Latent Concept-based Explanation of NLP Models

WARNING: The appendix contains a few examples which may be disturbing to the reader

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Abstract

Interpreting and understanding the predictions made by deep learning models poses a formidable challenge due to their inherently opaque nature. Many previous efforts aimed at explaining these predictions rely on input features, specifically, the words within NLP models. However, such explanations are often less informative due to the discrete nature of these words and their lack of contextual verbosity. To address this limitation, we introduce the Latent Concept Attribution method (LACOAT), which generates explanations for predictions based on latent concepts. Our foundational intuition is that a word can exhibit multiple facets, contingent upon the context in which it is used. Therefore, given a word in context, the latent space derived from our training process reflects a specific facet of that word. LACOAT functions by mapping the representations of salient input words into the training latent space, allowing it to provide latent context-based explanations of the prediction.

1 Introduction

The opaqueness of deep neural network (DNN) models is a major challenge to ensuring a safe and trustworthy AI system. Extensive and diverse research works have attempted to interpret and explain these models. One major line of work strives to understand and explain the prediction of a neural network model using the attribution of input words to prediction [Sundararajan et al., 2017b, Denil et al., 2014].

However, the explanation based solely on input words is less informative due to the discrete nature of words and the lack of contextual verbosity. A word consists of multifaceted aspects such as semantic, morphological, and syntactic roles in a sentence. Consider the word "trump" in Figure 1. It has several facets such as a verb, a verb with specific semantics, and a named entity representing a certain aspect such as tower names, family names, etc. We argue that given various contexts of a word in the

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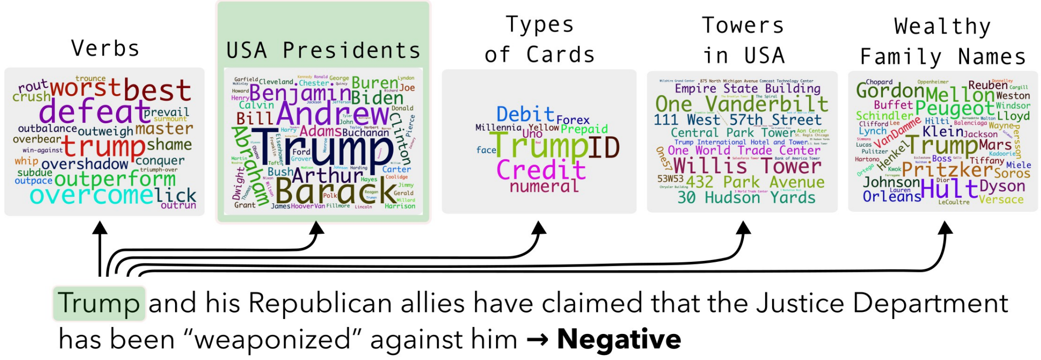


Figure 1: An example of various facets of word "trump"

training data, the model learns these diverse facets during training. Given a test instance, depending on the context a word appears, the model uses a particular facet of the input words in making the prediction. The explanation based on salient words alone does not reflect the facets of the word the model has used in the prediction and results in a less informed explanation.

Dalvi et al. [2022] showed that the latent space of DNNs represents the multifaceted aspects of words learned during training. The clustering of training data contextualized representations provides access to these multifaceted concepts, hereafter referred to as *latent concepts*. Given an input word in context at test time, we hypothesize that the alignment of its contextualized representation to a latent concept represents the facet of the word being used by the model for that particular input. We further hypothesize that this latent concept serves as a correct and enriched explanation of the input word. To this end, we propose the LAtent COncept ATtribution (LACOAT) method that generates an explanation of a model's prediction using the latent concepts. LACOAT discovers latent concepts of every layer of the model by clustering contextualized representations of words in the training corpus. Given a test instance, it identifies the most salient input representations of every layer with respect to the prediction and dynamically maps them to the latent concepts of the training data. The shortlisted latent concepts serve as an explanation of the prediction. Lastly, LACOAT integrates a plausibility module that generates a human-friendly explanation of the latent concept-based explanation.

2 Methodology

LACOAT consists of the following four modules:

- The first module, ConceptDiscoverer, discovers latent concepts of a model given a corpus.
- PredictionAttributor, the second module, selects the most salient words (along with their contextual representations) in a sentence with respect to the model's prediction.
- Thirdly, ConceptMapper, maps the representations of the salient words to the latent concepts discovered by ConceptDiscoverer and provides a latent concept-based explanation.
- PlausiFyer takes a latent concept explanation as input and generates a plausible and human-understandable explanation of the prediction.

Consider a sentiment classification dataset and a sentiment classification model as an example. LACOAT works as follows: ConceptDiscoverer takes the training dataset and the model as input and outputs latent concepts of the model. At test time, given an input sentence, PredictionAttributor identifies the most salient input representations with respect to the prediction. ConceptMapper maps these salient input representations to the training data latent concepts and provides them as an explanation of the prediction. PlausiFyer takes the test sentence and its concept-based explanation and generates a human-friendly and insightful explanation of the prediction.

Consider $\mathbb{M}$ represents the DNN model being interpreted, with L layers, each of size H. Let $\overrightarrow{z}_{w_i}$ be the *contextual representation* of a word w_i in an input sentence $\{w_1, w_2, ..., w_i, ...\}$. The representation can belong to any particular layer in the model, and LACOAT will generate explanations with respect to that layer.

2.1 ConceptDiscoverer

The words are grouped in the high-dimensional space based on various latent relations such as semantic, morphology and syntax [Mikolov et al., 2013, Reif et al., 2019]. With the inclusion of context i.e. contextualized representations, these groupings evolve into dynamically formed clusters representing a unique facet of the words called *latent concept* [Dalvi et al., 2022]. Figure 1 shows a few examples of latent concepts that capture different facets of the word "trump".

The goal of ConceptDiscoverer is to discover latent concepts given a model $\mathbb{M}$ and a dataset $\mathbb{D}$. We follow an identical procedure to Dalvi et al. [2022] to discover latent concepts. Specifically, for every word w_i in $\mathbb{D}$, we extract contextual representations $\overrightarrow{z}_{w_i}$. We then cluster these representations using agglomerative hierarchical clustering [Gowda and Krishna, 1978]. The distance between any two representations is computed using the squared Euclidean distance, and Ward's minimum variance criterion is used to minimize total within-cluster variance.

Each cluster represents a latent concept. Let $\mathcal{C} = C_1, C_2, ..., C_K$ represents the set of latent concepts extracted by ConceptDiscoverer, where each $C_i = w_1, w_2, ...$ is a set of words in a particular context. For sequence classification tasks, we also consider the [CLS] token (or a representative classification token) from each sentence in the dataset as a "word" and discover the latent concepts. In this case, a latent concept may consist of words only, [CLS] tokens only, or a mix of both.

