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Pathologies of Neural Models Make Interpretations Difficult

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Abstract

One way to interpret neural model predictions is to highlight the most important input features—for example, a heatmap visualization over the words in an input sentence. In existing interpretation methods for NLP, a word’s importance is determined by either input perturbation—measuring the decrease in model confidence when that word is removed—or by the gradient with respect to that word. To understand the limitations of these methods, we use input reduction, which iteratively removes the least important word from the input. This exposes pathological behaviors of neural models: the remaining words appear nonsensical to humans and do not match the words interpretation methods deem important. As we confirm with human experiments, the reduced examples lack information to support the prediction of any label, but models still make the same predictions with high confidence. To explain these counterintuitive results, we draw connections to adversarial examples and confidence calibration: pathological behaviors reveal difficulties in interpreting neural models trained with maximum likelihood. To mitigate their deficiencies, we fine-tune the models by encouraging high entropy outputs on reduced examples. Fine-tuned models become more interpretable under input reduction without accuracy loss on regular examples.

1 Introduction

Many interpretation methods for neural networks explain the model’s prediction as a counterfactual: how does the prediction change when the input is modified? Adversarial examples (Szegedy et al., 2014; Goodfellow et al., 2015) highlight the instability of neural network predictions by showing how small perturbations to the input dramatically change the output.

A common, non-adversarial form of model interpretation is feature attribution: features that are crucial for predictions are highlighted in a heatmap. One can measure a feature’s importance by input perturbation. Given an input for text classification, a word’s importance can be measured by the difference in model confidence before and after that word is removed from the input—the word is important if confidence decreases significantly. This is the leave-one-out method (Li et al., 2016b). Gradients can also reveal feature importance: a feature influences predictions if its gradient is a large positive value. Both perturbation and gradient-based methods can generate heatmaps, implying that the model’s prediction is highly influenced by the highlighted, important words.

Instead, we study how the model’s prediction is influenced by unimportant words. We use input reduction, iteratively removing unimportant words from the input while maintaining the model’s prediction. Intuitively, the words remaining after input reduction should be important for prediction. Moreover, the words should match the leave-one-out method’s selections, which closely align with

SQAD

<table>
<thead>
<tr>
<th>Context</th>
<th>In 1899, John Jacob Astor IV invested $100,000 for Tesla to further develop and produce a new lighting system. Instead, Tesla used the money to fund his Colorado Springs experiments.</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original</td>
<td>What did Tesla spend Astor’s money on?</td>
</tr>
<tr>
<td>Reduced</td>
<td>did</td>
</tr>
<tr>
<td>Confidence</td>
<td>0.78 → 0.91</td>
</tr>
</tbody>
</table>

Figure 1: SQUAD example from the validation set. Given the original Context, the model makes the same correct prediction (“Colorado Springs experiments”) on the Reduced question as the Original, with even higher confidence. For humans, the reduced question, “did”, is nonsensical.
human perception (Li et al., 2016b; Murdoch et al., 2018). However, rather than providing explanations of the original prediction, our reduced examples more closely resemble adversarial examples. The reduced input is meaningless to a human but retains the same model prediction with high confidence (Figure 1). Gradient-based input reduction exposes pathological model behaviors that contradict what one expects based on existing interpretation methods.

In Section 2, we construct these counterintuitive examples by augmenting input reduction with beam search and experiment with three tasks: SQUAD (Rajpurkar et al., 2016) for reading comprehension, SNLI (Bowman et al., 2015) for textual entailment, and VQA (Antol et al., 2015) for visual question answering. Input reduction with beam search consistently reduces the input sentence to very short lengths—often only one or two words—without lowering model confidence on its original prediction. The reduced examples appear nonsensical to humans, which we verify with crowdsourced experiments. In Section 3, we draw connections to adversarial examples and confidence calibration; we explain why the observed pathologies are a consequence of the overconfidence of neural models. This elucidates limitations of interpretation methods that rely on model confidence. In Section 4, we encourage high model uncertainty on reduced examples with entropy regularization. The pathological model behavior under input reduction is mitigated, leading to more reasonable reduced examples.

## 2 Input Reduction

To explain model predictions using a set of important words, we must first define importance. After defining input perturbation and gradient-based approximation, we describe input reduction with these importance metrics. Input reduction drastically shortens inputs without causing the model to change its prediction or significantly decrease its confidence. Crowdsourced experiments confirm that reduced examples appear nonsensical to humans: input reduction uncovers pathological model behaviors.

