). At each iteration \( \text{SparseAttacks} \) introduces in the hitting set \( \Gamma \) a large number of sparse adversarial attacks on the set of features \( F \setminus E \): it is in fact known \( [\text{Ignatiev and others, 2016}] \) that
attacks that use as few features as possible help convergence on instances that are hard (intuitively, a small set is harder to “hit” hence contributes substantially to the optimal solution compared to a longer one) SparseAttacks procedure is based on random search and it is inspired by recent works in image recognition and malware detection [Croce and others, 2020]; pseudo-code is reported in 2, while a detailed description follows in the next paragraph.

Sparse Adversarial Attacks In Algorithm 2 we present a method to generate sparse adversarial attacks against features (i.e., words) of a generic input text. GeneratePerturbations(k, n, Q) (line 2) returns a random population of n perturbations that succeed at changing N’s classification: for each successful attack p, a subset of k out of d features has been perturbed through a Fast Gradient Sign attack ⁹ (FGSM), while it is ensured that the point lies inside a convex region Q which in our case will be the ϵ-hyper-cube around the embedded text. If no perturbation is found in this way (i.e., population size of the attacks is zero, as in line 3), budget is decreased (line 4) and another trial of GeneratePerturbations(k, n, Q) is performed (e.g., with few features as targets and a different random seed to guide the attacks). Function AccuracyDrop(N, P) returns the best perturbation a where k is increasingly minimised (line 7). Algorithm terminates when either no attacks are possible (all the combinations of features have been explored) or after fixed number of iterations has been performed (line 1).

Algorithm 1: ORE computation via implicit hitting sets and sparse attacks

Data: a network N, the input text t, the initial set of features F, a network prediction ˆy, a cost function C against which the explanation is minimised

Result: an optimal ORE E

1. \[ \Gamma = \emptyset \]
2. while true do
3. \[ E = \text{MinimumHS}(\Gamma, C) \]
4. if Entails(E, (N \( \land \ B_{P,E}(t)) \rightarrow \hat{y}) \] then
5. \[ \text{return } E \]
6. else
7. \[ A = \text{SparseAttacks}(E, N) \]
8. \[ \Gamma = \Gamma \cup \{ A \} \]
9. end
10. end

Minimum Satisfying Assignment Explanations This approach, based on the method presented in [Dillig and others, 2012], finds an explanation in the form of an MSA, for which in turn a maximum universal subset (MUS) is required. For a given cost function C and text t, an MUS is a universal subset \( t' \) of words that maximises \( C(t') \). An MSA of the network M w.r.t the text is precisely a satisfying assignment of the formula \( \forall_{w \in t'}. M \rightarrow \hat{y} \) for some MUS \( t' \). In other words, an MSA is \( t \setminus t' \). The inputs to the MSA algorithm are: \( N \) which represents the network \( M \) in constraint form; text \( t \); cost function \( C \) and prediction \( \hat{y} \) for the input \( t \). The algorithm first uses the reversed sort function for the text \( t \) to optimize the search tree. The text is sorted by the cost of each word; then uses the recursive MUS algorithm to compute an MUS \( t' \). Finally, the optimal explanation \( (t \setminus t') \) is returned.

The inputs of the \( \text{mus} \) algorithm are: a set of candidate words \( cW \) that an MUS should be calculated for (equal to \( t \) in the first recursive call), a set of bounded words \( bW \) that may be part of an MUS, where \( \forall_{w \in bW}. w \) may be limited by \( \epsilon \)-ball or \( k \)-NN box closure, a lower bound \( L \), the network \( N \), a cost function \( C \), and a network prediction \( \hat{y} \). It returns a maximum-cost universal set for the network \( N \) with respect to \( t \), which is a subset of \( cW \) with a cost greater than \( L \), or the empty set when no such subset exists. The lower bound allows us to cut off the search when the current best result cannot be improved. During each recursive call, if the lower bound cannot be improved, the empty set is returned (line 1). Otherwise, a word \( w \) is chosen from the set of candidate words \( cW \) and it is determined whether the cost of the universal subset containing word \( w \) is higher than the cost of the universal subset without it (lines 5-12). Before definitively adding word \( w \) to \( bW \), we test whether the result is still satisfiable with \( \text{Entails} \) (line 5) i.e. still an explanation. The \( \text{shrink} \) method helps to reduce the set of candidate words by iterating through current candidates and checking using \( \text{Entails} \) whether they are necessary. This speeds-up the algorithm (as there are fewer overall calls to \( \text{Entails} \)). The recursive call at line 6 computes the maximum universal subset of \( \forall_{w \in bW}. N \rightarrow \hat{y} \), with adjusted \( cW \) and \( L \) as necessary. Finally within this \( \text{if} \) block, we compute the cost of the universal subset involving word \( w \), and if it is higher than the previous bound \( L \), we set the new lower bound to cost (lines 7-11). Lines 11-12 considers the cost of the universal subset \textit{not} containing word \( w \), in case it has higher cost, and if so, ⁹https://www.tensorflow.org/tutorials/generative/adversarial_fgsm
Algorithm 3: MUS computation, mus(bW, N, cW, t, C, L, y)