2.2 PredictionAttributor

Given an input instance s, the goal of PredictionAttributor is to extract salient input representations with respect to the prediction p from model $\mathbb{M}$. Gradient-based methods have been effectively used to compute the saliency of the input features for the given prediction, such as pure Gradient [Simonyan et al., 2014], Input x Gradient [Shrikumar et al., 2017] and Integrated Gradients (IG) [Sundararajan et al., 2017a]. In this work, we use IG as our gradient-based method as it is a well-established method from literature. However, LACOAT is agnostic to the choice of the attribution method, and any other method that identifies salient input representations can be used while keeping the rest of the pipeline unchanged.

Formally, we first use IG to get attribution scores for every token in the input s, and then select the top tokens that make up 50% of the total attribution mass (similar to top-P sampling).

2.3 ConceptMapper

At test time, given an input sentence PredictionAttributor provides the salient input representations. ConceptMapper maps each salient representation to a latent concept C_i of the training latent space. These latent concepts highlight a particular facet of the salient representations that is being used by the model and serve as an explanation of the prediction.

ConceptMapper uses a logistic regression classifier that maps a representation $\overrightarrow{z}_{w_i}$ to one of the K latent concepts. The model is trained using the representations of words from $\mathbb{D}$ that are used by ConceptDiscoverer as input features and the concept index (cluster id) as their label. Hence, for a concept C_i and a word $w_j \in C_i$, a training instance of the classifier is the input $x = \overrightarrow{z}_{w_j}$ and the output is $y = i$.

2.4 PlausiFyer

Interpreting latent concepts can be challenging due to the need for diverse knowledge, including linguistic, task-specific, worldly, and geographical expertise (as seen in Figure 1). PlausiFyer offers a user-friendly summary and explanation of the latent concept and its relationship to the input instance using a Large Language Model (LLM). Our intuition of natural language explanation is similar to Singh et al. [2023], however, we relied on latent concepts compared to most activated ngrams and the generation of synthetic data. Given an input sentence and the latent concept, we ask an LLM to explain the relationship between them. Due to space limitation, we present the prompts used for sequence labeling and classification tasks in App. C.

3 Experimental Setup

Data We use Parts-of-Speech (POS) Tagging, Toxicity classification (Toxicity), Sentiment Classification (Sentiment) and Natural Language Inference (NLI) tasks for our experiments. POS is a sequence labeling task while the other tasks are sequence classification tasks. We use the Penn TreeBank dataset [Marcus et al., 1993] for POS, Jigsaw Toxicity dataset [cjadams et al., 2017] for toxicity, the ERASER Movie Reviews dataset [Pang and Lee, 2004] for Sentiment and the MNLI dataset [Wang et al., 2019] for the NLI tasks. Appendix A provides the information about each dataset.

Models We fine-tune 12-layered pre-trained models; BERT-base-cased [Devlin et al., 2019], RoBERTa-base [Liu et al., 2019] and XLM-Roberta [Conneau et al., 2020] using the training datasets of the tasks considered. For Llama2-2-7b-chat-hf [Touvron et al., 2023], we use the base model without finetuning with zero-shot prompting for each task. We use *transformers* [Wolf et al., 2020] with the default settings and hyperparameters. Task-wise performance of the models is provided in App B. Tables 3, 4, 5, and 6.

Module-specific hyperparameters When extracting the activation and/or attribution of a word, we average the respective value over the word's subword units. We optimize the number of clusters K for each dataset as suggested by Dalvi et al. [2022]. We use $K = 600$ (POS, Toxicity) and $K = 400$ (Sentiment, MNLI) for `ConceptDiscoverer`.

Since the number of words in $\mathbb{D}$ can be very high, and the clustering algorithm is limited by the number of representations it can efficiently cluster, we filter out words with frequencies less than 5 and randomly select 20 contextual occurrences of every word with the assumption that a word may have a maximum of 20 facets. These settings are in line with Dalvi et al. [2022]. In the case of `[CLS]` tokens, we keep all of the instances.

We use a zero-vector as the baseline vector in `PredictionAttributor`'s IG, using 500 approximation steps. For `ConceptMapper`, we use the cross-entropy loss with L2 regularization and train the classifier with 'lbfgs' solver and 100 maximum iterations. To optimize the classifier and to evaluate its performance, we split the dataset $\mathcal{D}$ into train (90%) and test (10%). `ConceptMapper` used in the `LACOAT` pipeline is trained using the full dataset $\mathcal{D}$. Finally, for `PlausiFyer`, we use ChatGPT with a `temperature` of 0 and a `top_p` value of 0.95.

4 Evaluation

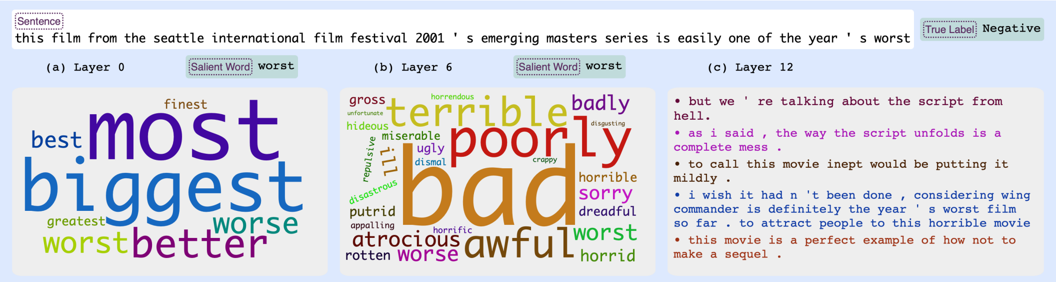
We perform a qualitative evaluation, a human evaluation, and a module-level evaluation of `LACOAT` to measure its correctness and efficacy. Due to space limitations, we mainly present the results of the qualitative evaluation and faithfulness evaluation. The human evaluation and the module-level evaluation of `LACOAT` is provided in Appendix E and F. Also, the full set of results for all tasks are presented in Apps. D, G, H, I.

4.1 Qualitative Evaluation

In this section, we qualitatively evaluate the usefulness of the latent concept-based explanation and the generated human-friendly explanation.

