# The Out-of-Distribution Problem in Explainability and Search Methods for Feature Importance Explanations

## Peter Hase, Harry Xie, and Mohit Bansal

Department of Computer Science University of North Carolina at Chapel Hill {peter, fengyu.xie, mbansal}@cs.unc.edu

## **Abstract**

Feature importance (FI) estimates are a popular form of explanation, and they are commonly created and evaluated by computing the change in model confidence caused by removing certain input features at test time. For example, in the standard Sufficiency metric, only the top-k most important tokens are kept. In this paper, we study several under-explored dimensions of FI explanations, providing conceptual and empirical improvements for this form of explanation. First, we advance a new argument for why it can be problematic to remove features from an input when creating or evaluating explanations: the fact that these counterfactual inputs are out-of-distribution (OOD) to models implies that the resulting explanations are socially misaligned. The crux of the problem is that the model prior and random weight initialization influence the explanations (and explanation metrics) in unintended ways. To resolve this issue, we propose a simple alteration to the model training process, which results in more socially aligned explanations and metrics. Second, we compare among five approaches for removing features from model inputs. We find that some methods produce more OOD counterfactuals than others, and we make recommendations for selecting a feature-replacement function. Finally, we introduce four search-based methods for identifying FI explanations and compare them to strong baselines, including LIME, Anchors, and Integrated Gradients. Through experiments with six diverse text classification datasets, we find that the only method that consistently outperforms random search is a Parallel Local Search (PLS) that we introduce. Improvements over the second best method are as large as 5.4 points for Sufficiency and 17 points for Comprehensiveness.

## 1 Introduction

Estimating feature importance (FI) is a common approach to explaining how learned models make predictions for individual data points [55, 49, 35, 61, 38, 12]. FI methods assign a scalar to each feature of an input representing its "importance" to the model's output, where a feature may be an individual component of an input (such as a pixel or a word) or some combination of components. Alongside these methods, many approaches have been proposed for evaluating FI estimates (also known as attributions) [44, 2, 14, 23, 21, 73]. Many of these approaches use test-time input ablations, where features marked as important are removed from the input, with the expectation that the model's confidence in its original prediction will decline if the selected features were truly important.

<sup>&</sup>lt;sup>1</sup>All supporting code for experiments in this paper is publicly available at <a href="https://github.com/peterbhase/ExplanationSearch">https://github.com/peterbhase/ExplanationSearch</a>.

For instance, according to the *Sufficiency* metric [14], the best FI explanation is the set of features which, if kept, would result in the highest model confidence in its original prediction. Typically the top-k features would be selected according to their FI estimates, for some specified *sparsity* level k. Hence, the final explanation e is a k-sparse binary vector in  $\{0,1\}^d$ , where d is the dimensionality of the chosen feature space. For an explanation e and a model f that outputs a distribution over classes p(y|x) = f(x), Sufficiency can be given as:

$$Suff(f, x, e) = f(x)_{\hat{y}} - f(Replace(x, e))_{\hat{y}}$$

where  $\hat{y} = \arg \max_y f(x)_y$  is the predicted class for x and the Replace function replaces features in x with some uninformative feature at locations corresponding to 0s in the explanation e.

The Replace function plays a key role in the definition of such metrics because it defines the *counterfactual* input that we are comparing the original input with. Though FI explanations are often presented without mention of counterfactuals, all explanations make use of counterfactual situations [40], and FI explanations are no exception. The only way we can understand what makes some features "important" to a particular model prediction is by reference to a counterfactual input which has its important features replaced with a user-specified (uninformative) feature.

In this paper, we study several under-explored dimensions of the problem of finding good explanations according to test-time ablation metrics including Sufficiency and a related metric, Comprehensiveness, with a focus on natural language processing tasks. We describe three primary contributions below.

First, we argue that standard FI explanations are heavily influenced by the out-of-distribution (OOD) nature of counterfactual model inputs, which results in *socially misaligned* explanations. We use this term, first introduced by Jacovi and Goldberg [25], to describe a situation where an explanation communicates a different kind of information than the kind that people expect it to communicate. Here, we do not expect the model prior or random weight initialization to influence FI estimates. This is a problem insofar as FI explanations are not telling us what we think they are telling us. We propose a training algorithm to resolve the social misalignment, which is to expose models to counterfactual inputs during training, so that counterfactuals are not out-of-distribution at test time.

Second, we systematically compare Replace functions, since this function plays an important role in evaluating explanations. To do so, we remove tokens from inputs using several Replace functions, then measure how OOD these ablated inputs are to the model. We compare methods that remove tokens entirely from sequences of text [44, 14], replace token embeddings with the zero embedding or a special token [35, 61, 2, 71, 61], marginalize predictions over possible counterfactuals [74, 31, 69], and edit the input attention mask rather than the input text. Following our argument regarding the OOD problem (Sec. 4), we recommend the use of some Replace functions over others.

Third, we provide several novel search-based methods for identifying FI explanations. While finding the optimal solution to  $\arg\max_e \mathrm{Suff}(f,x,e)$  is a natural example of binary optimization, a problem for which search algorithms are a common solution [46, 53, 4], we are aware of only a few prior works that search for good explanations [20, 50, 16]. We introduce our novel search algorithms for finding good explanations by making use of general search principles [46]. Based on experiments with two Transformer models and six text classification datasets (including FEVER, SNLI, and others), we summarize our core findings as follows:

- 1. We propose to train models on explanation counterfactuals and find that this leads to greater model robustness against counterfactuals and yields drastic differences in explanation metrics.
- 2. We find that some Replace functions are better than others at reducing counterfactual OOD-ness, although ultimately our solution to the OOD problem is much more effective.
- 3. We introduce four novel search-based methods for identifying explanations. Out of all the methods we consider (including popular existing methods), the only one that consistently outperforms random search is the Parallel Local Search (PLS) that we introduce, often by large margins of up to 20.8 points. Importantly, we control for the compute budget used by each method.

## 2 Related Work

**Feature Importance Methods.** A great number of methods have been introduced for FI estimation, drawing upon local approximation models [49, 50, 32], attention weights [26, 65, 72], model gradients [55, 54, 61, 56], and model-based feature selection [5, 3, 66, 45, 9, 12]. While search approaches are

regularly used to solve combinatorial optimization problems in machine learning [53, 6, 4, 17, 43], we know of only a few FI methods based on search [20, 50, 16]. Fong and Vedaldi [20] perform gradient descent in explanation space, while Ribeiro et al. [50] search for probably-sufficient subsets of the input (under a perturbation distribution). In concurrent work, Du and Xu [16] propose a genetic search algorithm for identifying FI explanations. We introduce several novel search algorithms for finding good explanations, including (1) a gradient search similar to Fong and Vedaldi [20], a (2) local heuristic search inspired by an adversarial attack method [17], (3) a global heuristic search, and (4) a parallel local search (PLS) making use of general search principles [46].

Choice of Replace Function. Past evaluations of explanation methods typically remove tokens or words from the text entirely [44, 14] or replace them with fixed feature values [23, 70]. Methods for creating explanations also use several distinct approaches, including (1) replacing token embeddings with the zero vector [35, 61, 2], (2) using a special token [71, 61], (3) marginalizing predictions over a random variable representing an unobserved token [74, 31, 69, 28], and (4) adversarially selecting counterfactual features [24]. Sturmfels et al. [59] carry out a case study involving a few Replace functions for a vision model, which they compare via test-time ablations with image blurring techniques, though the case study is not intended to be a full comparison of methods. Haug et al. [22] assess a number of Replace functions for explanation methods used with tabular data, but they compare between functions to use when generating explanations, rather than when evaluating explanations, for which they offer no recommendation. In addition to evaluating Replace functions from the above works, we also consider setting attention mask values for individual tokens to 0.

The Out-of-distribution Problem of Explanations. Many papers have expressed concerns over how removing features from an input may result in counterfactuals that are out-of-distribution to a trained model [71, 61, 20, 8, 23, 31, 24, 69, 60, 28, 48, 22, 52, 29, 63]. In response to the problem, some have proposed to marginalize model predictions over possible counterfactual inputs [74, 31, 69, 28], use counterfactuals close to real inputs [8, 52], weight their importance by their closeness to real inputs [48], or to adversarially select counterfactual features rather than use any user-specified features [24]. Others reject the whole notion of test-time ablations, preferring metrics based on train-time ablations [23]. Jethani et al. [29] propose a specialized model for evaluating explanations that is trained on counterfactual inputs in order to make them in-distribution, but since the evaluation model is distinct from the model used to solve the task, explanation metrics calculated using this evaluation model may not reflect the faithfulness of explanations to the task model. In concurrent work, Vafa et al. [63] independently adopt a solution equivalent to our Counterfactual Training with an Attention Mask Replace function, an approach which we empirically justify in Sec. 5. In general, prior works make arguments for their approach based on intuition or basic machine learning principles, such as avoiding distribution shift. In Sec. 4, we give a more detailed argument for preferring in-distribution counterfactuals on the basis of social alignment, a concept introduced by Jacovi and Goldberg [25], and we propose a solution to the OOD problem. Our solution allows for test-time evaluation of explanations of a particular model's decisions for individual data points, unlike similar proposals which either evaluate large sets of explanations all at once [23] or use a separate model trained specifically for evaluation rather than the blackbox model [29].

## 3 Problem Statement

Feature Importance Metrics. The problem we are investigating is to find good feature importance explanations for single data points, where explanation are evaluated under metrics using test-time ablations of the input. In this context, an explanation for an input in a d dimensional feature space is a binary vector  $e \in \{0,1\}^d$ , which may be derived from discretizing an FI estimate  $v \in \mathbb{R}^d$ . We consider two primary metrics, Sufficiency and Comprehensiveness [14]. Sufficiency measures whether explanations identify a subset of features which, when kept, lead the model to remain confident in its original prediction for a data point. Comprehensiveness, meanwhile, measures whether an explanation identifies all of the features that contribute to a model's confidence in its prediction, such that removing these features from the input lowers the model's confidence.

The Sufficiency metric for an explanation  $e \in \{0,1\}^d$  and model  $p(y|x) = f_{\theta}(x)$  is given as

$$Suff(f_{\theta}, x, e, s) = f_{\theta}(x)_{\hat{y}} - f_{\theta}(Replace_{s}(x, e))_{\hat{y}}$$
(1)

where  $\hat{y} = \arg \max_y f(x)_y$  is the predicted class for x, and the Replace<sub>s</sub> function retains a proportion s of the input features (indicated by e) while replacing the remaining features with some

user-specified feature. In order to control for the explanation sparsity, i.e. the proportion s of tokens in the input that may be retained, we average Sufficiency scores across sparsity levels in  $\{.05, .10, .20, .50\}$ , meaning between 5% and 50% of tokens in the input are retained [14]. A **lower** Sufficiency value is better, as it indicates that more of the model's confidence is explained by just the retained features (increasing  $f_{\theta}(\text{Replace}(x, e))_{\hat{y}}$ ).

Similarly, Comprehensiveness is given as  $\operatorname{Comp}(f_{\theta}, x, e, s) = f_{\theta}(x)_{\hat{y}} - f_{\theta}(\operatorname{Replace}_{s}(x, e))_{\hat{y}}$  but with sparsity values in  $\{.95, .90, .80, .50\}$ , as we are looking to remove features that are important to the prediction (while keeping most features). A **higher** Comprehensiveness value is better, as it indicates that the explanation selects more of the evidence that contributes to the model's confidence in its prediction (resulting in a lower  $f_{\theta}(\operatorname{Replace}(x, e))_{\hat{y}}$ ).

Overall Objective. Finally, our overall Sufficiency and Comprehensiveness objectives are given by averaging Suff (or Comp) scores across several sparsity levels. With a model p(y|x) = f(x), a single data point x with d features, and a set of sparsity levels S, the Sufficiency objective is optimized by obtaining a set  $E = \{e_i\}_{i=1}^{|S|}$  with one explanation per sparsity level as

$$\arg\max_{E} \frac{1}{|S|} \sum_{i=1}^{|S|} \mathrm{Suff}(f, x, e_i, s_i) \quad \text{s.t. } e_i \in \{0, 1\}^d \ \text{ and } \ \sum_{d} e_i^{(d)} \leq \mathrm{ceiling}(s_i \cdot d)$$

where the ceiling function rounds up the number  $s_i \cdot d$  of tokens to keep. When optimizing for Comprehensiveness, we use the Comp and  $\arg\min$  functions, and the inequality is flipped. In general, we will optimize this objective using a limited compute budget, further described in Sec. 6.2.

