

# Rationales for Sequential Predictions

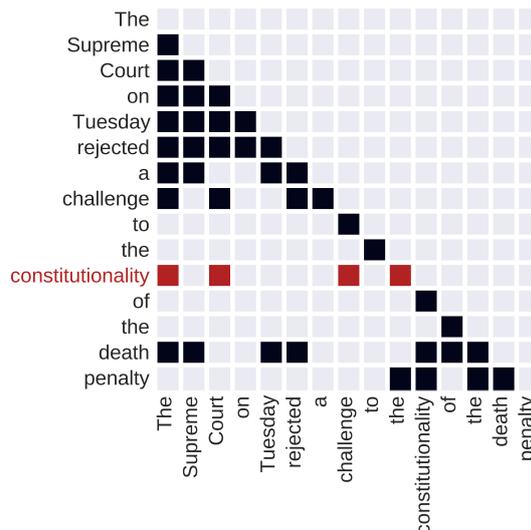
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## Abstract

Sequence models are a critical component of modern NLP systems, but their predictions are difficult to explain. We consider model explanations through *rationales*, subsets of context that can explain individual model predictions. We find sequential rationales by solving a combinatorial optimization: the best rationale is the smallest subset of input tokens that would predict the same output as the full sequence. Enumerating all subsets is intractable, so we propose an efficient greedy algorithm to approximate this objective. The algorithm, which is called greedy rationalization, applies to any model. For this approach to be effective, the model should form compatible conditional distributions when making predictions on incomplete subsets of the context. This condition can be enforced with a short fine-tuning step. We study greedy rationalization on language modeling and machine translation. Compared to existing baselines, greedy rationalization is best at optimizing the sequential objective and provides the most faithful rationales. On a new dataset of annotated sequential rationales, greedy rationales are most similar to human rationales.

## 1 Introduction

Sequence models are a critical component of tasks ranging from language modeling (Radford et al., 2019) to machine translation (Brown et al., 1993; Vaswani et al., 2017) to summarization (Rush et al., 2015). These tasks are dominated by complex neural networks. While these models produce accurate predictions, their decision making processes are hard to explain. Interpreting a model’s prediction is important in a variety of settings: a researcher needs to understand a model to debug it; a doctor using a diagnostic model requires justifications to validate a decision; a company deploying a language model relies on model explanations to detect biases appropriated from training data.



**Figure 1.** Rationales for sequential prediction on GPT-2. Each row is a predicted word. The darkened cells correspond to the context words found by greedy rationalization. To predict “constitutionality”, the model only needs “The”, “Court”, “challenge”, and “the”.

Interpretation takes many flavors (Lipton, 2018). We focus on *rationales*, i.e. identifying the most important subset of input tokens that leads to the model’s prediction. For example, consider the sentence: “The Supreme Court on Tuesday rejected a challenge to the constitutionality of the death penalty.” Suppose we would like to explain the decision of the model to generate “constitutionality.” While the model mathematically conditions on all the previous words, only some are critical to its predictions. In this case, the rationale produced by our algorithm includes “the”, “challenge”, and notably “Court”, but not phrases that add no information like “on Tuesday” (Figure 1).

Various rationale methods have been proposed for sequence classification, where each sequence has a single rationale (Lei et al., 2016; Chen et al., 2018; Jain et al., 2020). However, these methods cannot scale to sequence models, where each token in a sequence requires a different rationale.

This work frames the problem of finding sequence rationales as a combinatorial optimization: given a model, the best rationale is the smallest subset of input tokens that would predict the same token as the full sequence. Finding the global optimum in this setting is intractable, so we propose **greedy rationalization**, a greedy algorithm that iteratively builds longer rationales. This approach is efficient for many NLP models such as transformers. Moreover, it does not require access to the inner workings of a model, such as gradients.

Underlying this approach is an assumption that the model forms sensible predictions for incomplete subsets of the input. Although we can pass in incomplete subsets to neural models, there is no guarantee that their predictions on these subsets will be compatible with their predictions on full contexts (Arnold and Press, 1989). We show that compatibility can be learned by conditioning on randomly sampled context subsets while training a model. For large pretrained models like GPT-2 (Radford et al., 2019), fine-tuning is sufficient.