### 2.1 Importance from Input Gradient

Ribeiro et al. (2016) and Li et al. (2016b) define importance by seeing how confidence changes when a feature is removed: if removing a feature drastically changes a prediction, it must have been important. A natural approximation is to use the gradient (Baehrens et al., 2010; Simonyan et al., 2014). We formally define these importance metrics in natural language contexts and introduce the efficient gradient-based approximation. For each word in an input sentence, we measure its importance by the change in the confidence of the original prediction when we remove that word from the sentence. We switch the sign so that when the confidence decreases, the importance value is positive.

Formally, let \( x = \langle x_1, x_2, \ldots, x_n \rangle \) denote the input sentence, \( f(y \mid x) \) the predicted probability of label \( y \), and \( y = \text{argmax}_y f(y' \mid x) \) the original predicted label. The importance is then

\[
g(x_i \mid x) = f(y \mid x) - f(y \mid x_{-i}).
\]

To calculate the importance of each word in a sentence with \( n \) words, we need \( n \) forward passes of the model, each time with one of the words left out. This is highly inefficient, especially for longer sentences. Instead, we approximate the importance value with the input gradient. For each word in the sentence, we calculate the dot product of its word embedding and the gradient of the output with respect to continuous vector that represents the word: the embedding. The importance of \( n \) words can thus be computed with a single forward-backward pass. This gradient approximation has been used for various interpretation methods for natural language classification models (Li et al., 2016a; Arras et al., 2016); see Ebrahimi et al. (2017) for further details on the derivation. We use this approximation in all our experiments as it selects the same words for removal as an exhaustive search (no approximation).

### 2.2 Removing Unimportant Words

Instead of looking at the words with high importance values—what interpretation methods commonly do—we take a complementary approach and study how the model behaves when the supposedly unimportant words are removed. Intuitively, the important words should remain after the unimportant ones are removed.

Our input reduction process iteratively removes the unimportant words. At each step, we remove the word with the lowest importance value until the model changes its prediction. We experiment with three popular datasets: SQUAD (Rajpurkar et al., 2016) for reading comprehension, SNLI (Bowman et al., 2015) for textual entailment, and VQA (Antol et al., 2015) for visual question answering. In Section 3, we experiment with three popular datasets: SQUAD (Rajpurkar et al., 2016) for reading comprehension, SNLI (Bowman et al., 2015) for textual entailment, and VQA (Antol et al., 2015) for visual question answering.
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In SQuAD, each example is a context paragraph and a question. The task is to predict a span in the paragraph as the answer. We reduce only the question while keeping the context paragraph unchanged. The model we use is the DRQA Document Reader (Chen et al., 2017).

In SNLI, each example consists of two sentences: a premise and a hypothesis. The task is to predict one of three relationships: entailment, neutral, or contradiction. We reduce only the hypothesis while keeping the premise unchanged. The model we use is Bilateral Multi-Perspective Matching (BMPM) (Wang et al., 2017).

In VQA, each example consists of an image and a natural language question. We reduce only the question while keeping the image unchanged. The model we use is Show, Ask, Attend, and Answer (Kazemi and Elqursh, 2017).

During the iterative reduction process, we ensure that the prediction does not change (exact span for SQuAD); consequently, the model accuracy on the reduced examples is identical to the original. The predicted label is used for input reduction and the ground-truth is never revealed. We use the validation set for all three tasks.

Most reduced inputs are nonsensical to humans (Figure 2) as they lack information for any reasonable human prediction. However, models make confident predictions, at times even more confident than the original.

To find the shortest possible reduced inputs (potentially the most meaningless), we relax the requirement of removing only the least important word and augment input reduction with beam search. We limit the removal to the $k$ least important words, where $k$ is the beam size, and decrease the beam size as the remaining input is shortened. We empirically select beam size five as it produces comparable results to larger beam sizes with reasonable computation cost. The requirement of maintaining model prediction is unchanged.

With beam search, input reduction finds extremely short reduced examples with little to no decrease in the model’s confidence on its original predictions. Figure 3 compares the length of input sen-

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1Footnote: We set beam size to $\max(1,\ \min(k, L - 3))$ where $k$ is maximum beam size and $L$ is the current length of the input sentence.

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2.3 Humans Confused by Reduced Inputs

On the reduced examples, the models retain their original predictions despite short input lengths. The following experiments examine whether these predictions are justified or pathological, based on how humans react to the reduced inputs.

