Explaining Prediction Uncertainty of Pre-trained Language Models by Detecting Uncertain Words in Inputs

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Abstract

Estimating the predictive uncertainty of pre-trained language models is important for increasing their trustworthiness in NLP. Although many previous works focus on quantifying prediction uncertainty, there is little work on explaining the uncertainty. This paper pushes a step further on explaining uncertain predictions of post-calibrated pre-trained language models. We adapt two perturbation-based post-hoc interpretation methods, Leave-one-out and Sampling Shapley, to identify words in inputs that cause the uncertainty in predictions. We test the proposed methods on BERT and RoBERTa with three tasks: sentiment classification, natural language inference, and paraphrase identification, in both in-domain and out-of-domain settings. Experiments show that both methods consistently capture words in inputs that cause prediction uncertainty.

1 Introduction

Pre-trained language models (e.g., BERT; Devlin et al., 2019) light up the natural language processing (NLP) community by achieving remarkable performance across a wide range of NLP tasks (Liu et al., 2019; Yang et al., 2019; Gururangan et al., 2020; Brown et al., 2020). Nevertheless, there is a long debate on the trustworthiness of the predictions of pre-trained language models (Ribeiro et al., 2016, 2020; Chen and Ji, 2020; Huang et al., 2020). Estimating the uncertainty of model predictions provides insights into their trustworthiness (Desai and Durrett, 2020; Xu et al., 2020). If a model provides a prediction with high uncertainty (e.g. a nearly random guess), users would choose to not trust the prediction. A typical way to measure prediction uncertainty is to calibrate model outputs with the true correctness likelihood (Guo et al., 2017; Kong et al., 2020; Zhao et al., 2021), so that the predictive probabilities well represent the confidence of model predictions being correct. Higher prediction confidence indicates lower uncertainty (Xu et al., 2020; Jiang et al., 2021). Pre-trained language models can be calibrated during training by regularizing their outputs (Kumar et al., 2018; Kong et al., 2020) or inference stage via post-processing (e.g. temperature scaling; Guo et al., 2017; Zhao et al., 2021).

However, given a calibrated model, little is known about why it makes uncertain predictions on some instances. Although there is extensive work on explaining model predicted labels (Ribeiro et al., 2016; Lundberg and Lee, 2017; Chen et al., 2021), explaining prediction uncertainty is largely ignored. Explaining prediction uncertainty is an important complement to explaining predicted labels for understanding a model prediction behavior, especially when its prediction confidence is low (Anítorán et al., 2020). This work firstly explains model prediction uncertainty in NLP. Our hypothesis is there are some words in inputs containing redundant or noisy information that makes model predictions uncertain. We adapt two perturbation-based post-hoc interpretation methods, Leave-one-out (Li et al., 2016) and Sampling Shapley (Strumbelj and Kononenko, 2010), to explain uncertain predictions of pre-trained language models by identifying the words in inputs that cause prediction uncertainty. Note that different from previous applications of these two methods in attributing important words for explaining model predicted labels (Lundberg and Lee, 2017; Chen et al., 2020), we implement them in an opposite way, detecting uncertain words that drag down model prediction confidence.

We evaluate two pre-trained language models, BERT (Devlin et al., 2019) and RoBERTa (Liu et al., 2019), on three tasks, including sentiment classification, natural language inference, and paraphrase identification. For each task, we test on both in-domain and out-of-domain datasets. Experiments show that both methods consistently capture words in inputs that make model predictions
uncertain. Most of these words do not have specific meaning (redundant information) or oppose to ground-truth meaning (noisy information), either of which is not supportive for correct predictions. Leaving them out improves model prediction confidence on both in-domain and out-of-domain datasets.

2 Related Work

The problem of predictive uncertainty estimation and calibration has been well studied (Kuleshov and Liang, 2015; Gal and Ghahramani, 2016; Pereyra et al., 2017; Kumar et al., 2018; Liu et al., 2020; Jiang et al., 2021). Calibrated models can make uncertain predictions on some instances, while little is known about what causes prediction uncertainty. This work moves a step further to explain uncertain predictions.