In an empirical study, we compare greedy rationalization to various gradient- and attention-based explanation methods on language modeling and machine translation. Greedy rationalization best optimizes the objective, and its rationales are most faithful to the inner workings of the model. We additionally create a new dataset of annotated rationales based on the Lambada corpus (Paperno et al., 2016). We find that greedy rationales are most similar to human annotations, both on our dataset and on a labeled dataset of translation alignments.

## 2 Sequential Rationales

Consider a sequence of tokens,  $y_{1:T}$ , generated by some unknown process  $y_{1:T} \sim F$ . The goal of sequence modeling is to learn a probabilistic model  $p_\theta$  that approximates  $F$  from samples. Maximum-likelihood estimation is an effective way to train these models, where  $\theta$  is fit according to

$$\arg \max_{\theta} \mathbb{E}_{y_{1:T} \sim F} [\log p_\theta(y_{1:T})]. \quad (1)$$

Sequence models are typically factored into conditional distributions:

$$p_\theta(y_{1:T}) = f_\theta(y_1) \prod_{t=2}^T f_\theta(y_t | y_{<t}). \quad (2)$$

Here,  $f_\theta$  is the specific model parameterizing  $p_\theta$ , such as a transformer (Vaswani et al., 2017), and is

trained to take inputs  $y_{<t}$ . Going forward, we drop the dependence on  $\theta$  in the notation.

Word-level explanations are a natural way to interpret a sequence model: which words were instrumental for predicting a particular word? Would the same word have been predicted if some of the words had been missing?

Explanations may be straightforward for simpler models; for example, a bigram Markov model uses only the previously generated word to form predictions. However, the most effective sequence models have been based on neural networks, whose predictions are challenging to interpret (Lipton, 2018).

Motivated by this goal, we consider a sequence  $y_{1:T}$  generated by a sequence model  $p$ . At each position  $t$ , the model takes the inputs in the context  $y_{<t}$  and uses them to predict  $y_t$ . We are interested in forming *rationales*: subsets of the contexts that can explain the model’s prediction of  $y_t$ .<sup>1</sup>

What are the properties of a good rationale? Any of the contextual words  $y_{<t}$  can contribute to  $y_t$ . However, if a model makes the same prediction with only a subset of the context, that subset contains explanatory power on its own. A rationale is *sufficient* if the model would produce the same  $y_t$  having seen only the rationale (DeYoung et al., 2020). While rationales consisting of the full context would always be sufficient, they would be ineffective for explaining longer sequences. Intuitively, the smaller the rationale, the easier it is to interpret, so we also prioritize *brevity*.

We combine these desiderata and frame finding rationales as a combinatorial optimization: the best rationale of a word  $y_t$  is the smallest subset of inputs that would lead to the same prediction. Each candidate rationale  $S$  is an index set, and  $y_S$  denotes the subset of tokens indexed by  $S$ .<sup>2</sup> Denote by  $\mathcal{S} = 2^{[t-1]}$  the set of all possible context subsets. An optimal rationale is given by

$$\arg \min_{S \in \mathcal{S}} |S| \quad \text{s.t.} \quad \arg \max_{y'_t} p(y'_t | y_S) = y_t. \quad (3)$$

The constraint guarantees sufficiency, and the objective targets brevity. Although the objective may have multiple solutions, we only require one.

Optimizing Eq. 3 is hindered by a pair of computational challenges. The first challenge is that

<sup>1</sup>Our paradigm and method extend easily to conditional sequence models, such as those used for machine translation. For full details, refer to Appendix A.

<sup>2</sup>A sequence of tokens can be represented as a set of tuples: “The dog walks” becomes  $\{(1 : \text{The}), (2 : \text{dog}), (3 : \text{walks})\}$ .

solving this combinatorial objective is intractable; framed as a decision problem, it is NP-hard. We discuss this challenge in Section 3. The second challenge is that evaluating distributions conditioned on incomplete context subsets  $p(y'_t|y_S)$  involves an intractable marginalization over missing tokens. For now we assume that  $f(y'_t|y_S) \approx p(y'_t|y_S)$ ; we discuss how to enforce this condition in Section 4.

### 3 Greedy Rationalization

We propose a simple greedy algorithm, **greedy rationalization**, to approximate the solution to Eq. 3. The algorithm starts with an empty rationale. At each step, it considers adding each possible token, and it selects the one that most increases the probability of  $y_t$ . This process is repeated until the rationale is sufficient for predicting  $y_t$ .<sup>3</sup> Figure 2 provides an overview.