# 4 The Out-of-Distribution Problem in Explanations

In this section, we first give a full argument for why it is problematic for explanations to be created *or* evaluated using OOD counterfactuals. Then, we propose a solution to the OOD problem. We rely on this argument in our comparison of Replace functions in Sec. 5. We also assess our proposed solution to the OOD problem in Sec. 5 and later make use of this solution in Sec. 6.

The OOD problem for explanations occurs when a counterfactual input used to create or evaluate an explanation is out-of-distribution (OOD) to a model. Here, we take OOD to mean the input is not drawn from the data distribution used in training (or for finetuning, when a model is finetuned) [42]. In general, counterfactual data points used to produce FI explanations will be OOD because they contain feature values not seen in training, like a MASK token for a language model. A long line of past work raises concerns with this fact [71, 61, 20, 8, 23, 31, 24, 69, 60, 28, 48, 22, 52, 29, 63]. The most concrete argument on the topic originates from Hooker et al. [23], who observe that using OOD counterfactuals makes it difficult to determine whether model performance degradation is caused by "distribution shift" or by the removal of information. It is true that, for a given counterfactual, a model might have produced a different prediction if that counterfactual was in-distribution rather than out-of-distribution. But this is a question we cannot ask about a single, trained model, where there is no ambiguity about what causes a drop in model confidence when replacing features: the features in the input were replaced, and this changes that model's prediction. If the counterfactual was in-distribution, we would be talking about a different model, with a different training distribution. Hence, we believe we need a stronger argument for why we should not use OOD counterfactuals when explaining a trained model's behavior.

Our principal claim is that feature importance explanations for a standardly trained neural model are *socially misaligned*, which is undesirable. Jacovi and Goldberg [25] originally introduce this term as they describe shortcomings of explanations from a pipeline (select-predict) model, which is a kind of classifier designed to be interpretable. Explanations are socially misaligned when people expect them to communicate one kind of information, and instead they communicate a different kind of information. For example, if we expected an explanation to be the information that a model relied on in order to reach a decision, but the explanation was actually information selected after a decision was already made, then we would say that the explanations are socially misaligned. Our argument now proceeds in two steps: first, we outline what the social expectations are for feature importance explanations, and then we argue that the social expectations are violated due to the fact that counterfactuals are OOD.

We suggest that, for a particular trained model and a particular data point, people expect a feature importance explanation to reflect how the model has learned to interpret features as evidence for or against a particular decision.<sup>2</sup> This social expectation is upheld if FI explanations are influenced only by the interaction of an untrained model with a training algorithm and data. But our expectations are violated to the ex-

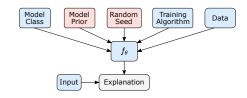


Figure 1: Causal diagram of a feature importance explanation for a trained model and an input.

tent that FI explanations are influenced by factors such as the choice of model prior and random seed (which we do not intend to influence FI explanations). We depict these possible upstream causes of individual FI explanations in Fig. 1. In fact, the model prior and random seed are influential to FI explanations when the counterfactuals employed in these explanations are OOD to the model. A simple example clearly illustrates the potential influence of model priors: Suppose one trained a BERT model to classify the sentiment of individual words using training data from a sentiment dictionary, then obtained feature importance explanations with the MASK token Replace function. In this situation, model predictions on counterfactual data are always equal to the prediction for a single MASK token,  $f_{\theta}$  (MASK). So, by construction, the MASK token never appears in the training data, but FI explanations for this model make use of the quantity  $f_{\theta}(MASK)$ . Since a model could not have learned its prediction  $f_{\theta}(MASK)$  from the data, this quantity will be largely determined by the model prior and other training hyperparameters, and therefore explanations based on this prediction are socially misaligned. Now, in general, we know that neural models are sensitive to random parameter initialization, data ordering (determined by the random seed) [15], and hyperparameters (including regularization coefficients) [10, 47, 64], even as evaluated on in-distribution data. For OOD data, then, a neural model will still be influenced by these factors, but the model has no data to learn from in this domain. As a result, FI explanations are socially misaligned to the extent that these unexpected factors influence the explanations (while the expected factors like data are not as influential). In other words, we do not expect explanations to influenced by random factors, the priors of the model designer, or uninterpretable hyperparameters, but we do expect them to be influenced by what the model learns from data.

The argument applies equally to explanation metrics. When metrics are computed using OOD counterfactuals, the scores are influenced by unexpected factors like the model prior and random seed, rather than the removal of features that a model has learned to rely on. As a result, the metrics are socially misaligned. They do not represent explanation quality in the way we expect them to.

The solution to the OOD problem is to align the train and test distributions, which we do by exposing the model to counterfactual inputs during training, a method we term Counterfactual Training. Since common explanation methods can require hundreds or thousands of model forward passes when explaining predictions [49, 61], explanations from these methods would be prohibitively expensive to obtain during training. We therefore propose to train with random explanations that remove most of the input tokens, which provides a good objective in theory for models to learn the counterfactual distribution that will be seen at test time [29]. Specifically, we double the inputs in each training batch, adding a Replace(x, e) version of each input (with the same label) according to a random explanation e with sparsity randomly selected from  $\{.05, .1, .2, .5\}$ . The resulting Counterfactual-Trained (CT) models make in-distribution predictions for both observed and counterfactual data points. While we cannot guarantee that this approach fully eliminates the influence of the model prior and random seed on FI explanations, the fact that explanations are influenced by what the model learns from data will resolve social misalignment to a great extent. We find that these models suffer only slight drops in test set accuracy, by 0.7 points on average across six datasets (see Table 3 in Supplement). But we observe that this approach greatly improves model robustness to counterfactual inputs, meaning the counterfactuals are now much more in-distribution to models (described further in Sec. 5). Similar to the goals of ROAR [23] and EVAL-X [29], our proposed solution also aims to align the train and test-time distributions. However, our approach allows for test-time evaluation of individual explanations for a particular trained model, while ROAR only processes large sets of explanations all at once and EVAL-X introduces a specialized model for evaluation, which may not reflect the faithfulness of explanations to the task model.

<sup>&</sup>lt;sup>2</sup>We mean "people" to refer to the typical person who has heard the standard description of these explanations, i.e. that they identify features that are "important" to a model decision. Of course, there will be some diversity in how different populations interpret feature importance explanations [19].

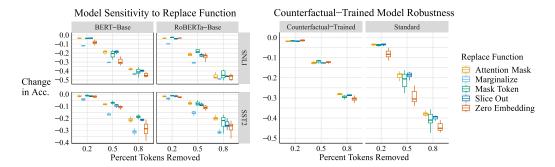


Figure 2: Model sensitivity to input ablations for several choices of Replace function and training algorithm. On the left we show the sensitivity of standardly trained models. On the right we show the effect of using Counterfactual-Trained models.

## 5 Analysis of Counterfactual Input OOD-ness

Here, we assess how out-of-distribution the counterfactual inputs given by Replace functions are to models, and we measure the effectiveness of Counterfactual Training. We do this before designing or evaluating explanation methods because, given our argument in Sec. 4, it is important to first identify which Replace function and training methods are most appropriate to use for these purposes.

**Experiment Design.** We compare between Replace functions according to how robust models are to test-time input ablations using each function, where the set of input features to be removed is fixed across the functions. We measure robustness by model accuracy, which serves as a proxy for how in-distribution or out-of-distribution the ablated inputs are. If we observe differences in model accuracies between Replace functions for a given level of feature sparsity, we can attribute the change in the input OOD-ness to the Replace function itself. In the same manner, we compare between Counterfactual-Trained (CT) models and standardly trained models (termed as Standard).

Specifically, we train 10 BERT-Base [13] and RoBERTa-Base [36] on two benchmark text classification datasets, SNLI [7] and SST-2 [58]. These are all Standard models, without the counterfactual training we propose. We use ten random seeds for training these models. Then, we evaluate how robust the models are to input ablations, where we remove a proportion of random tokens using one of five Replace functions (i.e. we Replace according to a random explanation). We evaluate across proportions in {0.2, 0.5, 0.8}. The five Replace functions we test are:

- 1. **Attention Mask.** We introduce this Replace function, which sets a Transformer's attention mask values for removed tokens to 0, meaning their hidden representations are never attended to.
- 2. **Marginalize.** This method marginalizes model predictions over counterfactuals drawn from a generative model  $p_{\phi}(x)$  of the data, i.e. as  $\arg\max_{y}\ln\sum_{\tilde{x}\sim p_{\phi}(\tilde{x}|x,e)}p_{\theta}(y|\tilde{x})p_{\phi}(\tilde{x}|x,e)$ , where  $p_{\phi}(\tilde{x}|x,e)$  is the distribution over tokens to be replaced given by e.g. BERT [74, 31, 8, 69].
- 3. MASK Token. In this method, we simply replace tokens with the MASK token.
- 4. **Slice Out**. This approach removes selected tokens from the input sequence itself, such that the resulting sequence has a lower number of tokens.
- 5. Zero Vector. Here, we set the token embeddings for removed tokens to the zero vector.

We train additional CT models for BERT-Base on SNLI, with ten random seeds per model, for all Replace functions except Marginalize, since this function is exceedingly expensive to use during Counterfactual Training. For further details, see the Supplement.

**Results for** Replace **functions.** We show the results of this experiment in Fig. 2, via boxplots of the drops in accuracy for each of the 10 models per condition. First, we describe differences in Replace functions for Standard models, then we discuss the effect of Counterfactual Training. On the left in Fig. 2, we see that Standard models are much more sensitive to some Replace functions than others. The Attention Mask and Mask Token functions are the two best methods. The best of these two methods outperforms the third best method by up to 1.61 points with BERT and SNLI (p = .0005),  $^3$ 

<sup>&</sup>lt;sup>3</sup>p-values for two-sided difference in means tests are calculated by block bootstrap with all data points and model seeds being resampled 100k times [18].

5.48 points with RoBERTa and SNLI ( $p < 1\mathrm{e} - 4$ ), 2.42 points with BERT and SST-2 (p = 0.0008), and 4.72 points with RoBERTa and SST-2 ( $p < 1\mathrm{e} - 4$ ). The other methods often far underperform the best method. For instance, with BERT on SST-2, Zero Embedding is up to 10.45 points worse than Mask Token ( $p < 1\mathrm{e} - 4$ ), and with RoBERTa on SST-2, Slice Out underperforms Attention Mask by up to 4.72 points ( $p < 1\mathrm{e} - 4$ ). Marginalize is regularly more than 10 points worse than the best method. Overall, we recommend that, when not using Counterfactual Training, researchers use either the Attention Mask or Mask Token Replace functions.

Counterfactual Training vs. Standard Training. On the right side of Fig. 2, we see the effect of Counterfactual Training on model robustness for several Replace functions. We find that counterfactual inputs are much less OOD for Counterfactual-Trained models than for Standard models, regardless of the Replace function used. The improvement in robustness is up to **22.9** points. Moreover, the difference between Replace functions is almost entirely erased, though we do observe a statistically significant difference between Attention Mask and Zero Embedding with 80% of tokens removed (by 2.23 points, p < 1e-4). Given these results, and following Sec. 4, we ultimately recommend that researchers use Counterfactual Training with the Attention Mask, Mask Token, or Slice Out Replace function whenever they intend to create FI explanations.

## 6 Explanation Methods and Experiments

## 6.1 Explanation Methods

We describe explanation methods we consider below, with implementation details in the Supplement.