For each task, we sample 200 examples that are correctly classified by the model and generate their reduced examples. In the first setting, we compare the human accuracy on original and reduced inputs. We recruit two groups of crowd workers and task them with textual entailment, reading comprehension, or visual question answering. We show one group the original inputs and the other the reduced. Humans are no longer able to give the correct answer, showing a significant accuracy loss on all three tasks (compare Original and Reduced in Table 1).

The second setting examines how random the reduced examples appear to humans. For each
of the original examples, we generate a version where words are randomly removed until the length matches the one generated by input reduction. We present the original example along with the two reduced examples and ask crowd workers their preference between the two reduced ones. The workers’ choice is almost fifty-fifty (the vs. Random in Table 1): the reduced examples appear almost random to humans.

These results leave us with two puzzles: why are the models highly confident on the nonsensical reduced examples? And why, when the leave-one-out method selects important words that appear reasonable to humans, the input reduction process selects ones that are nonsensical?

3 Making Sense of Reduced Inputs

Having established the incongruity of our definition of importance vis-à-vis human judgements, we now investigate possible explanations for these results.

We explain why model confidence can empower methods such as leave-one-out to generate reasonable interpretations but also lead to pathologies under input reduction. We attribute these results to two issues of neural models.

3.1 Model Overconfidence

Neural models are overconfident in their predictions (Guo et al., 2017). One explanation for overconfidence is overfitting: the model overfits the negative log-likelihood loss by learning to output low-entropy distributions over classes. Neural models are also overconfident on examples outside the training data distribution. As Goodfellow et al. (2015) observe for image classification, samples from pure noise can sometimes trigger highly confident predictions. These so-called rubbish examples are degenerate inputs that a human would trivially classify as not belonging to any class but for which the model predicts with high confidence. Goodfellow et al. (2015) argue that the rubbish examples exist for the same reason that adversarial examples
The Panthers used the San Jose State practice facility and stayed at the San Jose Marriott. The Broncos practiced at Stanford University and stayed at the Santa Clara Marriott.

Context: The Panthers used the San Jose State practice facility and stayed at the San Jose Marriott. The Broncos practiced at Stanford University and stayed at the Santa Clara Marriott.


Figure 5: A reduction path for a SQUAD example. The model prediction is always correct and its confidence stays high (shown on the left in parentheses) throughout the reduction. Each line shows the input at that step with an underline indicating the word to remove next. The question becomes unanswerable immediately after “Broncos” is removed in the first step. However, in the context of the original question, “Broncos” the input gradient considers it the least important word.

Figure 6: Heatmap generated with leave-one-out shifts drastically despite only removing the least important word (underlined) at each step. For instance, “advertisement”, is the most important word in step two but becomes the least important in step three.

3.2 Second-order Sensitivity

Thus far, we have seen that a neural model’s output changes wildly with small changes in its input. We call this first-order sensitivity, because interpretation based on input gradient is a first-order Taylor expansion of the model near the input (Simonyan et al., 2014). However, the interpretation (e.g., which words are important) also shifts drastically with small input changes (Figure 6). We call this second-order sensitivity.

The shifting heatmap suggests a mismatch between the model’s first- and second-order sensitivities. The heatmap shifts when, with respect to the removed word, the model has low first-order sensitivity but high second-order sensitivity.

Similar issues complicate comparable interpretation methods for image classification models. For example, Ghorbani et al. (2017) modify image inputs so the highlighted features in the interpretation change while maintaining the same prediction. To achieve this, they iteratively modify the input to maximize changes in the distribution of feature importance. In contrast, our shifting heatmap occurs by only removing the least impactful features without a targeted optimization. They speculate that the steepest gradient direction for the first- and second-order sensitivity values are generally orthogonal. Loosely speaking, the shifting heatmap suggests that the direction of the smallest gradient value can sometimes align with very steep changes in second-order sensitivity.
When explaining individual model predictions, the heatmap suggests that the prediction is made based on a weighted combination of words, as in a linear model, which is not true unless the model is indeed taking a weighted sum such as in a DAN (Iyyer et al., 2015). When the model composes representations by a non-linear combination of words, a linear interpretation oblivious to second-order sensitivity can be misleading.

4 Mitigating Model Pathologies

The previous section explains the observed pathologies from the perspective of overconfidence: models are too certain on rubbish examples when they should not make any prediction. Human experiments (Section 2.3) confirm that reduced examples fit the definition of rubbish examples. Hence, a natural way to mitigate pathologies is maximizing model uncertainty on the reduced examples.