Here is the algorithm. Begin with a rationale  $S^{(0)} = \emptyset$ . Denoting by  $[t-1] = \{1, \dots, t-1\}$ , the first rationale set is

$$S^{(1)} = \arg \max_{k \in [t-1]} p(y_t|y_k). \quad (4)$$

At each step, we iteratively add a single word to the rationale, choosing the one that maximizes the probability of the word  $y_t$ :

$$S^{(n+1)} = S^{(n)} \cup \arg \max_{k \in [t-1] \setminus S^{(n)}} p(y_t|y_{S^{(n)} \cup k}). \quad (5)$$

We continue iterating Eq. 5 until  $\arg \max_{y'_t} p(y'_t|y_{S^{(n)}}) = y_t$ . The procedure will always converge, since in the worst case,  $S^{(t-1)}$  contains the full context.

This procedure is simple to implement, and it is black-box: it does not require access to the inner workings of a model, like gradients or attention.

While greedy rationalization can be applied to any model, greedy rationalization is particularly effective for set-based models such as transformers. If we assume the rationale size  $m = |S|$  is significantly shorter than the size of the context  $t$ , greedy rationalization requires no extra asymptotic complexity beyond the cost of a single evaluation.

For transformers, the complexity of each evaluation  $f(y_t|y_{<t})$  is quadratic in the input set  $O(t^2)$ . Each step of greedy rationalization requires evaluating  $f(y_t|y_S)$ , but  $y_S$  can be significantly smaller

<sup>3</sup>The greedy approach is motivated by approximations to the set cover problem (Chvatal, 1979). Each set is a single context token, and a rationale is “covered” if it results in generating the true token.

than  $y_{<t}$ . A rationale of size  $m$  will require  $m$  steps to terminate, resulting in a total complexity of  $O(m^3t)$ . As long as  $m = O(t^{1/3})$ , greedy rationalization can be performed with the same asymptotic complexity as evaluating a transformer on the full input,  $O(t^2)$ . In Appendix C, we empirically verify the efficiency of greedy rationalization.

## 4 Model Compatibility

Greedy rationalization requires computing conditional distributions  $p(y_t|y_S)$  for arbitrary subsets  $S$ . Using an autoregressive model, this calculation requires marginalizing over unseen positions. For example, rationalizing a sequence  $y_{1:3}$  requires evaluating the candidate rationale  $p(y_3|y_1)$ , which marginalizes over the model’s predictions:

$$p(y_3|y_1) = \sum_k f(y_3|y_1, y_2 = k)f(y_2 = k|y_1).$$

Given the capacity of modern neural networks, it is tempting to pass in incomplete subsets  $y_S$  to  $f$  and evaluate this instead as  $f(y_t|y_S) \approx p(y_t|y_S)$ . However, since  $f$  is trained only on complete feature subsets  $y_{<t}$ , incomplete feature subsets  $y_S$  are out-of-distribution (Hooker et al., 2019). Evaluating  $f(y_3|y_1)$  may be far from the true conditional  $p(y_3|y_1)$ . In Figure 4, we show that indeed language models like GPT-2 produce poor predictions on incomplete subsets.

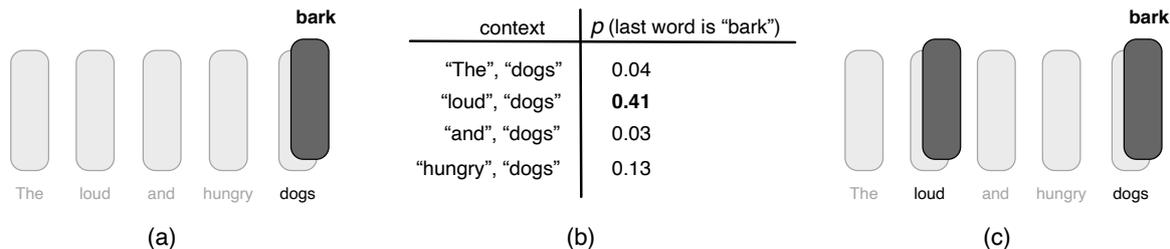
### 4.1 Fine-tuning for Compatibility

Ideally  $f(y_t|y_S)$  approximates  $p(y_t|y_S)$ , a property known as *compatibility* (Arnold and Press, 1989). Since training with Eq. 1 only evaluates  $f$  on complete contexts  $y_{<t}$ , its behavior on incomplete contexts  $y_S$  is unspecified. Instead, compatibility can be obtained by training to maximize