**Salience Methods.** One family of approaches we consider assigns a scalar *salience* to each feature of an input. The key property of these scores is that they allow one to rank-order features. We obtain binarized explanations through selecting the top-k features, or up to the top-k features when some scores are negative (suggesting they should not be kept). We list the methods below:<sup>4</sup>

- 1. LIME. LIME estimates FI by learning a linear model of a model's predicted probabilities with samples drawn from a local region around an input [49]. Though it is common to use the Slice Out Replace function with LIME, we use the Attention Mask Replace function (following Sec. 5), meaning we sample local attention masks rather than local input sequences.
- 2. Vanilla Gradients. We obtain model gradients w.r.t. the model input as salience scores, one early method for explanation [34]. We compute the gradient of the predicted probability w.r.t. input token embeddings, and we obtain a single value per token by summing along the embedding dimension.
- 3. Integrated Gradients. We evaluate the Integrated Gradients (IG) method of Sundararajan et al. [61]. This method numerically integrates the gradients of a model output w.r.t. its input along a path between the observed input and a user-selected baseline. Given our results in Sec. 5, we use a repeated MASK token embedding for our baseline  $\tilde{x}$  rather than the all-zero input suggested by Sundararajan et al. [61] for text models. We use the model's predicted probability as the output, and to obtain token-level salience scores, we sum the output of IG along the embedding dimension.

**Search Methods.** An alternative class of methods searches through the space of possible explanations. Search methods are regularly used to solve combinatorial optimization problems in machine learning [53, 6, 4, 17, 43]. All search methods use the Attention Mask Replace function, and the search space is restricted to explanations of the maximum allowable sparsity (or minimum, with Comprehensiveness), except for Anchors which takes a maximum number of features as a parameter.

- 1. Random Search. For each maximum explanation sparsity k (or minimum, for Comprehensiveness), we randomly sample a set of k-sparse explanations, compute the current objective for each of them, and choose the best explanation under the objective.
- 2. Anchors. Ribeiro et al. [50] introduce a method for finding a feature subset that almost always yields the same model prediction as its original prediction for some data point, as measured among data points sampled from a distribution centered on the original data point. Explanations are also preferred to have high coverage, meaning the feature subset is likely to be contained in a local sample. The solution is identified via a Multi-Armed Bandit method combined with a beam search.

<sup>&</sup>lt;sup>4</sup>In early experiments, we found that a parametric model (similar to [5, 3, 45]) performed far worse than other salience methods, and hence we leave out parametric models from further consideration.

- 3. Exhaustive Search. Exhaustive search returns the optimal solution after checking the entire solution space. This is prohibitively expensive with large inputs, as there is a combinatorial explosion in the number of possible explanations. However, we are able to exactly identify optimal explanations for short sequences, typically with 10 or fewer tokens.
- 4. Gradient Search. Fong and Vedaldi [20] propose to search through a continuous explanation space by gradient descent. We introduce a Gradient Search that uses discrete explanations, because continuous explanations do not reflect test-time conditions where discrete explanations must be used. For an input of length L, this method sequentially updates a continuous state vector  $s \in \mathbb{R}^L$  via gradient descent to minimize a regularized cross-entropy loss between the model prediction on the input x and the model prediction for Replace $(x, e_t)$ , where  $e_t$  is a discrete explanation sampled from a distribution  $p(e_t|s_t)$  using the Gumbel-Softmax estimator for differentiability [39, 27]. The regularizer maintains sparsity of the solution. The final explanation is obtained from the last state  $s_t$ .
- 5. Taylor Search. Inspired by HotFlip [17], this method explores the solution space by forecasting the change in the objective using a first-order Taylor approximation. Specifically, this is a local search method with a heuristic function computed as follows: We first calculate the gradient  $g \in \mathbb{R}^L$  of the cross-entropy loss (same loss as Gradient Search) with respect to the explanation  $e_t$ . Then we find the two indices i and j as the solution to  $\arg\max_{i,j} g^{(i)} g^{(j)}$ . The next state is obtained by setting  $e_t^{(i)} = 1$  and  $e_t^{(j)} = 0$ . This is a first-order approximation to the change in loss between the new and old state, based on the Taylor expansion of the loss [17]. Note when optimizing for Comprehensiveness, we use the  $\arg\min$ . Following Ebrahimi et al. [17], we ultimately use this search heuristic within a beam search, starting from a random explanation, with width w=3.
- 6. Ordered Search. Next, we introduce a global search algorithm, Ordered Search. This method searches through all explanations in an order given by a scoring function  $f:e\to\mathbb{R}$ . We only require that f is linear in e, as this allows for efficient ordering of the search space using a priority queue [4]. The algorithm proceeds by first estimating parameters for  $f_{\theta}$ , then searching through explanations in order of their score,  $\theta^T e$ . For the first stage, we obtain parameters for  $f_{\theta}$  from the per-token salience scores given by LIME, which is the best salience method evaluated in Sec. 6. In the second stage, we enumerate the search space in order of the score given by  $f_{\theta}$ . We allocate 25% of the compute budget to the first stage and 75% to the second (measured in terms of forward passes).
- 7. Parallel Local Search (PLS). Lastly, we again consider the class of local search algorithms, which have a long history of success with constrained optimization problems [46, 4]. We propose a parallelized local search algorithm (PLS) tailored to the problem at hand. Given a number r of parallel runs to perform, a proposal function Propose, and compute budget b per run, an individual search proceeds as follows: (1) Sample a random initial explanation  $e_1$  and compute the objective function for that explanation. (2) For the remaining budget of b-1 steps: sample a not-already-seen explanation  $e_t$  according to Propose and adopt  $e_t$  as the new state only if the objective is lower at  $e_t$  than at the current state. The Propose function samples not-already-seen explanations from neighboring states to the current state. We use r=10 parallel runs following tuning results.

## 6.2 Experimental Setup

**Data.** We compare the above explanation methods on six benchmark text classification datasets: SNLI [7], BoolQ [11], Evidence Inference [33], FEVER [62], MultiRC [30], and SST-2 [57]. One important distinction among these datasets is that BoolQ, FEVER, MultiRC, and Evidence Inference data points include both a *query* and an accompanying *document*. The query is typically critical information indicating how the model should process the document, and therefore we never replace query tokens. We use 500 test points from each dataset to compare methods. See Table 2 in the Supplement for dataset statistics, including average sequence length.

**Models.** We train ten seeds of BERT-Base models on each dataset [13], which we term Standard models. For each dataset we train another ten Counterfactual-Trained (CT) models using the Attention Mask Replace function, following the approach outlined in Sec. 4 (further details in Supplement).

**Controlling for Compute Budget.** We wish to control for the available compute budget in order to fairly compare explanation methods. Some explanations require a single forward and backward pass [55, 34], while others can require hundreds of forward and backward passes [61] or thousands of

Table 1: Explanation metrics across methods and datasets

		Sufficie	ency ↓	Comprehens	siveness †
Dataset	Method	Standard Model	CT Model	Standard Model	CT Model
SNLI	LIME Int-Grad Anchors Gradient Search	20.00 (2.02) 43.76 (3.27) 11.93 (1.53) 17.55 (1.47)	27.08 (1.68) 32.91 (2.36) 30.96 (1.87) 33.98 (1.43)	82.18 (2.82) 34.01 (2.55) 55.72 (2.60) 53.15 (2.53)	75.34 (1.93) 43.22 (2.28) 48.86 (2.38) 49.36 (1.95)
	Taylor Search Ordered Search Random Search PLS	6.91 (1.10) -1.45 (0.93) -1.54 (0.96) - <b>1.65</b> (1.07)	28.00 (1.46) 15.06 (1.37) 15.38 (1.39) <b>14.16</b> (1.38)	73.20 (2.57) 87.78 (2.41) 87.36 (2.47) <b>87.95</b> (2.55)	66.76 (2.12) 84.67 (1.61) 84.63 (1.68) <b>86.18</b> (1.45)
BoolQ	LIME Int-Grad Anchors Gradient Search Taylor Search Ordered Search Random Search PLS	2.15 (1.75) 20.78 (3.57) 11.98 (2.62) 5.12 (1.41) 6.01 (1.33) 0.09 (0.84) -0.58 (0.63) -1.17 (0.47)	-1.56 (0.63) 9.05 (1.53) 6.07 (1.06) 1.65 (0.81) 2.28 (0.87) -2.58 (0.70) -2.51 (0.70) -3.52 (0.88)	52.02 (3.69) 16.80 (1.57) 29.87 (4.17) 30.04 (2.58) 46.32 (3.89) 51.59 (3.52) 55.78 (3.71) 72.78 (4.06)	36.25 (3.45) 12.20 (1.68) 15.46 (1.97) 17.65 (1.85) 26.65 (2.68) 34.36 (3.34) 31.62 (3.06) 47.80 (3.57)
Evidence Inference	LIME Int-Grad Anchors Gradient Search Taylor Search Ordered Search Random Search PLS	-16.07 (2.84) 1.22 (4.42) 7.08 (4.70) -10.57 (2.58) -4.55 (2.66) -16.80 (2.75) -17.05 (2.83) <b>-20.76</b> (3.77)	-14.92 (1.38) -2.98 (1.68) 3.04 (0.99) -7.56 (1.46) -3.33 (1.27) -14.26 (1.36) -12.69 (1.30) -20.33 (2.65)	47.60 (5.66) 26.51 (2.68) 25.01 (6.52) 31.73 (4.43) 41.95 (5.63) 45.37 (5.53) 42.81 (6.00) <b>56.31</b> (9.81)	33.97 (4.22) 20.87 (2.57) 13.89 (1.55) 18.07 (2.13) 26.70 (3.00) 31.14 (3.73) 26.48 (3.15) 38.71 (3.91)
FEVER	LIME Int-Grad Anchors Gradient Search Taylor Search Ordered Search Random Search PLS	-0.24 (0.50) 9.72 (1.80) 6.19 (1.22) 0.66 (0.68) 4.17 (0.96) -1.26 (0.41) -1.51 (0.51) -2.04 (0.62)	0.39 (0.96) 4.99 (1.40) 6.36 (1.10) 2.63 (1.12) 4.20 (1.20) -0.01 (0.90) -1.24 (2.33) -3.66 (0.82)	33.86 (3.43) 17.81 (2.47) 20.82 (2.58) 19.26 (2.68) 24.51 (2.78) 31.79 (3.28) 32.47 (3.33) 37.72 (3.28)	22.06 (2.36) 13.69 (1.71) 11.94 (1.84) 11.44 (1.65) 15.62 (1.85) 18.90 (2.46) 18.84 (2.11) <b>24.07</b> (2.46)
MultiRC	LIME Int-Grad Anchors Gradient Search Taylor Search Ordered Search Random Search PLS	-5.20 (1.18) 13.19 (3.14) 5.40 (3.34) -0.09 (1.33) 7.54 (2.53) -6.43 (0.98) -7.42 (1.08) -10.17 (1.43)	-5.90 (1.19) 4.66 (1.71) 3.33 (1.27) -0.73 (1.18) 1.43 (1.47) -5.49 (1.13) -5.97 (1.22) -9.77 (1.49)	39.75 (4.84) 15.53 (3.39) 24.53 (8.77) 20.16 (2.92) 30.76 (4.04) 35.70 (4.40) 35.29 (4.59) 39.95 (5.44)	28.57 (2.18) 11.84 (1.31) 14.55 (1.66) 11.41 (1.13) 20.15 (1.83) 24.38 (2.03) 22.19 (1.81) 26.96 (2.19)

forward passes [49]. Since this is expensive to perform, we limit each method to a fixed number of forward and backward passes (counted together), typically 1000 in total, to obtain a single explanation.

## 6.3 Main Results

In Table 1, we show Suff and Comp scores across methods and datasets, for both the Standard and Counterfactual-Trained (CT) models. 95% confidence intervals are shown in parentheses, obtained by bootstrap with data and model seeds resampled 100k times. Bolded numbers are the best in their group at a statistical significance threshold of p < .05. We give results for SST-2 in the Supplement, including for Exhaustive Search since we use short sequences there, as well as for Vanilla Gradient as it performs much worse than other methods. We summarize our key observations as follows:

1. PLS performs the best out of all of the explanation methods, and it is the only method to consistently outperform Random Search. Improvements in Sufficiency are statistically significant for every dataset using both Standard and CT models, with differences of up to 12.9 points over

LIME and 7.6 points over Random Search. For Comprehensiveness, PLS is the best method in 9 of 10 comparisons, 7 of which are statistically significant, and improvements are as large as 20.8 points over LIME and 17 points over Random Search.