4.1.1 Evolution of Concepts

`LACOAT` generates the explanation for each layer with respect to a prediction, which shows the evolution of concepts in making the prediction. Figure 2 shows layers 0, 6 and 12's latent concept of the most attributed input token for RoBERTa fine-tuned on the sentiment task. We found that the initial layer latent concepts do not always align with the sentiment of the input instance and may represent a general language concept. Figure 2(a) shows the concept of comparative and superlative adjectives of both positive and negative sentiments. In the middle layers, the latent concepts evolved into concepts that align better with the sentiment of the input sentence. The latent concept of Figure 2(b) shows a mix of adjectives and adverbs of negative sentiment. In the sentiment task, the most attributed word in the last layer is `[CLS]` which resulted in latent concepts consisting of `[CLS]` representations of the



Sentence
this film from the seattle international film festival 2001 ' s emerging masters series is easily one of the year ' s worst

True Label Negative

(a) Layer 0 Salient Word worst

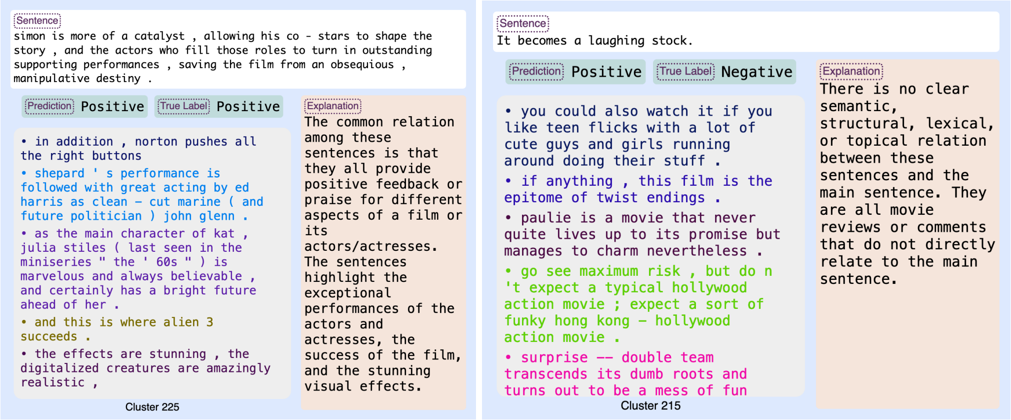
(b) Layer 6 Salient Word worst

(c) Layer 12

- but we ' re talking about the script from hell.
- as i said , the way the script unfolds is a complete mess .
- to call this movie inept would be putting it mildly .
- i wish it had n 't been done , considering wing commander is definitely the year ' s worst film so far . to attract people to this horrible movie
- this movie is a perfect example of how not to make a sequel .

Figure 2: Sentiment task: Latent concepts of the most attributed words in Layers 0, 6 and 12

most related sentences to the input. We randomly pick five [CLS] instances from the latent concept and show their corresponding sentences in the figure (see Figure 2(c)). We found that the last layer's latent concepts are best aligned with the input instance and its prediction and are the most informative explanation of the prediction. Then, we deepen our analysis of the explanations generated using the last layer only.



Sentence
simon is more of a catalyst , allowing his co - stars to shape the story , and the actors who fill those roles to turn in outstanding supporting performances , saving the film from an obsequious , manipulative destiny .

Prediction Positive True Label Positive

- in addition , norton pushes all the right buttons
- shepard ' s performance is followed with great acting by ed harris as clean – cut marine (and future politician) john glenn .
- as the main character of kat , julia stiles (last seen in the miniseries " the ' 60s ") is marvelous and always believable , and certainly has a bright future ahead of her .
- and this is where alien 3 succeeds .
- the effects are stunning , the digitalized creatures are amazingly realistic ,

Cluster 225

Explanation
The common relation among these sentences is that they all provide positive feedback or praise for different aspects of a film or its actors/actresses. The sentences highlight the exceptional performances of the actors and actresses, the success of the film, and the stunning visual effects.

(a) Sentiment: A positive labeled test instance correctly predicted by the model.

Sentence
It becomes a laughing stock.

Prediction Positive True Label Negative

- you could also watch it if you like teen flicks with a lot of cute guys and girls running around doing their stuff .
- if anything , this film is the epitome of twist endings .
- paulie is a movie that never quite lives up to its promise but manages to charm nevertheless .
- go see maximum risk , but do n 't expect a typical hollywood action movie ; expect a sort of funky hong kong – hollywood action movie .
- surprise -- double team transcends its dumb roots and turns out to be a mess of fun

Cluster 215

Explanation
There is no clear semantic, structural, lexical, or topical relation between these sentences and the main sentence. They are all movie reviews or comments that do not directly relate to the main sentence.

(b) Sentiment: A negatively labeled test instance that is incorrectly predicted as positive.

Figure 3: A few examples of LACOAT explanations for BERT using Sentiment task

4.1.2 Analyzing Last Layer Explanations

Correct prediction with correct gold label Figure 3a presents a case of correct prediction with latent-concept explanation and human-friendly explanation. In the case of sentence-level latent concepts (Figure 3a), it is harder to interpret compared to latent concepts consisting of words. However, PlausiFyer still highlights additional information about the relation between the latent concept and the input sentence. For example, it captures that the reason of positive sentiment in 3a is due to praising different aspects of a film and its actors and actresses.

Wrong prediction with correct gold label Figure 3b shows the predicted label is wrong. The input sentence has a negative sentiment but the model predicted it as positive. The instances of latent concepts show sentences with mixed sentiments such as "manages to charm" is positive, and "never quite lives up to its promise" is negative. This provides the domain expert an evidence of a possible wrong prediction. The PlausiFyer's *explanation* is even more helpful as it clearly states that "there is no clear ... relation between these sentences ...".

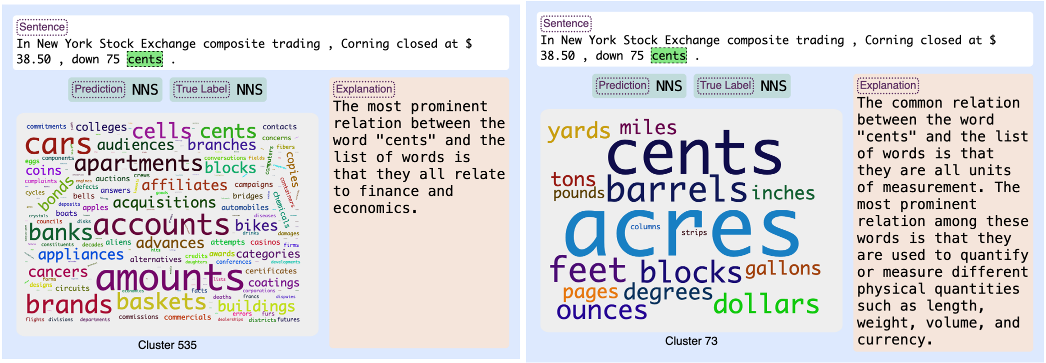
To study how the explanation would change if it is a correct prediction, we employ TextAttack [Morris et al., 2020] to create an adversarial example of the sentence in Figure 3b that flips its prediction. The new sentence replaces "laughing" with "kidding" which has a similar meaning but flipped the prediction to a correct prediction. Figure 7 in the appendix shows the full explanation of the augmented sentence. With the correct prediction, the latent concept changed and the *explanation*

		Faithfulness Metrics	
Dataset	Setting	Accuracy	% Label Flip
Sentiment	**Original**	96.31	-
	LACOAT	55.91	43.98
	Random	96.09	0.14
Toxicity	**Original**	91.55	-
	LACOAT	51.78	46.44
	Random	91.93	0.13
MNLI	**Original**	87.69	-
	LACOAT	82.08	8.83
	Random	88.12	0.55

Table 1: Faithfulness evaluation using the RoBERTa model. *Original* refers to the model's performance without any manipulation, *LACOAT* represents the performance after subtracting the most salient latent concept vector from the [CLS] vector, and Random is the average performance of the model after subtracting five random vectors from the [CLS] vector.

clearly expresses a negative sentiment "... all express negative opinions and criticisms ..." compared to the explanation of the wrongly predicted sentence.