4.1 Regularization on Reduced Inputs

To maximize model uncertainty on reduced examples, we use the entropy of the output distribution as an objective. Given a model \( f \) trained on a dataset \((X, Y)\), we generate reduced examples using input reduction for all training examples \(X\). Beam search often yields multiple reduced versions with the same minimum length for each input \(x\), and we collect all of these versions together to form \(\tilde{X}\) as the “negative” example set.

Let \( H(\cdot) \) denote the entropy and \( f(y|x) \) the probability of the model predicting \( y \) given \( x \). We fine-tune a model to maximize log-likelihood on regular examples and entropy on reduced examples:

\[
\sum_{(x,y)} \log(f(y|x)) + \lambda \sum_{\tilde{x} \in \tilde{X}} H(f(y|\tilde{x})),
\]

where hyperparameter \(\lambda\) trades-off between the two terms. Similar entropy regularization is used by Pereyra et al. (2017), but not in combination with input reduction; their entropy term is calculated on regular examples rather than reduced examples.

4.2 Regularization Mitigates Pathologies

On regular examples, entropy regularization does no harm to model accuracy, with a slight increase for SQUAD (Accuracy in Table 2).

After entropy regularization, input reduction produces more reasonable reduced inputs (Figure 7).

In the SQUAD example from Figure 1, the reduced question changed from “did” to “spend Astor money on ?“ after fine-tuning. The average length of reduced examples also increases across all tasks (Reduced length in Table 2). To verify that model overconfidence is indeed mitigated—that the reduced examples are less “rubbish” compared to before fine-tuning—we repeat the human experiments from Section 2.3.

Human accuracy increases across all three tasks (Table 3). We also repeat the vs. Random experiment: we re-generate the random examples to match the lengths of the new reduced examples from input reduction, and find humans now prefer the reduced examples to random ones. The increase in both human accuracy and preference suggests that the reduced examples are more reasonable; model pathologies have been mitigated.

This is promising, but do we need input reduction to reduce overconfidence? To provide a baseline, we fine-tune models using randomly reduced inputs (with the same lengths as input reduction). This baseline improves neither model accuracy nor interpretability (i.e., the reduced examples are just as short). Input reduction provides negative examples that curb overconfidence.

5 Discussion

Rubbish examples have been studied in images (Goodfellow et al., 2015; Nguyen et al., 2015), but to our knowledge not for NLP. Our input reduction gradually transforms a valid input into a rubbish example. We can often determine which word’s removal is the tipping point—for example, removing “Broncos” in Figure 5. These rubbish examples are interesting, as they are also adversarial: they resemble valid examples. In contrast, image rubbish examples generated from noise lie outside the training data distribution and resemble static.
In 1899, John Jacob Astor IV invested $100,000 for Tesla to further develop and produce a new lighting system. Instead, Tesla used the money to fund his Colorado Springs experiments. What did Tesla spend Astor’s money on? Colorado Springs experiments.

Original: Two man is dancing on the street
Answer: Contradiction
Before: dancing
After: two man dancing
Confidence: 0.977 → 0.706 → 0.717

Original: What color is the flower?
Answer: yellow
Before: flower?
After: What color is flower?
Confidence: 0.847 → 0.918 → 0.745

Table 3: Human Accuracy increases after fine-tuning the models. Humans also prefer gradient-based reduced examples over randomly reduced ones, indicating that the reduced examples are more meaningful to humans after regularization.

The robustness of NLP models has been studied extensively (Papernot et al., 2016; Jia and Liang, 2017; Iyyer et al., 2018; Ribeiro et al., 2018), and most studies define adversarial examples similar to the image domain: small perturbations to the input lead to large changes in the output. HotFlip (Ebrahimi et al., 2017) uses a gradient-based approach, similar to image adversarial examples, to flip the model prediction by perturbing a few characters or words. Our work and Belinkov and Bisk (2018) both identify cases where noisy user inputs become adversarial by accident: common misspellings break neural machine translation models; we show that incomplete user input can lead to unreasonably high model confidence.

Other failures of interpretation methods have been explored in the image domain. The sensitivity issue of gradient-based interpretation methods, similar to our shifting heatmaps, are observed by Ghorbani et al. (2017) and Kindermans et al. (2017). They show that various forms of input perturbation—from adversarial changes to simple constant shifts in the image input—cause significant changes in the interpretation. Ghorbani et al. (2017) make a similar observation about second-order sensitivity, that “the fragility of interpretation is orthogonal to fragility of the prediction”.