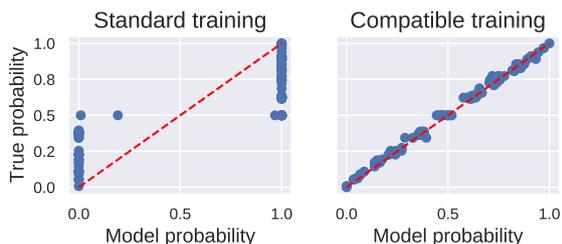
$$\mathbb{E}_{y_{1:T} \sim F} \mathbb{E}_{S \sim \text{Unif}(S)} \left[ \sum_{t=1}^T \log f(y_t|y_{S_{<t}}) \right], \quad (6)$$

where  $S \sim \text{Unif}(S)$  indicates sampling word subsets uniformly at random from the power set of all possible word subsets, and  $S_{<t}$  denotes the indices in  $S$  that are less than  $t$ . We approximate Eq. 6 with word dropout.<sup>4</sup> Jethani et al. (2021) show that the optimum of Eq. 6 is the distribution whose conditional distributions are all equal to the ground-truth conditionals.

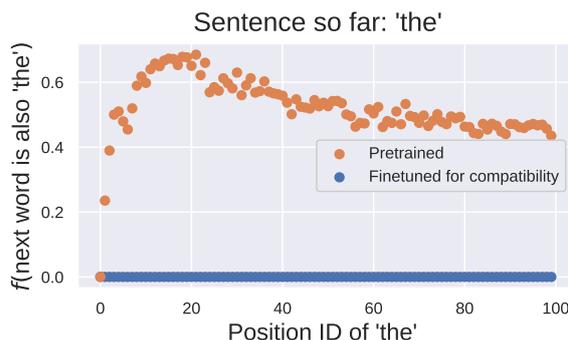
<sup>4</sup>In practice, we combine this objective with standard MLE training to learn compatible distributions while maintaining the performance of the original model. We also skew the word dropout distribution towards sparser rationales since we expect shorter rationales to be more common; see Appendix D.



**Figure 2.** One step of greedy rationalization. In (a), the rationale so far is a single word, “dogs.” In (b), each candidate token is considered and “loud” results in the best probability for “bark.” In (c), the token “loud” is added to the rationale. This process repeats until the most likely word is the model prediction.



**Figure 3.** Training with word dropout (right) results in compatible predictions for the majority-class synthetic language. The optimal compatibility is the dashed line.



**Figure 4.** Fine-tuning GPT-2 for compatibility removes pathological repeating on incomplete contexts. For a position  $t$ , the vertical axis gives  $f(y_{t+1} = \text{“the”} | y_t = \text{“the”})$ .

The intuition for Eq. 6 is straightforward: if the model sees incomplete contexts while training, it can approximate arbitrary incomplete distributions. Since  $f(y_t|y_S)$  approximates  $F(y_t|y_S)$  and  $f(y_t|y_{<t})$  approximates  $F(y_t|y_{<t})$ , all the conditional distributions are compatible.

## 4.2 Compatibility Experiments

To demonstrate the impact of training with the compatibility objective in Eq. 6, we consider a synthetic majority-class language over binary strings of 19 tokens. The first 17 are sampled uniformly from  $\{0, 1\}$ , and the 18th token is always ‘=’. The 19th token is 0 if there are more 0’s than 1’s in the first 17 tokens, and 1 otherwise.

We train two models: one using the standard objective in Eq. 1, the other using word dropout to optimize Eq. 6. Although both models have the same heldout perplexity on the full context, training with Eq. 6 is required to form compatible predictions on incomplete subsets. In Figure 3, we provide different models  $f$  with random subsets  $S$  and calculate the model’s probability that the last token is 1. A model that has only seen a few tokens should be less confident about the prediction of the final majority class, yet models trained without word dropout ignore this uncertainty.

Models do not need to be trained from scratch

with Eq. 6. A model can be pre-trained with Eq. 1, after which it can be fine-tuned for compatibility. As an example, when GPT-2 is not trained with word dropout, it makes insensible predictions for out-of-distribution sequences. For a sequence that contains only the token “the,” GPT-2 is trained to give reasonable predictions for  $p(y_2|y_1 = \text{“the”})$ . But when it has only seen the token “the” somewhere besides the first position of the sequence, the top prediction for the word after “the” is also “the”. Of course, following “the” with “the” is not grammatical. Fine-tuning for compatibility alleviates this problem (Figure 4).