Cross model analysis LACOAT provides an opportunity to compare various models in terms of how they learned and structured the knowledge of a task. Figure 4 compares the explanation of RoBERTa (4a) and XLMR (4b) for identical inputs. Both models predicted the correct label. However, their latent concept based explanation is substantially different. RoBERTa's explanation shows a large and diverse concept where many words are related to finance and economics. The XLMR's latent concept is rather a small focused concept where the majority of tokens are units of measurement. It is worth noting that both models are fine-tuned on identical data.


Sentence
In New York Stock Exchange composite trading , Corning closed at $ 38.50 , down 75 cents .

Prediction NNS
True Label NNS

Explanation
The most prominent relation between the word "cents" and the list of words is that they all relate to finance and economics.

(a) Explanation of the RoBERTa model

Sentence
In New York Stock Exchange composite trading , Corning closed at $ 38.50 , down 75 cents .

Prediction NNS
True Label NNS

Explanation
The common relation between the word "cents" and the list of words is that they are all units of measurement. The most prominent relation among these words is that they are used to quantify or measure different physical quantities such as length, weight, volume, and currency.

(b) Explanation of the XLMR model

Figure 4: Comparing explanation of RoBERTa and XLMR

4.2 Faithfulness Evaluation

We consider a salient latent concept highlighted by LACOAT to be faithful to the prediction if the ablation of that latent concept causes a change in prediction performance. We define ablation of a latent concept as removing the information of that latent concept from the prediction vector i.e. [CLS]. We calculate the vector of a latent concept by averaging the training representations that belong to the latent concept. At inference time, we ablate the most salient latent concept for a prediction by subtracting the latent concept vector from the [CLS] representation of the last layer and then perform the prediction. The prediction change represents the percentage of predictions that were altered after the manipulation. As a baseline, we manipulate using a random vector of the same magnitude to that of the salient latent concept vector and report the change in prediction.

Table 1 reports the model's accuracy and the percentage of altered predictions across all metrics. The results show that manipulating the `[CLS]` token representation using the LACOAT vector leads to significant performance drops and prediction changes across all datasets. In contrast, random vector manipulations have minimal impact on the model's performance and predictions. These findings suggest that the LACOAT vector plays a crucial role in the model's decision-making process. Comparing the results across different datasets, MNLI shows a relatively smaller drop in accuracy when manipulating the salient latent concept vector. We suspect this is due to the nature of the MNLI task, which requires reasoning over multiple sentences, with relevant information spread across multiple latent concepts. Nevertheless, the difference in results between the original accuracy and random vector confirms our hypothesis about the faithfulness of latent concepts.

5 Related work

The explainability methods can be approached by local explanations and global explanations targeting post-hoc analysis or introducing interpretability in the architecture [Madsen et al., 2023, Sundararajan et al., 2017b, Denil et al., 2014, Selvaraju et al., 2020, Kapishnikov et al., 2021, Zhao and Aletras, 2023, Kim et al., 2018, Ghorbani et al., 2019, Jourdan et al., 2023, Zhao et al., 2023, Ribeiro et al., 2016, Rajagopal et al., 2021]. Lyu et al. [2023] provides a survey of explainability methods in NLP. `LACOAT` is a local explanation method providing post-hoc explanations given an input instance. One of the common ways for local explanations is to interpret the model prediction based on the input features. However, such an explanation lacks contextual verbosity and it could not interpret the multifaceted roles of the input features.

Previous work attempted to explain and interpret NLP models using human-defined concepts [Kim et al., 2018, Abraham et al., 2022] and concepts extracted from hidden representations [Zhao et al., 2023, Ghorbani et al., 2019, Rajani et al., 2020, Geva et al., 2022]. Zhao et al. [2023], Kim et al. [2018] worked on the global explanation based on a surrogate model. We provide local explanations and we ensure the faithfulness of latent concepts by extracting them directly from the hidden representation without any supervised training. Rajani et al. [2020] used k-nearest neighbors of the training data to identify erroneous correlations and misclassified instances. Dalvi et al. [2022] analyzed latent concepts in their ability to represent linguistic knowledge. Our `ConceptDiscoverer` module is motivated by them. However, we propose a method to explain a model's prediction using latent concepts.

6 Conclusion

We presented `LACOAT` that provides a human-friendly explanation of a model's prediction. The qualitative evaluation and human evaluation showed that `LACOAT` explanations are insightful in explaining a correct prediction, in highlighting a wrong prediction and in comparing the explanations of models. The reliance on training data latent space enables interpreting how knowledge is structured in the network. Similarly, it enables the study of the evolution of predictions across layers. `LACOAT` promises human-in-the-loop in the decision-making process and is a step towards trust in AI. We discuss the limitations in App. J.

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A Datasets

B Finetuning Performance

We tuned several transformers BERT-base-cased, RoBERTa and XLM-RoBERTa. We used standard splits for training, development and test data that we used to carry out our analysis. The splits to preprocess the data are available through git repository[1]. See Table 3, Table 4, Table 5, and Table 6 for statistics and classifier accuracy.

[1] `https://github.com/nelson-liu/contextual-repr-analysis`

Table 2: The data statistics of each dataset used in the evaluation experiments and the number of tags to be predicted. POS [Marcus et al., 1993], Jigsaw Toxicity dataset [cjadams et al., 2017], the ERASER Sentiment dataset [Pang and Lee, 2004, Zaidan and Eisner, 2008] and the MNLI dataset [Wang et al., 2019]

Task	Train	Dev	Tags
Sentiment	13878	856	2
POS	36557	1802	48
Toxicity	9000	800	2
MNLI	9000	1200	3

Table 3: The fine-tuned performance of models, data statistics (number of sentences) on training, development, and test sets used in the finetuning, and the number of tags to be predicted for the POS tagging task. Model: BERT, RoBERTa, XLM-R

Task	Train	Dev	Test	Tags	BERT	RoBERTa	XLM-R
POS	36557	1802	1963	48	96.81	96.70	96.75

Table 4: The fine-tuned performance of models, data statistics (number of sentences) on training, development, and test sets used in the finetuning, and the number of tags to be predicted for the sentiment classification task. Model: BERT, RoBERTa, XLM-R