Previous work studies biases in the annotation process that lead to datasets easier than desired or expected which eventually induce pathological models. We attribute our observed pathologies primarily to the lack of accurate uncertainty estimates in neural models trained with maximum likelihood. SNLI hypotheses contain artifacts that allow training a model without the premises (Gururangan et al., 2018); we apply input reduction at test time to the hypothesis. Similarly, VQA images are surprisingly unimportant for training a model; we reduce the question. The recent SQuAD 2.0 (Rajpurkar et al., 2018) augments the original reading comprehension task with an uncertainty modeling requirement, the goal being to make the task more realistic and challenging. Question answering tasks such as Quizbowl combine knowing what to answer with when there is sufficient information to answer for the agent or an opponent (He et al., 2016).

Section 3.1 explains the pathologies from the overconfidence perspective. One explanation for overconfidence is overfitting: Guo et al. (2017) show that, late in maximum likelihood training, the model learns to minimize loss by outputting low-entropy distributions without improving validation accuracy. To examine if overfitting can explain the input reduction results, we run input reduction using DRQA model checkpoints from every training epoch. Input reduction still achieves similar results on earlier checkpoints, suggesting that better convergence in maximum likelihood training cannot fix the issues by itself—we need new training objectives with uncertainty estimation in mind.
5.1 Methods for Mitigating Pathologies

We regularize the model using input reduction’s reduced examples and improve its interpretability. This resembles adversarial training (Goodfellow et al., 2015), where adversarial examples are added to the training set to improve model robustness. The objectives are different: entropy regularization encourages high uncertainty on rubbish examples, while adversarial training makes the model less sensitive to adversarial perturbations.

Pereyra et al. (2017) apply entropy regularization on regular examples from the start of training to improve model generalization. A similar method is label smoothing (Szegedy et al., 2016). In comparison, we fine-tune a model with entropy regularization on the reduced examples for better uncertainty estimates and interpretations.

To mitigate overconfidence, Guo et al. (2017) use post-hoc fine-tuning a model’s confidence with Platt scaling. This method adjusts the softmax function’s temperature parameter using a small held-out dataset to align confidence with accuracy. However, because the output is calibrated using the entire confidence distribution, not individual values, this does not reduce overconfidence on specific inputs, such as the reduced examples.

5.2 Generalizability of Findings

To highlight the erratic model predictions on short examples and provide a more intuitive demonstration, we present paired-input tasks. On these tasks, the short lengths of reduced questions and hypotheses obviously contradict the necessary number of words for a human prediction (further supported by our human studies). We also apply input reduction to single-input tasks including sentiment analysis (Maas et al., 2011) and Quizbowl (Boyd-Graber et al., 2012), achieving similar results.

Interestingly, the reduced examples transfer to other architectures. In particular, when we feed fifty reduced SNLI inputs from each class—generated with the BiMPM model (Wang et al., 2017)—through the Decomposable Attention Model (Parikh et al., 2016), the same prediction is triggered 81.3% of the time.

6 Conclusion

We introduce input reduction, a process that iteratively removes unimportant input words while maintaining a model’s prediction. Combined with gradient-based importance estimates, we expose pathological behaviors of neural models. Without lowering model confidence original predictions, an input sentence can be reduced to the point where it appears nonsensical, often consisting of one or two words. Humans cannot understand the reduced examples, but neural models maintain their original predictions.

We explain these pathologies with known issues of neural models: overconfidence and sensitivity to small input changes. Inaccurate uncertainty estimates cause the the nonsensical reduced examples: the model is cannot lower its confidence on ill-formed inputs. The second-order sensitivity also explains why gradient-based interpretation methods contradict human expectations: a small change in the input can cause a minor change in the prediction but a large change in the interpretation. Input reduction’s many small perturbations—a stress test—can expose deeper issues of model overconfidence and oversensitivity that other methods cannot.

To properly interpret neural models, it is important to understand their fundamental characteristics: the nature of their decision surfaces, robustness against adversaries, and limitations of their training objectives. We explain fundamental difficulties of interpretation due to pathologies in neural models trained with maximum likelihood. Our work suggests several future directions to improve interpretability: more thorough evaluation of interpretation methods, better uncertainty and confidence estimates, and interpretation beyond bag-of-word heatmap.

More practically, NLP systems are often designed as pipelines: speech recognition or machine translation feeds into a downstream classification task. The classification is typically trained on uncorrupted English text. Input reduction suggests that both the outputs and confidences of such naïve pipelines should be treated with greater suspicion.

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2http://demo.allennlp.org/textual-entailment
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