There are extensive literatures on explaining model predicted labels by identifying salient features in inputs (Ribeiro et al., 2016; Lundberg and Lee, 2017; Chen et al., 2020; Sundararajan et al., 2017; Chen et al., 2021). However, these works ignore model prediction uncertainty. When a model makes an uncertain prediction, it is important to know what causes the uncertainty as the predicted label may be a random guess. Therefore, we claim to explaining predictive uncertainty as a complement to explaining predicted labels for better understanding model predictions.

There is a little work regarding explaining prediction uncertainty. Antorán et al. (2020) firstly explained uncertainty estimates in computer vision by generating a similar input which the model has low uncertainty on to identify uncertain features in the original input. However, this method is applied to differentiable probabilistic models for tabular and image data. To the best of our knowledge, there is no existing work on explaining uncertain predictions of pre-trained neural language models in NLP. Feng et al. (2018) observed prediction confidence increasing with input reduction. They focused on the pathologies of neural networks with reduced inputs that lack predictive information, while we focus on detecting the words in inputs that lead to uncertain predictions.

3 Explaining Uncertain Predictions

In this work, we consider models that are calibrated, so that we can know if their predictions are uncertain or not based on prediction confidence. Let \( f(\cdot) \) denote the model. Given an input \( \mathbf{x} = \{x_1, \ldots, x_N\} \) consisting of \( N \) words, the model output probabilities over classes are \( [f_1(\mathbf{x}), \ldots, f_C(\mathbf{x})] \), where \( f_c(\mathbf{x}) = P(y = c | \mathbf{x}) \) is the output probability on label \( c \in \{1, \ldots, C\} \), and \( C \) is the total number of classes. The probability on the predicted class \( \hat{y} \), i.e. \( f_{\hat{y}}(\mathbf{x}) \), represents model prediction confidence. The prediction uncertainty is computed as the entropy of the probability distribution over classes, \( H(Y | \mathbf{x}) = -\sum_{c=1}^{C} f_c(\mathbf{x}) \log f_c(\mathbf{x}) \). The higher the confidence, the lower the uncertainty. We define uncertain predictions with confidence lower than a threshold \( \tau \) which will be detailed in Section 4.2.

Recall that we assume there are some words in inputs containing redundant or noisy information that causes prediction uncertainty. An intuitive way to detect these words is removing different combinations of words and observing whether prediction confidence goes up. We adapt two perturbation-based methods, Leave-one-out (Li et al., 2016) and Sampling Shapley (Strumbelj and Kononenko, 2010), to explain uncertain predictions. Both methods identify the words in inputs that cause model prediction uncertainty. We consider these words as uncertain words. These two methods were previously implemented to find important words for model explanations (Li et al., 2016; Lundberg and Lee, 2017; Chen et al., 2020). Therefore, we need to modify their objective functions as follows.

**Leave-one-out.** This method evaluates the effect of each word on model prediction uncertainty by leaving it out and observing the output probability change on the predicted class. We define an uncertainty score for each word as

\[
S_i = f_{\hat{y}}(\mathbf{x}_{\setminus i}) - f_{\hat{y}}(\mathbf{x}),
\]

where \( \mathbf{x}_{\setminus i} \) denotes the input with the word \( x_i \) removed. The uncertainty score \( S_i \) quantifies how much the model prediction confidence can be improved when \( x_i \) is left out. In other words, \( S_i \) represents the uncertainty the word \( x_i \) contributes to the model prediction.