Finally, we find that that fine-tuning for compatibility does not hurt the heldout performance of the complete conditional distribution of each fine-tuned model (see Appendix D).

## 5 Connection to Classification Rationales

In this section, we discuss related approaches developed for classification, and why they cannot scale to sequence models. We also show that the combinatorial rationale objective in Eq. 3 is a global solution to a classification rationale-style objective.

In classification problems, a sequence  $x_{1:T}$  is associated with a label  $y$ . Rationale methods are commonly used in this setting (Lei et al., 2016; Chen et al., 2018; Yoon et al., 2018; Bastings et al., 2019; Jain et al., 2020; Jethani et al., 2021). The most common approach uses two models: one, a selection model  $q(S|x_{1:T})$ , provides a distribution over possible rationales; the other, the predictive model  $p(y|x_S)$ , makes predictions given only samples from the former model. Typically,  $p$  and  $q$  are optimized jointly to maximize

$$\mathbb{E}_{x,y \sim F} \mathbb{E}_{S \sim q(S|x,y)} [\log p(y|x_S) - \lambda |S|]. \quad (7)$$

Here,  $F$  is the ground truth, unknown data distribution, and  $\lambda$  is a regularizing penalty that encourages smaller rationales.

In practice, it is infeasible to adopt this objective for sequence models. Eq. 7 is centered on providing predictive models with only the words in its rationale. In sequential settings, each word requires its own rationale. Thus training with shared word representations would leak information across rationales. Training sequence models without sharing representations is computationally infeasible; it requires  $O(T^3)$  computations per sequence for transformer architectures.

Most classification rationale methods treat  $q(S|x_{1:T})$  as a probability distribution over all possible rationales. However, the  $q$  that maximizes Eq. 7 is deterministic for any  $p$ . To see this, note that  $q$  does not appear inside the expectation in Eq. 7, so it can place all its mass on a single mode. We provide a formal justification in Appendix B.

Since the optimal selection model  $q$  is a point-mass, the optimal rationale can be written as

$$\arg \min_{S \in \mathcal{S}} \lambda |S| - \log p(y|x_S). \quad (8)$$

This optimization is identical to the combinatorial optimization in Eq. 3, albeit with a soft constraint on the rationale’s prediction: the true label  $y$  is not required to be the maximum of  $p(y'|x_S)$ . In practice, this soft constraint sometimes results in empty rationales (Jain et al., 2020). Since we view sufficiency as a key component of a good rationale, Eq. 3 imposes a hard constraint on the rationale’s prediction.

## 6 Related Work

Finding rationales is similar to feature selection. While global feature selection has been a well-studied problem in statistics (Guyon and Elisseeff,

2003; Hastie et al., 2009; Bertsimas et al., 2016), instance-wise feature selection — where the goal is selecting features per-example — is a newer research area (Chen et al., 2018). We review local explanation methods used for NLP.

**Gradients.** Gradient-based saliency methods have long been used as a measure of feature importance in machine learning (Baehrens et al., 2010; Simonyan et al., 2013; Li et al., 2016a). Some variations involve word embeddings (Denil et al., 2014); integrated gradients, to improve sensitivity (Sundararajan et al., 2017); and relevance-propagation to track each input’s contribution through the network (Bach et al., 2015; Voita et al., 2021).

But there are drawbacks to using gradient-based methods as explanatory tools. Sundararajan et al. (2017) show that in practice, gradients are *saturated*: they may all be close to zero for a well-fitted function, and thus not reflect importance. Adversarial methods can also distort gradient-based saliences while keeping a model’s prediction the same (Ghorbani et al., 2019; Wang et al., 2020). We compare to gradient saliency methods in Section 8.

**Attention.** Recently, NLP practitioners have focused on using attention weights as explanatory tools. The literature has made a distinction between *faithfulness* and *plausibility*. An explanation is faithful if it accurately depicts how a model makes a decision (Jacovi and Goldberg, 2020); an explanation is plausible if it can be understood and interpreted by humans (Wiegrefe and Pinter, 2019). Practitioners have shown that attention-based explanations are generally not faithful (Jain and Wallace, 2019; Serrano and Smith, 2019), but that they may be plausible (Wiegrefe and Pinter, 2019; Mohankumar et al., 2020; Vashishth et al., 2019). Others show that attention weights should not be interpreted as belonging to single tokens since they mix information across tokens (Brunner et al., 2019; Kobayashi et al., 2020). Bastings and Filippova (2020) argue that general input saliency measures, such as gradients, are better suited for explainability than attention. We compare to attention-based methods in Section 8.