- 2. LIME is the best salience method on both Suff and Comp metrics, but it is still outperformed by Random Search on Sufficiency in 9 of 10 comparisons, by up to 21.5 points. LIME does appear to perform better than Random Search on Comprehensiveness with three of five datasets for Standard models and four of five with CT models, where the largest improvement over Random Search is 7.49 points.
- **3.** Suff and Comp scores are often much worse for CT models than for Standard models. With Random Search, for instance, Comp scores are worse for all datasets (by up to 24.16 points), and Suff scores are worse by 16.92 points for SNLI, though there are not large changes in Suff for other datasets. The differences here show that the OOD nature of counterfactual inputs can heavily influence metric scores, and they lend support to our argument about the OOD problem in Sec. 4. In particular, these metrics are more easily optimized when counterfactuals are OOD because it is easier to identify feature subsets that send the model confidence to 1 or 0.

Given the results above, we recommend that explanations be obtained using PLS for models trained with Counterfactual Training. Though explanation metrics are often worse for CT models, the only reason for choosing between Standard and CT models is that CT models' explanations are socially aligned, while Standard models' explanations are socially misaligned. It would be a mistake to prefer standardly trained models on the grounds that they are "more easily explained" when this difference is due to the way we unintentionally influence model behavior for OOD data points. When using CT models, however, we should be comfortable optimizing for Sufficiency and Comprehensiveness scores, and PLS produces the best explanations under these metrics.

We give additional results for RoBERTa and reduced search budgets in the Supplement.

#### 7 Conclusion

In this paper, we provide a new argument for why it is problematic to use out-of-distribution counterfactual inputs when creating and evaluating feature importance explanations. We present our Counterfactual Training solution to this problem, and we recommend certain Replace functions over others. Lastly, we introduce a Parallel Local Search method (PLS) for finding explanations, which is the only method we evaluate that consistently outperforms random search.

## 8 Broader Impacts and Limitations

There are several positive broader impacts of improved feature importance estimation methods and solutions to the OOD problem. When model developers and end users wish to understand the role of certain features in model decisions, FI estimation methods help provide an answer. Access to FI explanations can allow for (1) developers to check that models are relying on the intended features when making decisions, and not unintended features, (2) developers to discover which features are useful to a model accomplishing a task, and (3) users to confirm that a decision was based on acceptable features or dispute the decision if it was not. Our solution to the OOD problem helps align FI explanations with the kind of information that developers and users expect them to convey, e.g. by limiting the influence of the model prior on the explanations.

Nevertheless, there are still some risks associated with the development of FI explanations, mainly involving potential misuse and over-reliance. FI explanations are *not* summaries of data points or justifications that a given decision was the "right" one. When explanations are good, they reflect what the model has learned, but it need not be the case that what the model has learned is good and worth basing decisions on. It is also important to emphasize that FI explanations are not perfect, as there is always possibly some loss of information by making explanations sparse. Trust in and acceptance of these explanations should be appropriately calibrated to the evidence we have for their faithfulness. Lastly, we note that we cannot guarantee that our Counterfactual Training will eliminate the influence of the random seed and model prior on explanations, meaning that FI explanations for the models we consider will still not be perfectly socially aligned. It will be valuable for future work to further explore how these factors influence the explanations we seek for models.

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## References

- [1] David Alvarez-Melis, Hal Daumé III, Jennifer Wortman Vaughan, and Hanna Wallach. Weight of evidence as a basis for human-oriented explanations. *arXiv* preprint arXiv:1910.13503, 2019. URL https://arxiv.org/pdf/1910.13503.pdf. 24
- [2] Leila Arras, Ahmed Osman, Klaus-Robert Müller, and Wojciech Samek. Evaluating recurrent neural network explanations. In *Proceedings of the 2019 ACL Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP*, pages 113–126, Florence, Italy, August 2019. Association for Computational Linguistics. doi: 10.18653/v1/W19-4813. URL https://www.aclweb.org/anthology/W19-4813. 1, 2, 3
- [3] Seo-Jin Bang, Pengtao Xie, Wei Wu, and Eric P. Xing. Explaining a black-box using deep variational information bottleneck approach. *ArXiv*, abs/1902.06918, 2019. URL https://arxiv.org/abs/1902.06918, 2, 7, 18
- [4] Ricardo Baptista and Matthias Poloczek. Bayesian optimization of combinatorial structures. In *International Conference on Machine Learning*, pages 462–471. PMLR, 2018. URL http://proceedings.mlr.press/v80/baptista18a/baptista18a.pdf. 2, 3, 7, 8, 19
- [5] Jasmijn Bastings, Wilker Aziz, and Ivan Titov. Interpretable neural predictions with differentiable binary variables. In *ACL 2019*, pages 2963–2977, Florence, Italy, July 2019. Association for Computational Linguistics. doi: 10.18653/v1/P19-1284. URL https://www.aclweb.org/anthology/P19-1284. 2, 7, 18
- [6] David Belanger, Bishan Yang, and Andrew McCallum. End-to-end learning for structured prediction energy networks. In Doina Precup and Yee Whye Teh, editors, *Proceedings of the 34th International Conference on Machine Learning, ICML 2017, Sydney, NSW, Australia, 6-11 August 2017*, volume 70 of *Proceedings of Machine Learning Research*, pages 429–439. PMLR, 2017. URL http://proceedings.mlr.press/v70/belanger17a.html. 3, 7
- [7] Samuel R. Bowman, Gabor Angeli, Christopher Potts, and Christopher D. Manning. A large annotated corpus for learning natural language inference. In *EMNLP 2015*, 2015. URL https://arxiv.org/abs/1508.05326. 6, 8
- [8] Chun-Hao Chang, Elliot Creager, Anna Goldenberg, and David Duvenaud. Explaining image classifiers by counterfactual generation. In *ICLR*, 2019. URL https://arxiv.org/pdf/ 1807.08024.pdf. 3, 4, 6
- [9] Hanjie Chen and Yangfeng Ji. Learning variational word masks to improve the interpretability of neural text classifiers. In *EMNLP*, pages 4236–4251, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.347. URL https://www.aclweb.org/anthology/2020.emnlp-main.347. 2, 18
- [10] Marc Claesen and Bart De Moor. Hyperparameter search in machine learning. arXiv preprint arXiv:1502.02127, 2015. URL https://arxiv.org/pdf/1502.02127.pdf. 5
- [11] Christopher Clark, Kenton Lee, Ming-Wei Chang, Tom Kwiatkowski, Michael Collins, and Kristina Toutanova. BoolQ: Exploring the surprising difficulty of natural yes/no questions. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pages 2924–2936, Minneapolis, Minnesota, June 2019. Association for Computational Linguistics. doi: 10.18653/v1/N19-1300. URL https://www.aclweb.org/anthology/N19-1300. 8

- [12] Nicola De Cao, Michael Sejr Schlichtkrull, Wilker Aziz, and Ivan Titov. How do decisions emerge across layers in neural models? interpretation with differentiable masking. In EMNLP, pages 3243–3255, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.262. URL https://www.aclweb.org/anthology/2020.emnlp-main.262. 1, 2, 18, 24
- [13] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. In ACL 2019, 2019. URL https://arxiv.org/pdf/1810.04805.pdf. 6, 8
- [14] Jay DeYoung, Sarthak Jain, Nazneen Fatema Rajani, Eric Lehman, Caiming Xiong, Richard Socher, and Byron C. Wallace. Eraser: A benchmark to evaluate rationalized nlp models. In ACL 2020, volume abs/1911.03429, 2020. URL https://arxiv.org/pdf/1911.03429.pdf. 1, 2, 3, 4, 20
- [15] Jesse Dodge, Gabriel Ilharco, Roy Schwartz, Ali Farhadi, Hannaneh Hajishirzi, and Noah Smith. Fine-Tuning Pretrained Language Models: Weight Initializations, Data Orders, and Early Stopping. arXiv:2002.06305 [cs], February 2020. URL http://arxiv.org/abs/2002.06305. arXiv: 2002.06305. 5
- [16] Qingfeng Du and Jincheng Xu. Model-agnostic local explanations with genetic algorithms for text classification. In *The 33rd International Conference on Software Engineering & Knowledge Engineering*, 2021. URL https://ksiresearch.org/seke/seke21paper/paper040.pdf. 2, 3
- [17] Javid Ebrahimi, Anyi Rao, Daniel Lowd, and Dejing Dou. HotFlip: White-box adversarial examples for text classification. In *ACL*, pages 31–36, Melbourne, Australia, July 2018. Association for Computational Linguistics. doi: 10.18653/v1/P18-2006. URL https://www.aclweb.org/anthology/P18-2006. 3, 7, 8, 18
- [18] Bradley Efron and Robert J Tibshirani. An Introduction to the Bootstrap. CRC press, 1994. 6
- [19] Upol Ehsan, Samir Passi, Q Vera Liao, Larry Chan, I Lee, Michael Muller, Mark O Riedl, et al. The who in explainable ai: How ai background shapes perceptions of ai explanations. *arXiv* preprint arXiv:2107.13509, 2021. URL https://arxiv.org/pdf/2107.13509.pdf. 5
- [20] Ruth C Fong and Andrea Vedaldi. Interpretable explanations of black boxes by meaningful perturbation. In *Proceedings of the IEEE International Conference on Computer Vision*, pages 3429–3437, 2017. URL https://arxiv.org/pdf/1704.03296.pdf. 2, 3, 4, 8
- [21] Peter Hase and Mohit Bansal. Evaluating explainable ai: Which algorithmic explanations help users predict model behavior? In ACL 2020, 2020. URL https://arxiv.org/pdf/2005. 01831.pdf. 1
- [22] Johannes Haug, Stefan Zürn, Peter El-Jiz, and Gjergji Kasneci. On baselines for local feature attributions. In AAAI, 2021. URL https://arxiv.org/pdf/2101.00905.pdf. 3, 4
- [23] Sara Hooker, Dumitru Erhan, Pieter-Jan Kindermans, and Been Kim. A benchmark for interpretability methods in deep neural networks. In *Proceedings of the 33rd International Conference on Neural Information Processing Systems*, 2019. URL https://arxiv.org/abs/1806.10758. 1, 3, 4, 5
- [24] Cheng-Yu Hsieh, Chih-Kuan Yeh, Xuanqing Liu, Pradeep Ravikumar, Seungyeon Kim, Sanjiv Kumar, and Cho-Jui Hsieh. Evaluations and methods for explanation through robustness analysis. arXiv preprint arXiv:2006.00442, 2020. URL https://arxiv.org/pdf/2006.00442.pdf. 3, 4
- [25] Alon Jacovi and Yoav Goldberg. Aligning faithful interpretations with their social attribution. Transactions of the Association for Computational Linguistics, 9:294–310, 2021. URL https://direct.mit.edu/tacl/article/doi/10.1162/tacl\_a\_00367/98620/Aligning. 2, 3, 4