**Data:** a list of bounded words bW, a network N, a set of candidate words cW, the input text t, a cost function C against which the ORE is minimised, a lower bound for MUS L, a prediction y for the input

**Result:** a Maximum Universal Subset with respect to input text t

1. if cW = ∅ or (C(cW)) ≤ L then return ∅
2. best = ∅
3. choose w ∈ cW
4. bW = bW ∪ {w}, constW = cW \ {w}
5. if Entails,constW,(N \ B_{F,E}(constW)) \ y) then
   6. Y = mus(bW, N, shrink(N, bW, cW \ {w}), t, C, L - C(w), y)
   7. cost = C(Y) + C(w)
   8. if cost > L then
      9. best = Y ∪ {w}
   10. L = cost
11. Y = mus(bW \ {w}, N, cW \ {w}, t, C, L, y)
12. if C(Y) > L then best = Y
13. return best

updates best. Once one optimal explanation has been found, it is possible to compute all combinations of the input that match that cost, and then use Entails on each to keep only those that are also explanations.

Comparing MHS and MSA The MSA-based approach uses MUS algorithm to find maximum universal subset and then finds a MSA for that MUS. MUS is a recursive branch-and-bound algorithm [Dillig and others, 2012] that explores a binary tree structure. The tree consists of all the word appearing in the input cube. The MUS algorithm possibly explores an exponential number of universal subsets, however, the recursion can be cut by using right words ordering (i.e. words for which robustness query will answer false, consider words with the highest cost first) or with shrink method. MUS starts to work with a full set of candidate words, whereas the HS approach starts with an empty set of fixed words and tries to find an attack for a full set of bounded words. In each iteration step, the HS approach increases the set of fixed words and tries to find an attack. It is because a subset t′ ⊆ t is an MSA for a classifier M with respect to input text t iff t′ is a minimal hitting set of minimum falsifying set (see [Ignatiev and others, 2016] for details). To speed up the MSA algorithm, we use shrink procedure which reduces the set of candidate words, and for non-uniform cost function, words ordering (words with the highest cost are considered as the first candidates), while HS-based approach uses SparseAttacks routine to increase the hitting set faster.

Excluding words from MSA To exclude specific words from a smallest explanation we add one extra argument to the MSA algorithm input: the bW which represents bounded words. In this case the set cW = t \ bW. From now on the procedure

Algorithm 4: Computing smallest cost explanation

**Data:** a network N, an input text t, a cost function C for the input C, a prediction y.

**Result:** A smallest cost explanation for network N w.r.t. input text t

1. bW = ∅, cW = C, sce = ∅
2. textSortedByCost = sort(t)
3. maxus = mus(bW, N, cW, textSortedByCost, C, 0, y)
4. foreach c ∈ t do
   5. if c ∉ maxus then
      6. sce = sce ∪ c
   7. end
8. end
9. return sce

Algorithm 5: shrink algorithm shrink(bW, N, cW, C, C, L, y).

**Data:** a list of bounded words bW, a network N, a set of candidate words cW, a text t, a cost function C, a lower bound L, a prediction y for the input

**Result:** A set of the essential candidate words eW

1. eW = cW
2. foreach word ∈ cW do
   3. eW = eW \ {word}
   4. bW = bW ∪ {word}
   5. constW = C \ bw
   6. if Entails,constW,(N \ B_{F,E}(cW)) \ y) then
      7. eW = eW \ {word}
   8. end
9. bW = bW \ {word}
10. end
11. return eW

is the standard one.