**Local post-hoc interpretability.** Another class of methods provides local interpretability for pre-trained models. These approaches aim to explain a model’s behavior for a single example or for a small subset of inputs. LIME (Ribeiro et al., 2016) trains an interpretable model that locally approx-

imates the pretrained model. Alvarez-Melis and Jaakkola (2017) learn a causal relationship between perturbed inputs and their model outputs. These methods impose no constraints on the pretrained model. However, they are expensive – they require training separate models for each input region. In contrast, the method proposed here, greedy rationalization, can efficiently explain many predictions.

**Input perturbation.** Practitioners have also measured the importance of inputs by perturbing them (Zeiler and Fergus, 2014; Kádár et al., 2017). Occlusion methods (Li et al., 2016b) replace an input with a baseline (e.g. zeros), while omission methods (Kádár et al., 2017) remove words entirely. Li et al. (2016b) propose a reinforcement learning method that aims to find the minimum number of occluded words that would change a model’s prediction. Feng et al. (2018) use gradients to remove unimportant words to see how long it takes for the model’s prediction to change. They find that the remaining words are nonsensical and do not comport with other saliency methods. Others have shown that input perturbation performs worse than other saliency methods in practice (Poerner et al., 2018). These methods have mostly focused on subtractive techniques. For this reason, they are inefficient and do not aim to form sufficient explanations. In contrast, greedy rationalization efficiently builds up sufficient explanations.

## 7 Experimental Setup

There are two goals in our empirical studies. The first is to compare the ability of greedy rationalization to other approaches for optimizing the combinatorial objective in Eq. 3. The second is to assess the quality of produced rationales.

We measure the quality of rationales using two criteria: faithfulness and plausibility. An explanation is faithful if it accurately depicts how a model makes a decision (Jacovi and Goldberg, 2020); an explanation is plausible if it can be understood and interpreted by humans (Wiegrefe and Pinter, 2019). Although sufficiency is a standard way to measure faithfulness (DeYoung et al., 2020), all the rationales that satisfy the constraint of Eq. 3 are sufficient by definition. To measure plausibility, we compare rationales to human annotations. Since there do not exist language modeling datasets with human rationales, we collected annotations based on Lambada (Paperno et al., 2016). The data is available as part of this paper.

We compare greedy rationalization to a variety of gradient- and attention-based baselines (see Section 6). To form baseline sequential rationales, we add words by the order prescribed by each approach, stopping when the model prediction is sufficient. The baselines are:  $l_2$  gradient norms of embeddings (Li et al., 2016a), embedding gradients multiplied by the embeddings (Denil et al., 2014), integrated gradients (Sundararajan et al., 2017), attention rollout (Abnar and Zuidema, 2020), the last-layer transformer attention weights averaged-across heads, and all transformer attentions averaged across all layers and heads (Jain et al., 2020).

To compare rationale sets produced by each method to those annotated by humans, we use the set-similarity metrics described in DeYoung et al. (2020): the intersection-over-union (IOU) of each rationale and the human rationale, along with the token-level F1, treating tokens as binary predictions (either in the human rationale or out of it).

We use transformer-based models for all of the experiments.<sup>5</sup> We will release our fine-tuned GPT-2 model on Hugging Face (Wolf et al., 2019). For model and fine-tuning details, refer to Appendix D.

## 8 Results and Discussion

The experiments test sequential rationales for language modeling and machine translation. Appendix E contains full details for each experiment.

### 8.1 Language Modeling

**Long-Range Agreement.** The first study tests whether rationales for language models can capture long-range agreement. We create a template dataset using the analogies from Mikolov et al. (2013). This dataset contains word pairs that contain either a semantic or syntactic relationship. For each type of relationship, we use a predefined template. It prompts a language model to complete the word pair after it has seen the first word.

For example, one of the fifteen categories is countries and their capitals. We can prompt a language model to generate the capital by first mentioning a country and then alluding to its capital. To test long-range agreement, we also include a distractor sentence that contains no pertinent information about the word pair. For example, our

<sup>5</sup>We fine-tune each model for compatibility using a single GPU. That we can fine-tune GPT-2 Large (Radford et al., 2019) to learn compatible conditional distributions on a single GPU suggests that most practitioners will be able to train compatible models using a reasonable amount of computation.