- [26] Sarthak Jain and Byron C Wallace. Attention is not explanation. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pages 3543–3556, 2019. 2
- [27] Eric Jang, Shixiang Gu, and Ben Poole. Categorical reparameterization with gumbel-softmax. In *ICLR*, 2016. URL https://arxiv.org/pdf/1611.01144.pdf. 8, 18
- [28] Dominik Janzing, Lenon Minorics, and Patrick Blöbaum. Feature relevance quantification in explainable ai: A causal problem. In *International Conference on Artificial Intelligence and Statistics*, pages 2907–2916. PMLR, 2020. URL https://arxiv.org/pdf/1910.13413.pdf. 3, 4
- [29] Neil Jethani, Mukund Sudarshan, Yindalon Aphinyanaphongs, and Rajesh Ranganath. Have we learned to explain?: How interpretability methods can learn to encode predictions in their interpretations. In *International Conference on Artificial Intelligence and Statistics*, pages 1459–1467. PMLR, 2021. URL https://arxiv.org/pdf/2103.01890.pdf. 3, 4, 5
- [30] Daniel Khashabi, Snigdha Chaturvedi, Michael Roth, Shyam Upadhyay, and Dan Roth. Looking beyond the surface: A challenge set for reading comprehension over multiple sentences. In *Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long Papers)*, pages 252–262, New Orleans, Louisiana, June 2018. Association for Computational Linguistics. doi: 10.18653/v1/N18-1023. URL https://www.aclweb.org/anthology/N18-1023. 8
- [31] Siwon Kim, Jihun Yi, Eunji Kim, and Sungroh Yoon. Interpretation of NLP models through input marginalization. In *EMNLP*, pages 3154–3167, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.255. URL https://www.aclweb.org/anthology/2020.emnlp-main.255. 2, 3, 4, 6, 16
- [32] Himabindu Lakkaraju, Ece Kamar, Rich Caruana, and Jure Leskovec. Faithful and customizable explanations of black box models. In *Proceedings of the 2019 AAAI/ACM Conference on AI*, *Ethics, and Society*, pages 131–138, 2019. URL https://papers.nips.cc/paper/2017/file/8a20a8621978632d76c43dfd28b67767-Paper.pdf. 2
- [33] Eric Lehman, Jay DeYoung, Regina Barzilay, and Byron C. Wallace. Inferring which medical treatments work from reports of clinical trials. In *Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers)*, pages 3705–3717, Minneapolis, Minnesota, June 2019. Association for Computational Linguistics. doi: 10.18653/v1/N19-1371. URL https://www.aclweb.org/anthology/N19-1371. 8
- [34] Jiwei Li, Xinlei Chen, Eduard Hovy, and Dan Jurafsky. Visualizing and understanding neural models in nlp. arXiv preprint arXiv:1506.01066, 2015. URL https://arxiv.org/pdf/1506.01066.pdf. 7, 8, 17
- [35] Jiwei Li, Will Monroe, and Dan Jurafsky. Understanding neural networks through representation erasure. *arXiv preprint arXiv:1612.08220*, 2016. URL https://arxiv.org/pdf/1612.08220.pdf. 1, 2, 3
- [36] Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. Roberta: A robustly optimized bert pretraining approach. ArXiv, abs/1907.11692, 2019. URL https://arxiv.org/pdf/1907.11692.pdf. 6
- [37] Ilya Loshchilov and Frank Hutter. Decoupled weight decay regularization, 2017. URL https://arxiv.org/pdf/1711.05101.pdf. 19
- [38] Scott M Lundberg and Su-In Lee. A Unified Approach to Interpreting Model Predictions. In I. Guyon, U. V. Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems 30*, pages 4765–4774, 2017. URL http://papers.nips.cc/paper/7062-a-unified-approach-to-interpreting-model-predictions.pdf. 1

- [39] Chris J. Maddison, Andriy Mnih, and Yee Whye Teh. The concrete distribution: A continuous relaxation of discrete random variables. In *ICLR 2017*, 2017. URL https://arxiv.org/abs/1611.00712. 8, 18
- [40] Tim Miller. Explanation in artificial intelligence: Insights from the social sciences. Artif. Intell., 267:1–38, 2019. doi: 10.1016/j.artint.2018.07.007. URL https://doi.org/10.1016/j.artint.2018.07.007. 2
- [41] Takeru Miyato, Shin-ichi Maeda, Masanori Koyama, and Shin Ishii. Virtual adversarial training: a regularization method for supervised and semi-supervised learning. *IEEE transactions on pattern analysis and machine intelligence*, 41(8):1979–1993, 2018. URL https://arxiv.org/pdf/1704.03976.pdf. 25
- [42] Jose G Moreno-Torres, Troy Raeder, Rocío Alaiz-Rodríguez, Nitesh V Chawla, and Francisco Herrera. A unifying view on dataset shift in classification. *Pattern recognition*, 45(1):521–530, 2012. URL https://rtg.cis.upenn.edu/cis700-2019/papers/dataset-shift/dataset-shift-terminology.pdf. 4
- [43] Ramaravind Kommiya Mothilal, Amit Sharma, and Chenhao Tan. Explaining machine learning classifiers through diverse counterfactual explanations. In Mireille Hildebrandt, Carlos Castillo, Elisa Celis, Salvatore Ruggieri, Linnet Taylor, and Gabriela Zanfir-Fortuna, editors, *FAT\* '20: Conference on Fairness, Accountability, and Transparency*, pages 607–617. ACM, 2020. doi: 10.1145/3351095.3372850. URL https://doi.org/10.1145/3351095.3372850. 3, 7
- [44] Dong Nguyen. Comparing automatic and human evaluation of local explanations for text classification. In *NAACL-HLT 2018*, 2018. URL https://www.aclweb.org/anthology/N18-1097.pdf. 1, 2, 3
- [45] Bhargavi Paranjape, Mandar Joshi, John Thickstun, Hannaneh Hajishirzi, and Luke Zettlemoyer. An information bottleneck approach for controlling conciseness in rationale extraction. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing (EMNLP)*, pages 1938–1952, Online, November 2020. Association for Computational Linguistics. doi: 10.18653/v1/2020.emnlp-main.153. URL https://www.aclweb.org/anthology/2020.emnlp-main.153. 2, 7, 18
- [46] Marc Pirlot. General local search methods. *European journal of operational research*, 92(3): 493–511, 1996. 2, 3, 8
- [47] Philipp Probst, Anne-Laure Boulesteix, and Bernd Bischl. Tunability: Importance of hyper-parameters of machine learning algorithms. *J. Mach. Learn. Res.*, 20(53):1–32, 2019. URL https://arxiv.org/pdf/1802.09596.pdf. 5
- [48] Luyu Qiu, Yi Yang, Caleb Chen Cao, Jing Liu, Yueyuan Zheng, Hilary Hei Ting Ngai, Janet Hsiao, and Lei Chen. Resisting out-of-distribution data problem in perturbation of xai. *arXiv* preprint arXiv:2107.14000, 2021. 3, 4
- [49] Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. "Why Should I Trust You?": Explaining the predictions of any classifier. *Proceedings of the 22nd ACM SIGKDD International Conference on Knowledge Discovery and Data Mining*, 2016. URL https://arxiv.org/pdf/1602.04938.pdf. 1, 2, 5, 7, 9
- [50] Marco Tulio Ribeiro, Sameer Singh, and Carlos Guestrin. Anchors: High-precision model-agnostic explanations. In *AAAI Conference on Artificial Intelligence*, 2018. URL https://homes.cs.washington.edu/~marcotcr/aaai18.pdf. 2, 3, 7, 17
- [51] M. Robnik-Sikonja and I. Kononenko. Explaining classifications for individual instances. *IEEE Transactions on Knowledge and Data Engineering*, 20:589-600, 2008. URL http://lkm.fri.uni-lj.si/rmarko/papers/RobnikSikonjaKononenko08-TKDE.pdf. 24
- [52] Soumya Sanyal and Xiang Ren. Discretized integrated gradients for explaining language models. arXiv preprint arXiv:2108.13654, 2021. URL https://arxiv.org/pdf/2108.13654.pdf. 3, 4

- [53] Christian Schäfer. Particle algorithms for optimization on binary spaces. *ACM Transactions on Modeling and Computer Simulation (TOMACS)*, 23(1):1–25, 2013. URL https://arxiv.org/pdf/1111.0574.pdf. 2, 3, 7
- [54] Avanti Shrikumar, Peyton Greenside, and Anshul Kundaje. Learning important features through propagating activation differences. In *International Conference on Machine Learning*, pages 3145–3153, 2017. URL https://arxiv.org/pdf/1704.02685.pdf. 2
- [55] Karen Simonyan, Andrea Vedaldi, and Andrew Zisserman. Deep inside convolutional networks: Visualising image classification models and saliency maps. Workshop at International Conference on Learning Representations., 2013. URL https://arxiv.org/pdf/1312.6034.pdf. 1, 2, 8
- [56] Daniel Smilkov, Nikhil Thorat, Been Kim, Fernanda Viégas, and Martin Wattenberg. Smooth-grad: removing noise by adding noise. *arXiv preprint arXiv:1706.03825*, 2017. URL https://arxiv.org/pdf/1706.03825.pdf. 2
- [57] Richard Socher, Alex Perelygin, Jean Wu, Jason Chuang, Christopher D. Manning, Andrew Ng, and Christopher Potts. Recursive deep models for semantic compositionality over a sentiment treebank. In *Proceedings of the 2013 Conference on Empirical Methods in Natural Language Processing*, pages 1631–1642, Seattle, Washington, USA, October 2013. Association for Computational Linguistics. URL https://www.aclweb.org/anthology/D13-1170. 8
- [58] Richard Socher, Alex Perelygin, Jean Wu, Jason Chuang, Christopher D Manning, Andrew Y Ng, and Christopher Potts. Recursive deep models for semantic compositionality over a sentiment treebank. In *Proceedings of the 2013 conference on empirical methods in natural language processing*, pages 1631–1642, 2013. URL https://www.aclweb.org/anthology/D13-1170.pdf. 6, 20
- [59] Pascal Sturmfels, Scott Lundberg, and Su-In Lee. Visualizing the impact of feature attribution baselines. *Distill*, 5(1):e22, 2020. URL https://distill.pub/2020/attribution-baselines/. 3
- [60] Mukund Sundararajan and Amir Najmi. The many shapley values for model explanation. In *International Conference on Machine Learning*, pages 9269–9278. PMLR, 2020. URL https://arxiv.org/pdf/1908.08474.pdf. 3, 4
- [61] Mukund Sundararajan, Ankur Taly, and Qiqi Yan. Axiomatic attribution for deep networks. In *International Conference on Machine Learning*, pages 3319–3328, 2017. URL https://arxiv.org/pdf/1703.01365.pdf. 1, 2, 3, 4, 5, 7, 8
- [62] James Thorne, Andreas Vlachos, Christos Christodoulopoulos, and Arpit Mittal. FEVER: a large-scale dataset for fact extraction and VERification. In *Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long Papers)*, pages 809–819, New Orleans, Louisiana, June 2018. Association for Computational Linguistics. doi: 10.18653/v1/N18-1074. URL https://www.aclweb.org/anthology/N18-1074. 8
- [63] Keyon Vafa, Yuntian Deng, David M Blei, and Alexander M Rush. Rationales for sequential predictions. In *EMNLP*, 2021. URL https://arxiv.org/pdf/2109.06387.pdf. 3, 4
- [64] Jan N Van Rijn and Frank Hutter. Hyperparameter importance across datasets. In *Proceedings* of the 24th ACM SIGKDD International Conference on Knowledge Discovery & Data Mining, pages 2367–2376, 2018. URL https://arxiv.org/pdf/1710.04725.pdf. 5
- [65] Sarah Wiegreffe and Yuval Pinter. Attention is not not explanation. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pages 11–20, 2019. URL https://arxiv.org/pdf/1908.04626.pdf. 2
- [66] Maksymilian Wojtas and Ke Chen. Feature importance ranking for deep learning. In H. Larochelle, M. Ranzato, R. Hadsell, M. F. Balcan, and H. Lin, editors, *Advances*