**Sampling Shapley.** Leave-one-out is simple but ignores coalitions between words when quantifying their contributions to the uncertainty. The Shapley value (Shapley, 1953) stems from coalitional game theory provides an axiomatic solution to attribute the contribution of each word in a fair way. However, the exponential complexity \( (O(2^N)) \) of com-
putting Shapley value is intractable. Sampling Shapley (Strumbelj and Kononenko, 2010) provides a solvable approximation to Shapley value via sampling. Specifically, for a word $x_i$, its uncertainty score is computed as

$$S_i = \frac{1}{M} \sum_{m=1}^{M} f^*(x_i^{(m)}) - f^*(x_i^{(m)} \cup x_i),$$  

(2)

where $M$ is the number of samples, and $x_i^{(m)} \subseteq x_i$ contains a subset of words in $x_i$. The uncertainty score quantifies the overall contribution of the word $x_i$ to model prediction uncertainty over all $M$ ensembles. In experiments, we set $M = 200$. 

4 Experiments

4.1 Models and Datasets

We evaluate two pre-trained language models, BERT (Devlin et al., 2019) and RoBERTa (Liu et al., 2019). The two models are fine-tuned on three downstream tasks: sentiment classification, natural language inference, and paraphrase identification. Each task contains an in-domain/out-of-domain dataset pair. Specifically, IMDB (Maas et al., 2011)/Yelp (Zhang et al., 2015) for sentiment classification, SNLI (Bowman et al., 2015)/MNLI (Williams et al., 2018) for natural language inference, and QQP (Iyer et al., 2017)/TwitterPPDB (TPPDB) (Lan et al., 2017) for paraphrase identification. More details about the models and datasets are in Appendix A.1. For each task, we train the models on the in-domain training set and test them on both in-domain and out-of-domain test sets. The test results are in Table 1. RoBERTa performs better than BERT. The prediction performance of both models drops on out-of-domain test sets.

Posterior Calibration. We follow Desai and Durrett (2020) and calibrate the models on each dataset via temperature scaling (Guo et al., 2017). Specifically, we use the development set to learn a temperature $T$ which corrects model output probabilities by dividing non-normalized logits before the softmax function. Then the learned $T$ is applied to modify model outputs on the test set. In experiments, we linearly search for an optimal temperature $T$ between $[0, 10]$ with a granularity of 0.01, which empirically performs well.

We evaluate model calibration with Expected Calibration Error (ECE) (Guo et al., 2017) (see more details in Appendix A.2). We report the learned temperature scalars and ECEs before and after calibration in Table 5 in Appendix A.2. Temperature scaling performs effectively in decreasing model calibration errors on both in-domain and out-of-domain datasets. This enables us to further explain uncertain predictions based on calibrated confidence. We apply temperature scaling to correct model outputs in the following experiments.

4.2 Detecting Uncertain Words

For each model, we test it on 1000 randomly selected examples per dataset. We select the examples which the model has correct but uncertain predictions on (with confidence lower than the empirical threshold $\tau = 0.8$). Leave-one-out and Sampling Shapley respectively.

Table 1: Prediction accuracy (%) of different models on in-domain and out-of-domain test sets.

| Models  | IMDB  | SNLI  | QQP  | Yelp | MNLI | TPPDB |
|---------|-------|-------|------|------|------|-------|
| BERT    | 91.32 | 89.70 | 90.40| 87.68| 69.94| 87.03 |
| RoBERTa | 93.11 | 90.96 | 91.19| 92.35| 75.57| 86.15 |

Figure 1: Prediction confidence changes with uncertain words deleted. The suffix “-L” and “-S” represent the uncertain words are identified by Leave-one-out and Sampling Shapley respectively.
Sampling Shapley are applied to explain each one of these examples by computing word uncertainty scores introduced in section 3.

Both interpretation methods capture uncertain words in inputs. Figure 1 shows the prediction confidence changing with the identified uncertain words removed iteratively from the one with the highest uncertainty score. All curves increase first and reach to peak values, indicating both Leave-one-out (“-L”) and Sampling Shapley (“-S”) identify uncertain words in inputs. Both models achieve higher prediction confidence on in-domain datasets than on out-of-domain datasets.