Task	Train	Dev	Test	Tags	BERT	RoBERTa	XLM-R
Sentiment	13878	1516	2726	2	94.53	96.31	93.80

Table 5: The fine-tuned performance of models, data statistics (number of sentences) on training, development, and test sets used in the finetuning, and the number of tags to be predicted for the toxicity classification task. Model: BERT, RoBERTa, XLM-R

Task	Train	Dev	Test	Tags	BERT	RoBERTa	XLM-R
Toxicity	159570	63977	89185	2	91.53	91.55	91.53

Table 6: The fine-tuned performance of models, data statistics (number of sentences) on training, development, and test sets used in the finetunings, and the number of tags to be predicted for the MNLI task. Model: BERT, RoBERTa, XLM-R

Task	Train	Dev	Test	Tags	BERT	RoBERTa	XLM-R
MNLI	393000	19650	19650	3	84.00	87.69	84.54

C Task-specific Prompts used with `PlausiFyer`

We use the following prompt for the sequence classification task:

```
Do you find any common semantic, structural, lexical and topical relation between
these sentences with the main sentence? Give a more specific and concise summary
about the most prominent relation among these sentences.

main sentence: {sentence}
{sentences}
No talk, just go.
```

and the following prompt for the sequence labeling task:

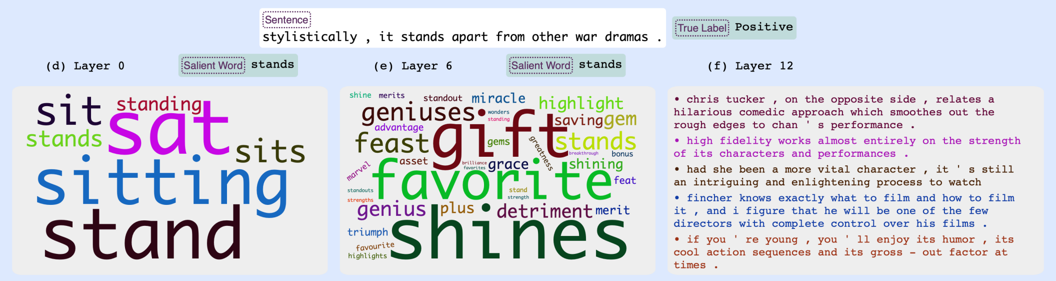
```
Do you find any common semantic, structural, lexical and topical relation between
the word highlighted in the sentence (enclosed in [[ ]]) and the following list
of words? Give a more specific and concise summary about the most prominent
relation among these words.

Sentence: {sentence}
List of words: {words}
Answer concisely and to the point.
```

We did not provide the prediction or the gold label to LLM to avoid biasing the explanation.

D Qualitative Evaluation - More Examples in POS tagging and sentiment classification tasks

D.1 Example for the Evolution of Concepts

Figure 5 presents the other example of latent concepts of the salient words in layers 0, 6, and 12. Similarly to the example shown in Figure 2, the latent concept of this example shows that the different forms of the verb "sit" are not aligned with its usage in the input instance. The concept in the middle layer aligns better with the sentiment of the input sentence (Figure 5(b)). Most words of layer 6's latent concept match the sentiment of the input sentence. We also randomly pick five [CLS] instances from the latent concept and show their corresponding sentences in the figure (see Figure 5(c)). The concept of the last layer is best aligned with the input sentence.



stylistically , it stands apart from other war dramas .

- chris tucker , on the opposite side , relates a hilarious comedic approach which smoothes out the rough edges to chan ' s performance .
- high fidelity works almost entirely on the strength of its characters and performances .
- had she been a more vital character , it ' s still an intriguing and enlightening process to watch
- fincher knows exactly what to film and how to film it , and i figure that he will be one of the few directors with complete control over his films .
- if you ' re young , you ' ll enjoy its humor , its cool action sequences and its gross - out factor at times .

Figure 5: Sentiment task: Examples of the latent concepts of the most attributed words in layers 0, 6 and 12

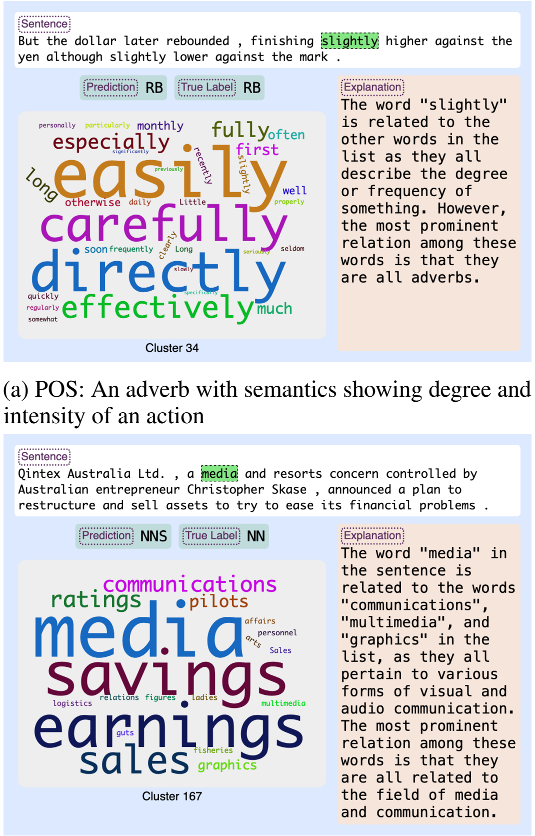
D.2 Example for the last layer explanation analyzing

Correct prediction with correct gold label Figure 6a shows a correct prediction case in POS tagging task. PlausiFyer discovers relation between the latent concept and the input sentence. For example, it captures that the adverbs in Figure* have common semantics of showing degree or frequency.

Wrong prediction with correct gold label Figure 6b presents a wrong prediction case. The prediction is Noun; however, the the majority of words in the latent concepts are plural Nouns, giving evidence of a possibly wrong prediction. In addition, the *explanation* did not capture any morphological relationship between the concept and the input word.

Adversarial Example of the Sentence in Figure 3b The augmented sentence has a similar meaning word "kidding" instead of "laughing" (See Figure 7). The predicted label of the sentence becomes Positive, which is matched to the gold label. The latent concept of the "kidding" is more aligned with the sentence than the original one.

Correct Predicted Label with Incorrect Gold Label The automatic labeling of latent concepts based on the model's class provides an opportunity to analyze the wrong predictions of the model with respect to the concept labels. We specifically observe the wrong predictions of test instances. We discovered that many of the wrong prediction cases were not caused by misclassification of the



Sentence

But the dollar later rebounded , finishing slightly higher against the yen although slightly lower against the mark .

Prediction RB

True Label RB

Explanation

The word "slightly" is related to the other words in the list as they all describe the degree or frequency of something. However, the most prominent relation among these words is that they are all adverbs.