- in Neural Information Processing Systems, volume 33, pages 5105-5114. Curran Associates, Inc., 2020. URL https://proceedings.neurips.cc/paper/2020/file/36ac8e558ac7690b6f44e2cb5ef93322-Paper.pdf. 2, 18
- [67] Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, et al. Huggingface's transformers: State-of-the-art natural language processing. *ArXiv*, pages arXiv–1910, 2019. 20
- [68] Thomas Wolf, Lysandre Debut, Victor Sanh, Julien Chaumond, Clement Delangue, Anthony Moi, Pierric Cistac, Tim Rault, Rémi Louf, Morgan Funtowicz, Joe Davison, Sam Shleifer, Patrick von Platen, Clara Ma, Yacine Jernite, Julien Plu, Canwen Xu, Teven Le Scao, Sylvain Gugger, Mariama Drame, Quentin Lhoest, and Alexander M. Rush. Transformers: State-of-the-art natural language processing. In *Proceedings of the 2020 Conference on Empirical Methods in Natural Language Processing: System Demonstrations*, pages 38–45, Online, October 2020. Association for Computational Linguistics. URL https://www.aclweb.org/anthology/2020.emnlp-demos.6. 19
- [69] Jihun Yi, Eunji Kim, Siwon Kim, and Sungroh Yoon. Information-theoretic visual explanation for black-box classifiers. arXiv preprint arXiv:2009.11150, 2020. URL https://arxiv.org/ pdf/2009.11150.pdf. 2, 3, 4, 6, 16, 17
- [70] Fan Yin, Zhouxing Shi, Cho-Jui Hsieh, and Kai-Wei Chang. On the faithfulness measurements for model interpretations, 2021. URL https://arxiv.org/pdf/2104.08782.pdf. 3
- [71] Omar Zaidan, Jason Eisner, and Christine Piatko. Using "Annotator Rationales" to Improve Machine Learning for Text Categorization. In *Human Language Technologies 2007: The Conference of the North American Chapter of the Association for Computational Linguistics; Proceedings of the Main Conference*, pages 260–267, Rochester, New York, April 2007. Association for Computational Linguistics. URL https://www.aclweb.org/anthology/N07-1033. 2, 3, 4
- [72] Ruiqi Zhong, Steven Shao, and Kathleen McKeown. Fine-grained sentiment analysis with faithful attention. arXiv preprint arXiv:1908.06870, 2019. URL https://arxiv.org/pdf/1908.06870.pdf. 2
- [73] Yilun Zhou, Serena Booth, Marco Tulio Ribeiro, and Julie Shah. Do feature attribution methods correctly attribute features? *arXiv preprint arXiv:2104.14403*, 2021. URL https://arxiv.org/pdf/2104.14403.pdf. 1
- [74] Luisa M Zintgraf, Taco S Cohen, Tameem Adel, and Max Welling. Visualizing deep neural network decisions: Prediction difference analysis. In *ICLR*, 2017. URL https://arxiv.org/ pdf/1702.04595.pdf. 2, 3, 6

# A Method Implementation and Hyperparameter Tuning Details

#### A.1 Replace Functions

- 1. **Attention Mask.** To make this a differentiable function, we compute the function by taking the element-wise product between the attention distribution and the binary attention mask, then renormalizing the attention probabilities to sum to 1. The difference between this approach and deleting a token from an input text is that positional embeddings for retained tokens are unchanged.
- 2. **Marginalize.** As in Kim et al. [31], we use a pretrained BERT-Base as our generative model (or a RoBERTa-Base model, when the classifier is a RoBERTa model). The final prediction is obtained from the marginal log probability as  $\arg\max_y \ln\sum_{\tilde{x}\sim p_\phi(\tilde{x}|x,e)} p_\theta(y|\tilde{x})p_\phi(\tilde{x}|x,e)$ , where  $p_\phi(\tilde{x}|x,e)$  is the distribution over imputed tokens. Since computing this marginal distribution is quite expensive, we adopt a Monte Carlo approximation common to past work [31, 69]. Using a subset of SNLI validation data, we tune the number of samples over sizes in {10, 25, 50, 100}, selecting for maximum robustness. Surprisingly, 10 samples performed the best in terms of robustness, though the margin was small over the other values. Consequently, we select a value of 10, which also allows us to evaluate this method at scale due to its relative computational

efficiency. This finding is similar to the results in Yi et al. [69], who ultimately use a value of 8 samples for Monte Carlo estimation of the marginal distribution. This method is still over ten times slower than other Replace functions given the need to perform many MLM forward passes.

- 3. MASK Token. Described in main paper.
- 4. Slice Out. Desribed in main paper.
- 5. **Zero Vector**. Described in main paper.

#### A.2 Explanation Methods

**LIME.** For a data point x, we train a model  $m_{\phi}$  minimizing an MSE weighted by the kernel  $\pi$  and regularized by  $\Omega$ ,

$$\sum_{i=1}^{N} \pi(x, \tilde{x}_i) (m_{\phi}(\tilde{x}_i) - f_{\theta}(\tilde{x}_i)_{\hat{y}})^2 + \Omega(\phi)$$

where  $f_{\theta}(x)_{\hat{y}}$  is the task model's predicted probability, local samples  $\tilde{x}_i$  have attention masks that are imputed with a random number of 0s, and  $\Omega$  is the default auto regularization in the LIME package.

We next specify the form of the weight function  $\pi$ , the regularization method  $\Omega$ , and the distribution of perturbed data points  $p(\tilde{x}|x_i)$ , which are all set to the default LIME package settings. The weight function  $\pi$  is an exponential kernel on the negative cosine similarity between data points multiplied by 100. The perturbation distribution is over binary vectors: in every sample, a uniformly random number of randomly located elements are set to 0, and the remainder are kept as 1. Lastly,  $\Omega$  is to perform forward selection when there are no more than 6 features (i.e. perform greedy local search in the space of possible feature sets, starting with no features and adding one feature at a time). When there are more than six features, ridge regression is used, then the top k features according to the product of their feature weight and the observed feature value (0 or 1 in our case). We use the regression weights as the final salience scores.

**Vanilla Gradient.** We obtain model gradients w.r.t. the model input as salience scores, one early method for explanation [34]. We compute the gradient of the predicted probability w.r.t. input token embeddings, and we obtain a single value per token by summing along the embedding dimension.

**Integrated Gradients.** The salience for an input x with baseline  $\tilde{x}$  is given as

$$(x - \tilde{x}) \times \int_{\alpha=0}^{1} \frac{\partial f(\tilde{x} + \alpha(x - \tilde{x}))}{\partial x} d\alpha.$$

We use the input embeddings of a sequence as x. By the Completeness property of IG, token-level salience scores still sum to the difference in predicted probabilities between the observed input and the baseline.

**Random Search.** Using a subset of SNLI validation points, we tune this method over two possible search spaces: the space of all k-sparse explanations, when the sparsity levels allows up to k tokens to be retained (or no lower than k tokens, for Comprehensiveness), and the space of all allowably sparse explanations. We find it preferable to restrict the search space to exactly k-sparse explanations. We adopt this same search space for all other search methods.

Anchors. We use the anchor-exp package made available by Ribeiro et al. [50] for our experiments, with two modifications. First, we limit the compute budget used in this method to 1000 forward passes (as with all search methods). Second, thoughwe sample locally around inputs using the default argument masking\_str='UNKWORDZ', we use the Attention Mask Replace function for computing the model forward pass, as we do with all search methods. Besides this, we call explain\_instance with default parameters, and we refer the reader to Ribeiro et al. [50] for additional details. Note that we distinguish results on Sufficiency and Comprehensiveness in terms of the maximum number of features selected by the explanation. Additionally, this method has over a 3x slower wall-clock runtime compared to our search methods used with the same compute budget (in terms of model forward passes), and as a result we are constrained to reporting results across a smaller number of model seeds for each dataset (between 3 and 10, rather than always 10).

**Gradient Search.** For an input of length L, this method sequentially updates a continuous state vector  $s \in \mathbb{R}^L$  via gradient descent in order to minimize a regularized cross-entropy loss between the original model prediction  $\hat{y}$  and the predicted probability given the input  $\tilde{x} = \text{Replace}(x, e_t)$ . The explanation  $e_t$  is sampled as follows:  $e^{(d)} \sim \text{Gumbel-Softmax}(s^{(d)})$ , for d = 1 : L. The new state is  $s_{t+1} \leftarrow s_t - \alpha \nabla_s \mathcal{L}(\hat{y}, f(\tilde{x})_{\hat{y}})$ , though note that we use an AdamW optimizer for this step. By virtue of the differentiable Attention Mask Replace function and the Gumbel-Softmax estimator [39, 27], this loss is differentiable w.r.t. s. The regularizer is an  $\ell_2$  penalty on the difference between the expected sparsity  $\sum_{d=1}^L \sigma(s^{(d)})$  and a target sparsity, set to ceiling  $(.05 \cdot L)$ , which is designed to encourage searching through sparse explanations. The final salience scores are given by s, with the probabilistic interpretation that  $\sigma(s_i)$  is the probability that token s is in the optimal explanation.

We observe that this search method is equivalent to fitting a non-parametric model to the dataset with the objective  $\mathcal{L}$  given above. Recently, many parametric models have been proposed for sampling explanations for individual data points [5, 3, 66, 45, 9, 12]. In early experiments, we found that a parametric model performed far worse than this non-parametric approach, and hence we leave out parametric models from further consideration. This is perhaps unsurprising given how hard it may be to learn a map from inputs to good explanations for all data.

Now we give more details to checkpoint selection, weight initialization, regularization, and tuning for Gradient Search. For checkpoint selection: we select the search state that achieves the best Sufficiency (or Comprehensiveness) as measured once every m gradient updates. We do so because checking these metrics consumes some of the available compute budget (see Supplement B.3), and therefore we check the metric value at intervals for purposes of checkpointing. In our experiments, we check the metric every 20 gradient updates and search until the total budget has been consumed. For initialization: a random initial starting point is sampled from a Multivariate Normal distribution centered around 0, with  $\Sigma = I$ . For regularization and other tuning details, we perform sequential line searches over hyperparameters, according to Sufficiency scores on a subset of BoolQ data points. To tune a specific hyperparameter, we set all other hyperparameters to some default values. We refer to the hyperparameters we use after tuning as "final" hyperparameters, which are listed in the table below (note: Number of Samples is the number of sampled explanations per gradient update).

Hyperparameter	Default	Final	Range
Number of Samples	10	1	1, 10, 20, 40
Optimizer	AdamW	AdamW	AdamW, SGD
Scheduler	None	None	None, Linear, Step, Cosine
Learning Rate	0.2	0.1	0.01, 0.05, 0.1, 0.2, 0.4
Sparsity Weight	1e-3	1e-3	1e-1, 5e-2, 1e-2, 5e-3, 1e-3, 5e-4, 0
Target Sparsity	0.1	0.05	0.03, 0.05, 0.1, 0.2, 0.3, 0.4

**Taylor Search.** At time step t, the state is an explanation  $e_t$ , and a heuristic is evaluated on neighboring states in order to select the next state to compute the objective on. The search space is all k-sparse explanations, and therefore neighboring states are those with Hamming distance 2 to the current state (with one retained token being hidden and one hidden token being retained). The heuristic is the projected change in the cross-entropy loss between the model's original prediction  $\hat{y}$  and this label's probability given the input Replace(x,e), for a proposed explanation e, which is computed as such: We first calculate the gradient  $g \in \mathbb{R}^L$  of the cross-entropy loss with respect to the explanation  $e_t$ , which is possible with the differentiable Attention Mask Replace function. Then, when optimizing for Sufficiency, we find the two indices i and j as the solution to  $\arg\max_{i,j} g^{(i)} - g^{(j)}$  such that the sparsity is maintained by flipping both tokens, meaning  $e^{(i)} = 1$  ( $x^{(i)}$  is retained) and  $e^{(j)} = 0$  ( $x^{(j)}$  is hidden). The next state is obtained by setting  $e^{(i)}_t$  and  $e^{(j)}_t$  to these values. This is a first-order approximation to the change in loss between the new and old state, based on the Taylor expansion of the loss [17]. Note when optimizing for Comprehensiveness, we use the  $\max$  min. Following Ebrahimi et al. [17], we ultimately use this search heuristic within a beam search, starting from a random explanation, with width w = 3.

Hyperparameters for Taylor Search are listed below. We performed tuning with Taylor Search for Sufficiency on a subset of BoolQ validation points, and ultimately we selected the largest, best performing pair of values given the available compute budget.

Hyperparameter	Default	Final	Range
Beam Width	2	5	1,2,3,4,5
Number of Steps	50	50	50, 100, 200

**Ordered Search.** More complicated forms for f, such as being quadratic in e, would make finding the optimum of the function computationally intractable, let alone a full rank-ordering of solutions [4].

Using Sufficiency scores on a subset of SNLI validation data, we tune over the ratio between compute budget used in estimating the model  $f_{\theta}$  (i.e. salience scores) and the budget used for the search. Out of 1000 steps, we consider using up to m steps for estimating the salience scores via LIME, where  $m \in \{10, 100, 200, 250, 500, 750\}$ , ultimately using m = 250.