7.3 Details on the Experimental Results

Datasets and Test Bed

As mentioned in the Experimental Evaluation Section, we have tested MSA and HS approaches for finding optimal cost explanations respectively on the SST, Twitter and IMDB datasets. For each task, we have selected a sample of 40 input texts that maintain classes balanced (i.e., half of the examples are negative, half are positive). Moreover, we inserted inputs whose polarity was exacerbated (either very negative or very positive) as well as more challenging examples that machines usually misclassify, like double negations or mixed sentiments etc. Further details in Table 1.

Models Setup

We performed our experiments on FC and CNNs with up to 6 layers and 20K parameters. FC are constituted by a stack of Dense layers, while CNNs additionally employ Convolutional and MaxPool layers: for both CNNs and FC the decision is taken through a softmax layer, with Dropout that is added after each layer to improve generalization during...
Figure 8: Examples of Optimal Robust Explanations - highlighted in blue -. OREs were extracted using kNN boxes with 25 neighbors per-word: fixing words in an ORE guarantees the model to be locally robust. The examples come from the IMDB dataset, model employed is a FC network with 100 input words (accuracy 0.81).

Figure 9: Examples of explanations that were enabled by the adversarial attacks routine. Timeout was set to 2 hours.

Figure 10: How an explanation grows when either $\epsilon$ (top) or $k$ (bottom) is increased. Model considered is a fully connected with 50 input words on SST dataset (0.89 accuracy). On the left a positive review that is correctly classified, on the right a negative review that is misclassified (i.e., the model’s prediction is negative). For specific ranges of $\epsilon$ the Oracle cannot extract an explanation (timeout, highlighted in red).
Table 1: Datasets used for training/testing and extracting explanations. We report various metrics concerning the networks and the training phase (included accuracy on Test set), while in Table 1.2 we report the number of texts for which we have extracted explanations along with the number of words considered when calculating OREs: samples were chosen to reflect the variety of the original datasets, i.e., a mix of long/short inputs equally divided into positive and negative instances.

| Inputs (Train, Test) | TWITTER | SST | IMDB |
|----------------------|---------|-----|------|
| 1.55M, 50K           | 117.22K | 1.82K | 25K, 25K |
| Output Classes       | 2       | 2   | 2    |
| Input Length (max, max. used) | 88, 50   | 52, 50 | 2315, 100 |
| Neural Network Models | FC, CNN | FC, CNN | FC, CNN |
| Neural Network Layers (min, max) | 3, 6     | 3.6  | 3.6   |
| Accuracy on Test Set (min, max) | 0.77, 0.81 | 0.82, 0.89 | 0.69, 0.81 |
| Number of Networks Parameters (min, max) | 3K, 18K | 1.3K, 10K | 5K, 17K |

Table 1.2: Explanations

| ϵ    | Explanation Length | MSA Execution Time | HS Execution Time |
|------|--------------------|--------------------|-------------------|
| 0.01 | 5 ± 5              | 8.08 ± 7.9         | 63.70 ± 63.69     |
| 0.05 | 5.5 ± 4.5          | 176.22 ± 175.92    | 339.96 ± 334.66   |
| 0.1  | 7.5 ± 2.5          | 2539.75 ± 2539.14  | 3563.4 ± 3535.84  |

Table 2: Comparison between MSA and HS in terms of execution time for different values of ϵ, and the corresponding explanation length.

**Example 1** Calculating all of the smallest explanations for an input (ϵ = 0.05, FC network, 10 input words, 5 dimensional embedding, SST dataset):

Input: ['strange', 'funny', 'twisted', 'brilliant', 'and', 'macabre', '<PAD>', '<PAD>', '<PAD>', '<PAD>']

Explanations (5 smallest, len=6.0): 
- ['strange', 'funny', 'twisted', 'brilliant', '<PAD>'], ['<PAD>']
- ['strange', 'funny', 'twisted', '<PAD>']
- ['strange', 'twisted', '<PAD>']
- ['strange', 'twisted', 'brilliant', '<PAD>']
- ['strange', 'twisted', 'and', '<PAD>']

**Example 2** Decision bias, as Derrida cannot be excluded (ϵ = 0.05, FC network, 10 input words, 5 dimensional embedding, SST dataset):

Input: ['Whether', 'or', 'not', 'you', 'are', 'enlightened', 'by', 'any', 'Derrida']

Exclude: ['Derrida']

Explanation: ['Whether', 'or', 'are', 'enlightened', 'by', 'any', 'of', 'Derrida']