(a) POS: An adverb with semantics showing degree and intensity of an action

Sentence

Qintex Australia Ltd. , a media and resorts concern controlled by Australian entrepreneur Christopher Skase , announced a plan to restructure and sell assets to try to ease its financial problems .

Prediction NNS

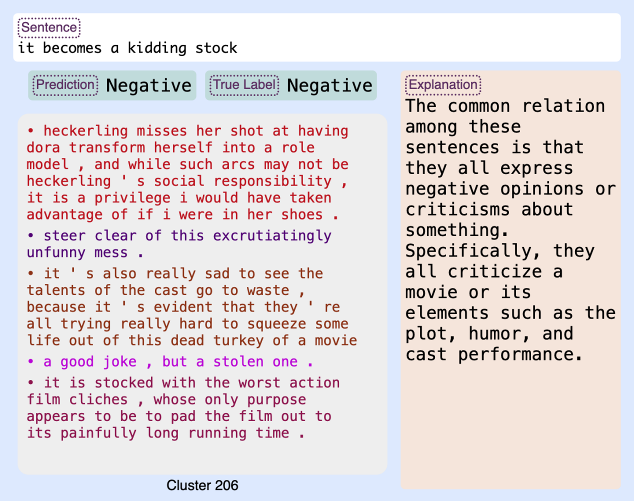
True Label NN

Explanation

The word "media" in the sentence is related to the words "communications", "multimedia", and "graphics" in the list, as they all pertain to various forms of visual and audio communication. The most prominent relation among these words is that they are all related to the field of media and communication.

(b) POS: An incorrect prediction that can be detected from the latent concept

Figure 6: A few examples of LACOAT explanations for BERT using POS tasks



Sentence

it becomes a kidding stock

Prediction Negative

True Label Negative

- heckerling misses her shot at having dora transform herself into a role model , and while such arcs may not be heckerling ' s social responsibility , it is a privilege i would have taken advantage of if i were in her shoes .
- steer clear of this excrutiatingly unfunny mess .
- it ' s also really sad to see the talents of the cast go to waste , because it ' s evident that they ' re all trying really hard to squeeze some life out of this dead turkey of a movie
- a good joke , but a stolen one .
- it is stocked with the worst action film cliches , whose only purpose appears to be to pad the film out to its painfully long running time .

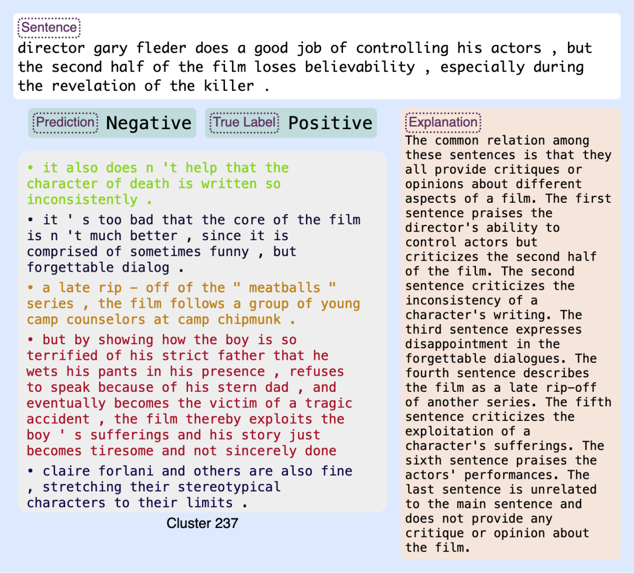
Cluster 206

Explanation

The common relation among these sentences is that they all express negative opinions or criticisms about something. Specifically, they all criticize a movie or its elements such as the plot, humor, and cast performance.

Figure 7: An augmented example for the test instance in Figures 3b: The augmented sentence replaced the “laughing” with “kidding” which has a similar meaning. The label of the augmented sentence becomes positive, which is matched with the gold label. The new predicted latent concept is more closely aligned with the main sentence. The model may not learn the implicit meaning of the “laughing stock” in the sentence.

models but were due to the fact that the gold label was annotated incorrectly. Figure 8 shows an


Sentence

director gary fleder does a good job of controlling his actors , but the second half of the film loses believability , especially during the revelation of the killer .

Prediction Negative

True Label Positive

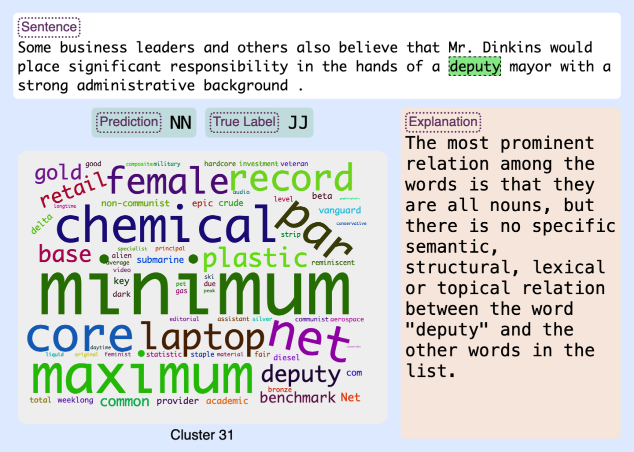
- it also does n 't help that the character of death is written so inconsistently .
- it ' s too bad that the core of the film is n 't much better , since it is comprised of sometimes funny , but forgettable dialog .
- a late rip – off of the " meatballs " series , the film follows a group of young camp counselors at camp chipmunk .
- but by showing how the boy is so terrified of his strict father that he wets his pants in his presence , refuses to speak because of his stern dad , and eventually becomes the victim of a tragic accident , the film thereby exploits the boy ' s sufferings and his story just becomes tiresome and not sincerely done
- claire forlani and others are also fine , stretching their stereotypical characters to their limits .

Cluster 237

Explanation

The common relation among these sentences is that they all provide critiques or opinions about different aspects of a film. The first sentence praises the director's ability to control actors but criticizes the second half of the film. The second sentence criticizes the inconsistency of a character's writing. The third sentence expresses disappointment in the forgettable dialogues. The fourth sentence describes the film as a late rip-off of another series. The fifth sentence criticizes the exploitation of a character's sufferings. The sixth sentence praises the actors' performances. The last sentence is unrelated to the main sentence and does not provide any critique or opinion about the film.

Figure 8: A correct prediction but incorrect gold label: The test instance emphasizes the movie's shortcomings and uses the word "especially" to highlight the flaws. The explanation is rather long but it correctly highlights that the sentences are about "critiques or opinions"


Sentence

Some business leaders and others also believe that Mr. Dinkins would place significant responsibility in the hands of a deputy mayor with a strong administrative background .