**Parallel Local Search.** Here we specify the Propose function used in Parallel Local Search, and we describe some additional implementation details, some comparisons we performed with Simulated Annealing, and tuning for the number of parallel searches r. The Propose function samples new explanations by starting a random walk from the current explanation that ends when a not-before-seen explanation is encountered. As in Taylor Search, neighboring states have Hamming distance 2. Though we parallelize this search method, we maintain a shared set of previously-seen explanations and compute the Propose function serially at each step so that we never compute the more expensive objective function on the same explanations.

A similar algorithm, Simulated Annealing, uses a probabilistic update condition that favors exploration early on in the search and exploitation later in the search [4]. We find it preferable to use a deterministic update rule, moving to the new state if and only if its objective value is better than the old state. Lastly, following tuning results, we use r=10 parallel runs for all experiments, meaning that each run has a budget b=100 when the overall method budget is 1000 forward passes. The value of r is tuned over the set  $\{1,5,10,25\}$ . We note that using a value greater than 1 significantly improves the wall-clock runtime of this algorithm, as the batched forward passes performed when r searches are done in parallel are much more efficient than performing a greater number of forward passes with only 1 input.

#### **A.3** Model Training Details and Experiment Runtimes

We now give implementation details for training models on our six datasets. The models include BERT-Base or RoBERTa-Base models drawn from the Hugging Face Transformers library [68], trained with AdamW [37] using a learning rate of 1e-5, and in general we select the best model training checkpoint according to the validation set accuracy. When training models for our analysis of counterfactual OOD-ness in Sec. 5, we train Standard models for 20 epochs and Counterfactual-Trained models for 10 epochs, since in the latter case we effectively double the number of inputs per batch. For our explanation evaluation experiments in Sec. 6, we train all models for 10 epochs. Note that in every experiment we train ten models using ten different random seeds.

All experiments are conducted on a NVIDIA RTX 2080 GPU. Wall-clock runtimes for training models are: for Sec. 5 experiments, .6 hours per SNLI model and 1 hour per SST-2 model; for Sec. 6, training one model takes 4.8 hours for FEVER, .7 hours for BoolQ, 1.5 hours for SNLI, 2.9 hours for MultiRC, 1.7 for Evidence Inference, and 3.9 hours for SST-2.

For analysis and explanation evaluation experiments, we report the following runtimes: Sec. 5 experiments take up to 12 hours for robustness analysis for each Replace function (across seeds, models, and datasets), except for Marginalize which takes close to 48 hours. We give max runtimes across datasets for obtaining and evaluating explanations to provide an upper bound on wall-clock runtime given the variable sequence lengths between datasets, meaning we report runtimes for the Evidence Inference dataset. With a compute budget of 1000 forward/backward passes, we find observe that obtaining a set of explanations at one sparsity level using 500 points for one BERT-Base model takes 2.5 hours for LIME, 2.5 minutes for Vanilla Gradient, 11 hours for Integrated Gradients, 10 hours for Gradient Search, 17 hours for Anchors, 5 hours for Taylor Search, 3 hours for Ordered Search, 5 hours for Random Search, and 5 hours for Parallel Local Search.

Table 2: Dataset statistics

Dataset	# Classes	Split	Size	Avg. document length	Avg. query length
SNLI	3	Train Validation Test	5000 9823 9807	24.8 24.4 24.4	- - -
BoolQ	2	Train Validation	9427 3270	121.9 119.8	9.4 9.3
FEVER	2	Train Validation Test	97957 6122 6111	342.3 291.2 278.7	10.4 10.7 10.7
Evidence Inference	3	Train Validation Test	7958 972 959	483.1 484.4 482.0	25.3 23.6 27.0
SST-2 2	2	Train Validation Test	67349 872 1821	11.3 23.2 10.8*	- - -
MultiRC 2	2	Train Validation Test	24029 3214 4848	326.9 326.1 314.8	21.2 20.7 20.8

## **B** Experimental Details

#### **B.1** Data Preprocessing

We use datasets as prepared by the ERASER dataset suite [14], which are publicly available and distributed under the original licenses for each dataset (including Creative Commons and MIT License),<sup>5</sup> as well as SST-2 which is publicly available under a Creative Commons license [58].<sup>6</sup> Note that BoolQ has only one split for evaluation. Additionally, note that for experiments in Sec. 6, we use a subset of 50k points for training models on SNLI, and we use the 500 shortest SST-2 test points according to the number of tokens given by the BERT tokenizer [67] in order to compare with exhaustive search for this dataset.

For preprocessing, input text is split by spaces into a list of words. We tokenize each word independently and concatenate the resulting tokens. Each input consists of a document section and a query section. The document section contains the document while the query section contains the question. The two sections are separated by [SEP]. The entire input is preceded by a [CLS] token and followed by a [SEP] token. For inputs longer than 512 tokens (the maximum input length for our task model Bert), we truncate the input document so that the entire input is shorter or equal to 512 tokens.

#### **B.2** Analysis of Counterfactual Input OOD-ness Details

In this evaluation, the tokens to be hidden from the model are selected uniformly at random without replacement. We sample 10 random masks per data point and take the majority prediction on the corresponding 10 ablated data points as the model's overall prediction. The exception to this procedure is Marginalize, since it is much more computationally expensive than other methods, and therefore we use only one random explanation per input. Note that we use a subset of 10k train points for each task, and we perform this experiment on validation splits because the experiment motivates method design choices in Sec. 6.1.

<sup>&</sup>lt;sup>5</sup>http://www.eraserbenchmark.com/

 $<sup>^6</sup> h ttps://www.kaggle.com/atulanandjha/stanford-sentiment-treebank-v2-sst2$ 

Table 3: Model accuracies

Dataset	Standard Acc.	CT Acc.
SNLI	85.84 (0.69)	85.08 (0.71)
BoolQ	74.16 (1.62)	73.76 (1.62)
FEVER	89.66 (0.76)	89.72 (0.76)
Evidence Inference	58.81 (3.12)	57.35 (3.13)
SST-2	92.89 (1.18)	92.43 (1.21)
MultiRC	68.96 (1.30)	67.76 (1.32)

Table 4: Explanation metrics for SST-2

		Sufficiency ↓		Comprehensiveness ↑		
Dataset	Method	Standard Model	CT Model	Standard Model	CT Model	
	LIME	1.98 (0.84)	5.92 (0.93)	52.42 (2.92)	45.75 (2.49)	
	Anchors	3.44 (0.96)	17.69 (1.64)	30.03 (3.13)	24.19 (2.54)	
	Taylor Search	0.09 (0.50)	5.02 (0.79)	45.65 (3.11)	38.91 (2.70)	
SST-2	Ordered Search	-0.91 (0.47)	2.69 (0.79)	56.24 (2.82)	49.21 (2.48)	
	Random Search	-0.91 (0.48)	2.70 (0.79)	56.11 (2.85)	48.98 (2.49)	
	PLS	-0.91 (0.51)	2.68 (0.85)	56.28 (2.84)	49.25 (2.53)	
	Exhaustive Search	-0.91 (0.51)	2.68 (0.85)	56.29 (2.84)	49.26 (2.53)	

## **B.3** Compute Budget Details

In this section we describe how the compute budget is spent by each explanation method. Note that we consider both creating and evaluating explanations to draw from the available compute budget, because some methods compute the Suff and Comp metrics while obtaining an explanation, whereas others leave these metrics to be checked after an explanation is settled on. We describe the standard case in this paper of 1000 forward and backward passes per final metric value.

- 1. LIME uses 996 forward passes to obtain an explanation, then 4 forward passes to obtain a final metric value (one per sparsity level).
- 2. Vanilla Gradient uses only a single forward and backward passes. This is our only method that uses a fixed compute budget.
- 3. Integrated Gradients uses 498 forward and backward passes and 4 forward passes to obtain the final metric value.
- 4. Taylor Search uses no more than 1000 forward passes, given the beam width and number of steps described in Supplement A.
- 5. The remaining search methods (including Ordered Search, Random Search, Parallel Local Search) all use 1000 forward passes in total, since these methods involve exactly computing the objective value at each step, so the metrics do not need to be recomputed after explanations are obtained.

# C Additional Results

**SST-2 Results.** Here we discuss results for SST-2, which are shown in Table 4. Our primary observation here is that most of the search methods we consider perform as well as Exhaustive Search (for sequences short enough to exhaustively search). The closest to Exhaustive Search is Parallel Local Search, which exactly identifies the optimal explanation for the Sufficiency metric and comes within .01 of the optimal Comprehensiveness value. Meanwhile, the best salience method (LIME) underperforms these search methods by between 2.86 and 3.86 points, showing that salience methods fall well behind search methods in this scenario.

Search Method Performance Over Time. In Figure 3, we show search performance across time steps for the three best performing search methods, Random, Ordered, and Parallel Local. Note that Ordered Search begins at step 251 since the first 250 forward passes are allocated to computing LIME, and Parallel Local Search begins at step 10 since we use 10 parallel runs. We see that Parallel Local outperforms Random early on and then continues to remain the preferable method, as differences at step 1000 are statistically significant at p < .05. In fact, for FEVER, where the search space is larger,

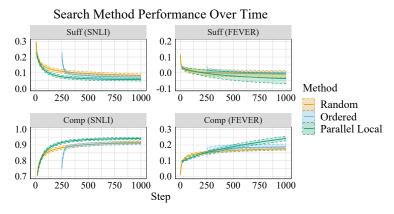


Figure 3: Search method performance over time on FEVER and SNLI with Counterfactual-Trained models, for searches that ran for 1000 forward passes. Shaded areas represent 95% confidence intervals accounting for seed variance using 10 random seeds.

Parallel Local will clearly continue to improve with additional compute, while Random and Ordered plateau in performance by 1000 steps.

Each of these search methods tends to achieve good performance even by 250 steps. We report results using this **reduced search budget** across datasets in Table 5 in the Supplement. We find that search methods outperform salience methods in 15 of 24 comparisons (with 8 favoring LIME), suggesting that search methods can outperform salience methods even with a far smaller compute budget. This is relevant if, for instance, one needs to obtain explanations at multiple sparsity levels with a single compute budget for all of the explanations, which could be useful for applications requiring all explanations to be visualized at once (or visualized on demand with no latency).

**Counterfactual-Trained Model Accuracy.** In Table 3, we show model accuracies on test sets for standardly trained models (Standard) and Counterfactual-Trained (CT) models, with 95% confidence intervals reflecting sample variance in parentheses. These accuracies are from the single best performing seed for each dataset, according to dev set accuracies, out of 10 trained models. Note that for SST-2, we report dev set numbers as test labels are unavailable.

We observe that differences in accuracies are typically less than 1 point between the two training algorithms. On average across the datasets, the difference is about 0.7 points. This is a small but consistent gap, and hence it will be valuable for future work to study the causes of this gap and identify ways to align the train and explanation-time distributions without losing any model accuracy on test data.

**Results with Reduced Search Budget.** In Table 5, we give results for a reduced search budget of 1000 forward passes across sparsity levels, i.e. 250 per sparsity level. This setup favors salience-based methods which can easily give explanations at varying sparsity levels. With too many sparsity levels, this evaluation is heavily biased toward salience-based methods, since it spreads the compute for search methods across sparsity levels. We use a constant budget per sparsity for results in the main paper because we view the use of multiple sparsity levels as an attempt to average results across possible desired settings, and explanations at multiple sparsities may not always be needed. But ultimately, user preferences will dictate whether explanations at multiple levels of sparsity are desired. This discussion aside, the results are as follows: compared to the best salience-based method, LIME, search methods are preferable in 15 of 24 comparisons, while LIME is preferable in 8 of 24 comparisons (at statistical significance of p < .05). Comparing within search methods, PLS is preferable to Random Search 7 times and Random Search is preferable one time (at p < .05). We observe that LIME performs best on Comprehensiveness, and therefore we suggest that LIME may be the best method when explanations are desired at many sparsity levels, the compute budget is heavily limited, and one is optimizing for Comprehensiveness. Otherwise, PLS remains the preferable method.