	Length	Ratio	Ante	No D
Grad norms	22.5	4.1	<b>1.0</b>	0.06
Grad x emb	38.0	7.4	0.99	0.01
Integrated grads	28.1	5.2	0.99	0.00
Attention rollout	36.9	7.1	<b>1.0</b>	0.12
Last attention	16.7	2.9	0.99	0.13
All attentions	14.5	2.6	<b>1.0</b>	0.02
Greedy	<b>7.1</b>	<b>1.2</b>	<b>1.0</b>	<b>0.43</b>

**Table 1.** Language modeling faithfulness on long-range agreement with templated analogies. “Ratio” refers to the approximation ratio of each method’s rationale length to the exhaustive search minimum. “Ante” refers to the percent of rationales that contain the true antecedent. “No D” refers to the percent of rationales that do not contain any tokens from the distractor.

template for this category is,

When my flight landed in **Japan**, I converted my currency and slowly fell asleep. (I had a terrifying dream about my grandmother, but that’s a story for another time). I was staying in the capital,

Here, the parenthetical clause is a distractor sentence, since it contains no relevant information about predicting the capital of Japan. The correct capital, “Tokyo,” is predicted by GPT-2 both with and without the distractor. We use this template for all of the examples in the country capital category, swapping the antecedent “Japan” for each country provided in Mikolov et al. (2013).

We feed the prompts to GPT-2, which completes each analogy. To measure faithfulness, we calculate the percent of rationales that contain the true antecedent, and the percent of rationales that do not contain any words in the distractor. We only use examples where the prediction is the same both with and without the distractor. We also perform exhaustive rationale search on the objective in Eq. 3. This search is highly inefficient, so we only complete it for 40 examples. To measure the approximation ratio, we divide the size of the rationale found by each method by the exhaustive rationale size.

Table 1 contains the results on the compatible model.<sup>6</sup> Although all methods contain the true antecedents in their rationales, greedy rationalization has by far the least distractors in its rationales. The rationales are also universally shorter for greedy rationalization, and closer to the optimal rationales, justifying our greedy assumption.

<sup>6</sup>To show that fine-tuning GPT-2 for compatibility is not hurting the baselines, we also perform the baseline methods on a pretrained GPT-2 without fine-tuning; see Appendix E.

	Length	IOU	F1
Gradient norms	52.9	0.13	0.21
Gradient x embedding	64.8	0.11	0.19
Integrated gradients	59.1	0.11	0.19
Attention rollout	73.5	0.09	0.17
Last attention layer	43.2	0.17	0.27
All attention layers	35.8	0.24	0.33
Greedy	<b>14.1</b>	<b>0.27</b>	<b>0.37</b>

**Table 2.** Language modeling plausibility on rationale-annotated Lambada.

**Annotated Rationales.** To test the plausibility of rationales for language models, we collect a dataset of human annotations. We base the collection on Lambada (Paperno et al., 2016). Lambada is constructed so that humans need to use both local and global context to reliably predict a missing word. By its construction it is guaranteed to have non-trivial rationales.

Our goal is to collect rationales that are both minimal and sufficient for humans. We run an annotation procedure with two roles: a selector and a predictor. First, the selector sees the full passage and ranks the words in order of how informative they are for predicting the final word. Next, the predictor sees one word at a time chosen by the selector, and is asked to predict the final word of the passage. The words the predictor saw before guessing the correct word form a human rationale. This rationale selection method is inspired by Rissanen Data Analysis (Rissanen, 1978; Perez et al., 2021), which uses a minimum description length metric to estimate feature importances. We rely on human annotators to estimate information gains.

Since it could be trivial for humans to predict the final word if it also appears in the context, we only include examples that do not repeat a word. We collect annotations for 107 examples, which we also release publicly. We compare the rationales produced by each method to the annotated rationales. In the analysis, we only include the 62 examples that GPT-2 predicts correctly.

Table 2 shows that the greedy rationales are most similar to the human-annotated rationales. Greedy rationalization is also the most effective at minimizing the combinatorial objective in Eq. 3, as its rationales are by far the shortest. Figure 5 contains examples of rationales for this dataset.