Prediction NN

True Label JJ

Cluster 31

Explanation

The most prominent relation among the words is that they are all nouns, but there is no specific semantic, structural, lexical or topical relation between the word "deputy" and the other words in the list.

Figure 9: An incorrect prediction (noun vs adjective) based on a latent concept made up of a mixture of nouns and adjectives: the "deputy" in this case is an adjective. The prediction aligns with a mixed cluster that contains both nouns and adjectives and the model may not learn to distinguish the "noun" and "adjective" in this case. The latent concept explanation is useful for the user to know that the model has used a mixed latent space for the prediction. The Explanation is rather wrong since it mentions that all these words are nouns.

example in which the main sentence and the explanation sentence share the same sentiment. We can see that the sentence provides critiques of the different aspects of the film. But the gold label of this sentence is positive. We think the gold label for this sentence is incorrect.

Incorrect Prediction in POS tagging Task Figure 9 presents an incorrect prediction in the POS tagging task. The prediction is aligned with a mixed concept that consists of nouns and adjectives. According to the latent concept explanation, we know that the model may not learn to distinguish the "noun" and "adjective", which causes the incorrect prediction.

E Human Evaluation

We perform two human evaluations; one aimed at evaluating the usefulness of `LACOAT`'s explanation in understanding a prediction (`LACOAT` Effectiveness) and the other compares `LACOAT` with other explanation methods.

E.1 `LACOAT` Effectiveness

We conduct a human evaluation using four annotators across 50 test samples. Specifically, given an explanation (e.g. Figure 6), all annotators are asked to answer five questions (Q1-Q5) that aimed at evaluating the usefulness of `LACOAT`. We have four annotators across 100 test samples. Specifically, given an explanation (e.g. Figure 6), three annotators are asked to answer the following five questions:

1. Regardless of the prediction, can you see any relation between the original input and the concept used by the model? (Yes/No)
2. Given the prediction, does the *latent concept* help you understand why the model made that prediction? (Helps/Neutral/Hinders)
3. Given the prediction, does the *explanation* help you understand why the model made that prediction? (Helps/Neutral/Hinders)
4. Does the explanation *accurately* describe the latent concept? (Yes/No)
5. Is the explanation *relevant* to the task at hand? (Yes/No)

Q1 evaluates whether `LACOAT` attributes the correct concept to a given prediction, while *Q2* and *Q3* measure the efficacy of `LACOAT`'s output in helping a user understand the prediction. *Q4* and *Q5* evaluates the output of `PlausiFyer`. They specifically separate out the cases where the explanation was accurate but irrelevant to the task at hand.

Table 7 shows the consolidated labels by picking the majority label in case of Yes/No questions and averaging the annotations in case of the rest. The evaluation shows that the latent concept itself was not only relevant to the task at hand, but also helped the user understand the model's prediction. The results for the helpfulness of the explanation text were mixed, with the majority of the annotations stating that it did not help or hinder their process. However, upon inspection, we see that the explanation was mostly helpful in all the cases where the model made the correct prediction, and not helpful when the prediction was incorrect. Qualitatively analyzing the explanation text for incorrect prediction shows that `PlausiFyer` mostly outputs "There is no relationship between the sentences and the concepts", which was deemed as hindering by most of the annotators. While such an explanation may serve as an indicator of a potential problem in the prediction, improving the prompt may result in a response that is indicative of the issue with the prediction. We leave this exploration for the future. Table 7 also shows the agreement between the annotators using Fleiss' Kappa. Since not all samples were annotated by all annotators, we compute the average Fleiss' kappa of each annotator with the consolidated annotation. The agreement ranges from *Fair* to *Substantial* across the five questions.

E.2 Comparison with other Methods

Despite a number of explanation methods proposed in the literature, it is hard to draw a comparison between them due to the difference in granularity of explanation, type of explanation and the methodology used. We design a human evaluation, asking evaluators to give a score between 1 to 3 to each of three explanations generated by IG, `LACOAT` and Cockatiel [Jourdan et al., 2023]. The annotation setup allows to rank multiple methods with the same usefulness rating. A total of

Table 7: **Top**: Consolidated label distribution for Q1-Q5. Fleiss' κ scores are computed by averaging each annotator with the consolidated annotation. The consolidated labels and agreement scores are shown for all the samples, as well as partitioned into those where the model prediction was correct/incorrect. **Bottom**: Percentage of samples where LACOAT is ranked similar or better than other methods. A* represents the average preference of LACOAT per annotator.

Top	Labels	Correct Samples	Incorrect Samples	All Samples	
				Annotation	Fleiss κ
Q1	Yes/No	28 / 0	20 / 2	48 / 2	0.35
Q2	Helps/Neutral/Hinders	27 / 1 / 0	17 / 5 / 0	44 / 6 / 0	0.41
Q3	Helps/Neutral/Hinders	16 / 10 / 2	1 / 19 / 2	17 / 29 / 4	0.61
Q4	Yes/No	17 / 11	5 / 17	22 / 28	0.47
Q5	Yes/No	17 / 11	6 / 16	23 / 27	0.80

Bottom	A1	A2	A3	A4	Consolidated	Average Cohen's κ
LACOAT ↑	85%	72%	77%	87%	89%	0.37

400 annotations were collected using four evaluators where each test instance is evaluated by all annotators. We ask four annotators to rank 100 samples where they see the original input, gold label, predicted label, and explanations by three methods: LACOAT, IG and COCKATIEL. LACOAT explanations are shown across three layers (layer 0, 6 and 12), while IG explanations are shown for layer 0 and COCKATIEL for layer 12. The annotators are asked to rank each method from 1 to 3 in terms of usefulness in understanding the reason for the prediction where 1 implies the method was very useful while 3 implies it was not useful. The annotation allows for the annotator to rank multiple methods with the same usefulness rating, e.g. for a particular sample, both LACOAT and COCKATIEL can have the rank 1. This setting is intentional since the output of explanation methods is not directly comparable to each other due to the difference in their design and the targeted form and granularity of explanation.

The second part of Table 7 shows the percentage of samples for which each of the annotators ranked LACOAT to be the same or better than both IG and Cockatiel. The consolidated ranking is computed by averaging the ranks across users. The average Cohen's κ indicates *Fair agreement* between each annotator and the consolidated ranking. The results show that LACOAT explanation is more useful in understanding the prediction compared to other methods. Also, the results suggested that LACOAT is preferred or equally preferred by all annotators. The average Cohen's κ further shows a "fair agreement" between annotators and the consolidated ranking where consolidated ranking is the average rank across users.