Table 5: Explanations metrics with a reduced search budget

		Sufficie	Sufficiency ↓		iveness ↑
Dataset	Method	Standard Model	CT Model	Standard Model	CT Model
	Vanilla Grad	59.41 (2.42)	63.41 (0.81)	7.08 (1.63)	5.84 (1.06)
SNLI	LIME (1000)	20.00 (2.02)	27.09 (1.68)	82.17 (2.82)	75.34 (1.94)
SNLI	Ordered Search (250)	-1.19 (0.87)	16.23 (1.45)	87.01 (2.40)	83.31 (1.73)
	Random Search (250)	-1.34 (0.90)	16.82 (1.46)	86.10 (2.52)	82.45 (1.82)
	PL Search (250)	<b>-1.50</b> (0.96)	<b>15.30</b> (1.37)	<b>87.25</b> (2.42)	<b>84.57</b> (1.68)
	Vanilla Grad	30.81 (3.44)	16.40 (2.13)	2.43 (0.70)	2.25 (0.73)
BoolQ	LIME (1000)	2.14 (1.75)	-1.56 (0.64)	52.03 (3.67)	<b>36.26</b> (3.44)
DoolQ	Ordered Search (250)	1.44 (1.29)	-1.71 (0.70)	43.33 (3.18)	27.78 (3.00)
	Random Search (250)	0.09 (0.82)	-1.84 (0.66)	49.46 (3.55)	27.58 (2.74)
	PL Search (250)	<b>-0.56</b> (0.57)	<b>-2.61</b> (0.68)	<b>54.85</b> (3.78)	31.98 (2.97)
	Vanilla Grad	20.76 (4.14)	12.96 (2.13)	2.92 (1.31)	1.57 (0.56)
Evidence	LIME (1000)	-16.07 (2.84)	-14.93 (1.38)	<b>47.61</b> (5.66)	<b>33.97</b> (4.19)
Inference	Ordered Search (250)	-14.47 (2.65)	-11.67 (1.34)	39.69 (4.83)	26.51 (3.15)
	Random Search (250)	-15.28 (2.67)	-10.86 (1.28)	38.79 (5.46)	23.65 (2.80)
	PL Search (250)	-16.18 (3.14)	-13.78 (2.53)	41.90 (8.96)	25.27 (2.78)
	Vanilla Grad	19.63 (2.39)	13.21 (1.81)	1.52 (0.60)	1.02 (0.41)
FEVER	LIME (1000)	-0.24 (0.50)	1.36 (2.13)	<b>33.86</b> (3.44)	<b>22.06</b> (4.10)
ILVLK	Ordered Search (250)	-0.73 (0.40)	1.00 (0.90)	28.70 (3.18)	16.30 (2.26)
	Random Search (250)	-1.16 (0.50)	-0.30 (2.07)	29.13 (3.18)	16.58 (1.91)
	PL Search (250)	-1.06 (0.44)	-0.36 (2.04)	25.81 (2.87)	15.22 (1.84)
	Vanilla Grad	21.16 (3.47)	11.80 (1.38)	3.75 (1.18)	1.74 (0.79)
MultiRC	LIME (1000)	-5.20 (1.19)	<b>-5.91</b> (1.19)	<b>39.75</b> (4.80)	<b>28.57</b> (2.18)
Withit	Ordered Search (250)	-5.02 (1.03)	-4.16 (1.10)	33.26 (4.25)	21.95 (1.92)
	Random Search (250)	<b>-6.08</b> (1.17)	-4.86 (1.20)	32.31 (4.30)	19.95 (1.67)
	PL Search (250)	-5.20 (1.30)	-4.91 (1.27)	28.38 (3.85)	17.46 (1.49)
	Vanilla Grad	47.26 (3.79)	46.83 (1.41)	2.56 (0.71)	3.01 (1.00)
SST-2	LIME (1000)	1.97 (0.84)	5.92 (0.93)	52.42 (2.93)	45.74 (2.52)
551-2	Ordered Search (250)	-0.91 (0.47)	2.71 (0.79)	55.90 (2.84)	48.96 (2.50)
	Random Search (250)	-0.91 (0.46)	2.73 (0.75)	55.44 (2.52)	48.31 (2.18)
	PL Search (250)	-0.91 (0.47)	2.69 (0.79)	56.14 (2.84)	49.08 (2.50)

Table 6: Explanation metrics for RoBERTa-Base models

Dataset	Method	Sufficiency $\downarrow$	Comprehensiveness †
SNLI	LIME	24.42 (1.65)	71.30 (2.63)
	Random Search	11.52 (1.46)	81.43 (2.59)
	PLS	<b>9.73</b> (1.41)	<b>83.44</b> (2.31)
FEVER	LIME	1.22 (0.81)	25.09 (2.56)
	Random Search	1.10 (0.78)	22.46 (2.50)
	PLS	<b>-0.40</b> (0.63)	<b>27.61</b> (2.68)

**Results with RoBERTa Models.** Shown in Table 6, we give a comparison between LIME, Random Search, and PLS using RoBERTa-Base as our task model, as opposed to the BERT-Base setting in the main paper experiments. Results are given for a subset of datasets, with the same compute budget as in the main paper, using 10 Counterfactual-Trained RoBERTa-Base models on each dataset. We observe similar trends and improvements using PLS as with BERT-Base. PLS is the best method in each condition and consistently outperforms Random Search, unlike LIME.

Weight of Evidence Metrics. Note that we can also measure the Sufficiency and Comprehensiveness metrics in terms of a difference in log-odds (i.e. weight of evidence) rather than probabilities, which reflects differences in evidence for classes before this evidence is compressed to the bounded

Table 7: Explanation metrics with weight of evidence

		Sufficiency ↓		Comprehensiveness ↑	
Dataset	Method	Diff. in Probs	WoE	Diff. in Probs	WoE
Evidence Inference	LIME Random Search PLS	-14.93 (1.38) -12.71 (1.29) <b>-20.33</b> (2.46)	-0.98 (0.14) -0.81 (0.13) <b>-1.44</b> (0.14)	33.97 (4.17) 26.50 (3.15) 38.71 (3.52)	1.76 (0.29) 1.35 (0.21) <b>2.09</b> (0.25)
MultiRC	LIME Random Search PLS	-5.90 (1.19) -6.58 (1.20) <b>-9.77</b> (1.45)	-0.33 (0.09) -0.39 (0.09) <b>-0.63</b> (0.13)	<b>28.57</b> (2.18) 22.79 (1.78) 26.96 (2.05)	<b>1.54</b> (0.17) 1.24 (0.13) 1.45 (0.16)

probability scale [51, 1]. In this case, Sufficiency e.g. is computed as

$$Suff_{WoE}(f_{\theta}, x, e) = \ln \frac{f_{\theta}(x)_{\hat{y}}}{f_{\theta}(x)_{\neg \hat{y}}} - \ln \frac{f_{\theta}(\text{Replace}(x, e))_{\hat{y}}}{f_{\theta}(\text{Replace}(x, e))_{\neg \hat{y}}}$$
(2)

where  $f_{\theta}(x)_{\neg \hat{y}}$  is the sum of all class probabilities except the predicted class, meaning each term is the log-odds in favor of  $\hat{y}$ . In Sec. 6 we describe results for the standard difference-in-probabilities version of each metric as well as the weight-of-evidence versions.

In Table 7, we compare the default difference-in-probability version of our metric (reported in the main paper) with the weight-of-evidence version, which is used by [51, 1]. We do not observe any notable differences in the trends between the metrics. We report one case where a hypothesis test is statistically significant with WoE but not the difference in probabilities; however, the difference between p-values is negligible (p = .052 vs. p = .030).

#### **D** Discussion

**Should We Prefer Counterfactual-Trained Models If They Are Harder to Explain?** This question is raised by the fact that Suff and Comp scores are often worse for CT models (see Sec. 6). We suggest that the only reason for choosing between Standard and CT models is that CT models' explanations are not influenced by the model prior and random seed to the extent that Standard models' explanations are, as we argued in Sec. 4. If one prefers explanations (and explanation metrics) to reflect what a model *has learned from the data*, rather than the model prior and random seed, one would prefer to use CT models. It would be a mistake to prefer the standardly trained models on the grounds that they are "more easily explained" when this difference is due to the way we unintentionally influence model behavior for out-of-distribution data points.

In Defense of Searching For Explanations. De Cao et al. [12] argue against using a certain kind of search to find feature importance explanations on the grounds that it leads to "over-aggressive pruning" of features that a model does in fact rely on for its output. In their case, the objective of the search method is to find "a subset of features (e.g. input tokens) ... [that] can be removed without affecting the model prediction." They suggest that this method is susceptible to *hindsight bias*, asserting that "the fact that a feature can be dropped does not mean that the model 'knows' that it can be dropped and that the feature is not used by the model when processing the example." They provide the example of a model that (successfully) counts whether there are more 8s than 1s in a sequence, where they take issue with the fact that the search method would return a single 8 as its explanation for any sequence with more 8s than 1s, since this preserves the model prediction of "more 8s than 1s." The problem with this explanation, it is said, is that it removes digits that are most certainly being counted by the model when it comes to its decision. They provide empirical evidence that a learned model does in fact count all 8s and 1s before deciding which are more numerous.

One response to this argument is that if one obtains the optimal solution to an optimization problem and is not satisfied with it, then the objective must not be capturing everything that we care about, and the issue is not with the optimization method (i.e. search) that is employed. In the case at hand, we should first note that the objective is actually under-specified. De Cao et al. [12] suppose the search method returns the *maximal set* of tokens that can be removed while maintaining the model prediction, but the objective is not given with any preference for explanation *sparsity* (only that the removed tokens are a "subset" of the input). However, De Cao et al. [12] would take issue with

search-based explanations regardless of whether the search method returns the minimal or maximal subset of tokens that can be removed without changing the model prediction. This is because they want the explanation to identify tokens that are "used by the model when processing the example." This criterion is not formalized, but the problem must be that it is a different criterion than the search objective, which is to find a feature subset that preserves the model prediction. After formalizing the notion of a feature being "used by a model," one should then be able to search for good explanations under the corresponding objective.

**Explanation Distribution at Train Time.** We reiterate that, to exactly match train and test-time distributions, models would be trained on counterfactual inputs drawn from explanation methods themselves, rather than simply random explanations. For now, this remains prohibitively expensive, as it would increase the number of forward passes required during training by up to 1000x depending on the budget to be used when explaining predictions. We explored methods based on training on the true counterfactual distribution (i.e., based on real explanations) to a limited extent, such as using real explanations only in the last training epoch. However, this alerted us to a few obstacles in such approaches: (1) this training distribution is non-stationary, as the FI explanations will change potentially with each gradient update, (2) these experiments were still quite expensive and required selecting a specific model checkpoint as the final model, which might not perform as well on accuracy metrics, and (3) we found that the Suff and Comp metrics were sometimes similar to Standard models, suggesting that these models were ultimately not as robust to the counterfactuals as the CT models were (see Conclusion 3 in Sec. 6.3). Future work in reducing the costs of obtaining explanations will help set the stage for more closely aligning the train and test time explanation distributions. In this regard, there may be applicable insights to draw from work on efficiently improving model robustness to local perturbations, such as Miyato et al. [41].

Another question that arises during training is whether applying the Replace function to  $x_i$  implies that the label  $y_i$  should change. It may *seem* problematic, for example, to fit a model to (Replace(x,e), y) pairs if removing even a small number of tokens in x tends to flip the label. However, we note that what the model sees is an input with, e.g., MASK tokens in place of some tokens, and what an optimal model will do in this situation is make a prediction based on what evidence is available to it, with the knowledge that some features that could have influenced the label have been removed from the input. That is, based on the overall data distribution, such a model should produce appropriately calibrated outputs for inputs where most of the visible evidence suggests the labels to be  $y_1$ , while if the removed evidence had been visible, the label could be seen to be  $y_2$ .

Measuring Compute Budget. While we use the number of forward and backward passes as our compute budget for each method, wall-clock time will continue to be a useful and practical measure of compute for comparing methods. We note that batching forward passes on a GPU will significantly speed up method runtimes for a single data point while keeping the number of forward passes constant. In our experiments, this means that PLS is very efficient compared to Gradient Search, which does not batch inputs in the forward or backward pass. We use forward and backward passes as the unit of our compute budget since this is the fundamentally rate-limiting step in obtaining explanations, but practitioners will do well to compare methods with respect to wall-clock time as well.