It is worth noting that the top few words added by the baselines are quite relevant; after 5 tokens, the “All attention layers” baseline has a better F1 and IOU than greedy rationalization. However,

Target word: grow

"Just who is going to pay for this special feed grain anyway? It must cost a bit if it's that special."  
 "You're going to pay, obviously," replied Mitch, "since your cows will be eating it. On the other hand, Joe will be **planting** and irrigating the grain. He'll do all the work to **make it** \_\_\_\_\_"

Target word: refuse

It was the kind of smile that I'd seen before. The kind the boxer gave me right before he killed me in that **dirty** fight.

"I **have a proposition** for you" he began, pulling his hands down from under his chin and pushing out of the chair. "**One that you won't be able to** \_\_\_\_\_"

**Figure 5.** Examples from our annotated Lambada dataset. **Highlighted text** denotes greedy rationales, and **bolded text** denotes human-annotated rationales.

	Mean Crossovers		Crossover Rate	
	Source	Target	Source	Target
Grad norms	0.41	0.50	<b>0.06</b>	0.07
Grad x emb	6.22	5.63	0.42	0.42
Integrated grads	1.93	1.53	0.22	0.12
Last attention	0.56	2.49	0.08	0.24
All attentions	0.60	0.83	0.08	0.11
Greedy	<b>0.11</b>	<b>0.16</b>	0.08	<b>0.03</b>

**Table 3.** Translation faithfulness with distractors. "Mean crossovers" refers to the average number of crossovers per rationale, and "Crossover rate" refers to the fraction of rationales that contain at least one.

the baselines struggle to form sufficient rationales, which hurts their overall performance.

## 8.2 Machine Translation

**Distractors.** To measure faithfulness, we take a transformer trained on IWSLT14 De-En (and fine-tuned for compatibility), and generate translations for 1000 source sequences. We then randomly concatenate each source sequence with a distractor (before or after). We know that each target sequence is generated from the original source. Thus, we can evaluate rationales by penalizing them for "crossing over" to the distractor.

**Table 3** contains the results. Greedy rationalization has by far the fewest average number of crossovers per rationale. Although the percent of source rationales that cross over is slightly higher than the percent using gradient norms, the percentage on the target side is superior.

**Annotated Alignments.** To test plausibility, we compare the rationales to human-labeled word

	Length	AER ↓	IOU	F1	Top1
Grad norms	10.3	0.82	0.31	0.16	0.62
Grad x emb	13.0	0.89	0.16	0.12	0.40
Integrated grads	11.0	0.84	0.27	0.14	0.45
Last attention	10.7	0.83	0.28	0.15	0.59
All attentions	10.6	0.82	0.32	0.15	<b>0.65</b>
Greedy	<b>5.0</b>	<b>0.77</b>	<b>0.41</b>	<b>0.23</b>	0.64

**Table 4.** Translation plausibility with annotated alignments. The first four columns correspond to using the full rationale found by each method; the last column "Top1" refers to the accuracy of the first token added by each method. AER refers to alignment error rate.

alignments. Using a dataset containing 500 annotated alignments for German-English translation,<sup>7</sup> we compute rationales for each method using the ground truth targets. We measure similarity to the labeled rationales by computing alignment error rate (AER) (Och and Ney, 2000), along with computing the IOU and F1 between sets. To separate the requirement that the rationale be sufficient from each method's global ordering of tokens, we also compare top-1 accuracies, which measure whether the top token identified by each baseline is present in the labeled alignment set.

**Table 4** contains the results. The rationales learned by greedy rationalization are more similar to human-labeled alignments than those provided by gradient and attention methods. Many methods have similar top-1 accuracies — indeed, the best top-1 accuracy comes from averaging all attention layers. This reinforces the notion that although the baselines may be able to capture first-order information, they struggle to form sufficient rationales.

## 9 Conclusion

We proposed an optimization-based algorithm for rationalizing sequence predictions. Although exact optimization is intractable, we developed a greedy approach that efficiently finds good rationales. Moreover, we showed that models can be fine-tuned to form compatible distributions, thereby circumventing an intractable marginalization step. In experiments, we showed that the greedy algorithm is effective at optimization, and that its rationales are more faithful and plausible than those of gradient- and attention-based methods. We hope that our research, along with the release of an annotated dataset of sequence rationales, catalyzes further research into this area.

<sup>7</sup><https://www-i6.informatik.rwth-aachen.de/goldAlignment/>

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