Sampling Shapley performs better than Leave-one-out. In Figure 1, the confidence starts decreasing after the peak value as the further removed words contain supportive information. The peaks of Sampling Shapley appear later than those of Leave-one-out, indicating Sampling Shapley can capture more uncertain words. The curves of Sampling Shapley decline slower than those of Leave-one-out, meaning Sampling Shapley is less likely to identify informative words as uncertain words.

Removing uncertain words maintains major semantic similarity. We define the number of words deleted till prediction confidence reaches the peak as the Maximum Uncertain Words (MUW). We check the semantic similarity (SIM) between the original inputs and the reduced inputs with MUW words removed via Universal Sentence Encoder (USE) (Cer et al., 2018). The MUW and SIM of different models are in Table 3. The reduced inputs maintain major semantic meaning of the original inputs, which means they are not potential adversaries that trigger models to make over-confident predictions.

4.3 Visualizations

Table 2 shows the top 5 uncertain tokens identified by Leave-one-out or Sampling Shapley on IMDB/Yelp datasets (see full results in Table 6 in Appendix A.3). Most uncertain words do not have specific meaning (e.g. stop words), containing redundant information. Some contain noisy information, such as negations (e.g. “not”) or sentiment words (e.g. “great” and “awesome” in Yelp). This indicates that the knowledge (e.g. sentiment words) a model learns from in-domain datasets (e.g. IMDB) still influences its predictions on out-of-domain datasets (e.g. Yelp).

Table 7 in Appendix A.3 visualizes the generated explanations by Leave-one-out and Sampling Shapley. The identified uncertain words can confuse model predictions, such as positive words “delicious”, “great” in the negative Yelp review, and overlapped words “she”, “notes” in the contradicted MNLI example. Removing uncertain words helps improve model prediction confidence.

5 Conclusion

In this paper, we propose to explain uncertain predictions of two pre-trained language models, BERT and RoBERTa, which are post-calibrated. We adapt two methods, Leave-one-out and Sampling Shapley, successfully identifying the words in inputs that cause model prediction uncertainty. Experiments show that detecting and deleting uncertain words can improve model prediction confidence on both in-domain and out-of-domain datasets.
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Datasets | C | L | #train | #dev | #test
--- | --- | --- | --- | --- | ---
IMDB | 2 | 268 | 20000 | 5000 | 25000
Yelp | 2 | 138 | 50000 | 60000 | 38000
SNLI | 3 | 14 | 549367 | 4921 | 4921
MNLI | 3 | 22 | 391176 | 4772 | 4907
QQP | 2 | 11 | 363176 | 20207 | 20215
TPPDB | 2 | 15 | 42200 | 4685 | 4649

Table 4: Summary statistics of the datasets, where C is the number of classes, L is average sentence length, and # counts the number of examples in the train/dev/test sets.

A. Supplement of Experiments

A.1 Models and Datasets

We adopt the pretrained BERT-base and RoBERTa-base models from Hugging Face\textsuperscript{1}. For sentiment classification, we utilize movie reviews IMDB (Maas et al., 2011) as the in-domain dataset and Yelp reviews (Zhang et al., 2015) as the out-of-domain dataset. For natural language inference, the task is to predict the semantic relationship between a premise and a hypothesis as entailment, contradiction, or neutral. The Stanford Natural Language Inference (SNLI) corpus (Bowman et al., 2015) and Multi-Genre Natural Language Inference (MNLI) (Williams et al., 2018) are used as the in-domain and out-of-domain datasets respectively. The task of paraphrase identification is to judge whether two input texts are semantically equivalent or not. We adopt the Quora Question Pairs (QQP) (Iyer et al., 2017) as the in-domain dataset, while using the TwitterPPDB (TPPDB) (Lan et al., 2017) as the out-of-domain dataset. Table 4 shows the statistics of the datasets.

A.2 Expected Calibration Error

The Expected Calibration Error (ECE) (Guo et al., 2017) measures the difference between prediction confidence and accuracy, i.e.

\[
ECE = \sum_{k=1}^{K} \frac{|B_k|}{n} |acc(B_k) - conf(B_k)|, \tag{3}
\]

where the total n predictions are partitioned into K equally-spaced bins, B_k represents the predictions fall into the kth bin, acc(·) and conf(·) compute the average accuracy and confidence in each bin respectively. For a perfect calibration, acc(B_k) = conf(B_k), k ∈ {1, …, K}. In this work, we set K = 10.

A.3 Visualizations

\textsuperscript{1}\url{https://github.com/huggingface/pytorch-transformers}

| Models | In-domain | Out-of-domain |
| --- | --- | --- |
| BERT | | |
| T | 2.83 | 1.61 | 2.19 | 2.63 | 2.33 | 3.42 |
| pre-ECE | 8.03 | 7.49 | 8.09 | 10.20 | 21.62 | 12.38 |
| post-ECE | 3.54 | 3.20 | 3.80 | 4.19 | 4.88 | 7.17 |

| RoBERTa | | |
| T | 2.43 | 1.88 | 2.49 | 2.18 | 2.47 | 3.71 |
| pre-ECE | 6.50 | 7.11 | 7.99 | 6.82 | 18.56 | 13.52 |
| post-ECE | 3.10 | 2.30 | 4.26 | 2.17 | 3.28 | 8.19 |

Table 5: Post-hoc calibration results. T is the learned temperature. pre-ECE and post-ECE represent the ECEs on test sets before and after calibration respectively.
Table 6: Top 5 uncertain tokens identified by Leave-one-out or Sampling Shapley for different models on different datasets.

| Models/Dataset | Method          | Prediction      | Explanation                                                                                           |
|----------------|-----------------|-----------------|-------------------------------------------------------------------------------------------------------|
| BERT/IMDB      | Leave-one-out   | Positive (0.67 → 0.90) | i could not believe how well this kid did on screen you will completely forget that they are actors and loose yourself in the movie it is like watching home movies with a twist i recomend this to everyone highly |
| RoBERTa/Yelp   | Sampling Shapley| Negative (0.71 → 0.90) | i was hoping the previous reviewer had merely had a bad stay and or the property had updated since then but no such luck n n the beds here are rocks it felt like i was sleeping on a box spring instead of a mattress and a really had and painful one at that when we got up in the morning that phrase in quotations as it implies we had a good night’s sleep which we didn’t my husband pointed out that the side of the mattress was slumping so it was probably very old definitely not marriott standard n n wireless internet was slow but a cat 5 was provided in the room for laptops that got internet up to speed just fine n n break fast when i had it was good perhaps previous reviewer came down late a little on the crowded side but the biscuits were delicious n n all in all the stay was great except for the beds but unfortunately that’s a huge thing that needs to be good when you’re staying at a hotel sorry guys |
| RoBERTa/SNLI   | Leave-one-out   | Entailment (0.71 → 0.94) | A photographer with bushy dark hair takes a photo of a skate boarder at an indoor park . The person with the camera photographs the person skating . |
| BERT/MNLI      | Sampling Shapley| Contradiction (0.73 → 0.93) | i ’ ve got it down in my notes if you want to see them . ” she extended the woven cords . she found it impossible to share her notes with anyone . |
| BERT/QQP       | Leave-one-out   | Nonparaphrases (0.76 → 0.96) | can india and pakistan be friends ? why should india and pakistan be friends ? |
| RoBERTa/TPPDB  | Sampling Shapley| Nonparaphrases (0.76 → 0.92) | How to take great vacation photos , no fancy camera required . New York Times Most Viewed Stories How to Take Great Vacation Photos |

Table 7: Visualizations of uncertainty explanations for different models on different datasets, where prediction confidence changes are shown in brackets when uncertain words (in red color) are removed.