F Module Specific Evaluation

The correctness of LACOAT depends on the performance of each module it comprised off. The ideal way to evaluate the efficacy of these modules is to consider gold annotations. However, they are not available for any module. To mitigate this limitation, we design various constrained scenarios where certain assumptions can be made about the representations of the model. For example, the POS model optimizes POS tags so it is highly probable that the last layer representations form latent concepts that are a good representation of POS tags as suggested by various previous works [Kovaleva et al., 2019, Durrani et al., 2022]. One can assume that for `ConceptDiscoverer`, the last layer latent concepts will form groupings of words based on specific tags and for `PredictionAttributor`, the input word at the position of the predicted tag should reside in a latent concept that is dominated by the words with the same tag. In the following, we evaluate the correctness of these assumptions.

Latent Concept Annotation For the sake of evaluation, we annotated the latent concepts automatically using the class labels of each task. Given a latent concept, we annotate it with a certain class if more than 90% of the words in the latent concept belong to that class. In the case of POS, the latent concepts will be labeled with one of the 44 tags. For sentiment, the class labels, *Positive* and *Negative*, are at sentence level. We tag a latent concept as *Positive/Negative* if 90% of its tokens

Table 8: Number of clusters for each polarity: "Neg" for negative Label, "Pos" for positive, and "Mix" for mix label. The total number of clusters is 400.

	Sentiment								
	BERT			**RoBERTa**			**XLM-R**		
Layer	Neg	Pos	Mix	Neg	Pos	Mix	Neg	Pos	Mix
Layer 0	49	1	350	45	0	355	55	0	345
Layer 1	53	1	346	50	0	350	58	0	342
Layer 2	51	1	348	49	0	351	62	0	338
Layer 3	53	0	347	60	0	340	62	0	338
Layer 4	57	0	343	52	0	348	69	0	331
Layer 5	56	0	344	51	0	349	68	0	332
Layer 6	57	0	343	45	1	354	59	1	340
Layer 7	51	0	349	56	2	342	68	0	332
Layer 8	49	0	351	116	25	259	71	0	329
Layer 9	66	4	330	226	126	48	82	7	311
Layer 10	125	31	244	235	140	25	257	92	51
Layer 11	174	49	177	258	120	22	256	110	34
Layer 12	230	81	89	254	126	20	105	270	25

([CLS] or words) belong to sentences labeled as *Positive/Negative* in the training data. The latent concepts that do not fulfill the criteria of 90% for any class are annotated as *Mixed*.

F.1 `ConceptDiscoverer`

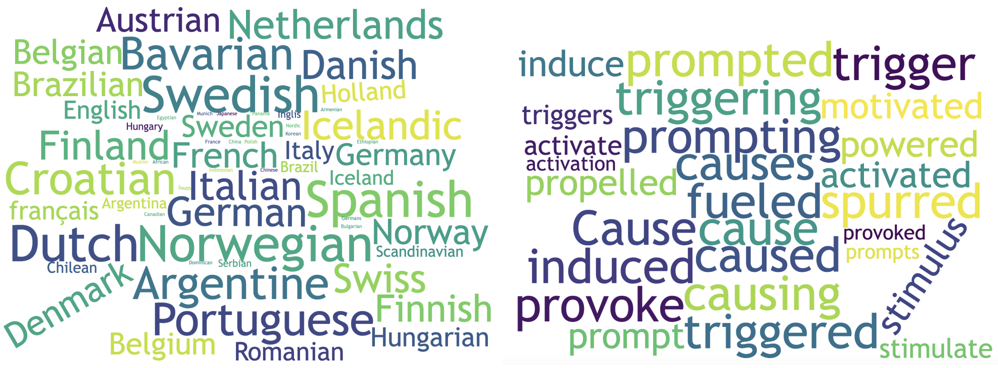
`ConceptDiscoverer` identifies latent concepts by clustering the representation. We question whether the discovered latent concepts are a true reflection of the properties that a representation possesses. Using `ConceptDiscoverer`, we form latent concepts of the last layer and automatically annotate them as described above. We found 87%, 83% and 86% of the latent concepts of BERT, RoBERTa and XLMR that perfectly map to a POS tag respectively. We further analyzed other concepts where 90% of the words did not belong to a single tag. We found them to be of compositional nature i.e. a concept consisting of related semantics like a mix of adjectives and proper nouns about countries such as Swedish and Sweden (App. Figure 10). For sentiment, we found 78%, 95%, and 94% of the latent concepts of BERT, RoBERTa, and XLMR to consist of either Positive or Negative sentences. The high number of class-based clusters of RoBERTa and XLMR show that at the 12th layer, the majority of their latent space is separated based on these two classes (see Table 8 for detailed results).

We also found that the concepts are not always formed aligning to the output class. Some concepts are formed by combining words from different classes. For example in Figure 10a, the concept is composed of nouns (specifically countries) and adjectives that modify these country nouns. Similarly, Figure 10b describes a concept composed of different forms of verbs.

Moreover, Table 8 provides the number of clusters for each polarity in the sentiment classification task. It shows that the majority of latent concepts are class-based clusters at the last layer for the BERT, RoBERTa, and XLMR models.

Table 9: Accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept.

	POS		Sentiment	
Layers	BERT	RoBERTa	BERT	RoBERTa
9	92.38	86.97	31.94	99.59
10	92.79	89.64	99.57	99.69
11	93.39	89.95	99.71	99.48
12	93.95	90.04	99.25	99.27



(a) (b)

Figure 10: Compositional concepts: (a) A cluster representing countries (NNP) and their adjectives (JJ), (b) Different form of verbs (Gerunds, Present and Past participles).

Table 10: Saliency-based method (95%): accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept in the POS tagging task. Model: BERT-base-cased, RoBERT-base, XLM-R

	POS		
Layer	BERT	RoBERTa	XLM-R
Layer 0	13.76	11.13	11.97
Layer 1	12.75	13.58	11.91
Layer 2	15.51	15.60	12.99
Layer 3	17.61	17.25	22.88
Layer 4	23.81	20.30	32.08
Layer 5	37.03	23.28	48.44
Layer 6	64.83	32.52	67.94
Layer 7	77.90	48.61	80.11
Layer 8	86.96	73.88	85.83
Layer 9	88.98	82.56	89.30
Layer 10	89.99	83.24	89.94
Layer 11	90.68	84.61	90.19
Layer 12	92.16	85.67	90.18

F.2 `PredictionAttributor`

We question whether the salient input representation correctly represents the latent space of the output. This specifically evaluates `PredictionAttributor`.We calculate the number of times the representation of the most salient word/`[CLS]` token maps to the latent concept of the identical label as that of the prediction. We expect a high alignment at the top layers for `PredictionAttributor` to be correct.

We do not include `ConceptMapper` when evaluating this and conduct the experiment using the training data only where we already know the alignment of a salient representation and the latent concept. Table 9 shows the results across the last four layers (See Tables 10, 11 for full results). For POS, we observed a successful match of above 90% for all models. We observed the mismatched cases and found them to be also of a compositional nature i.e. latent concepts comprised of semantically related words (see Figure 10 for examples).

For sentiment, more than 99% of the time, the last layer's salient representation maps to the predicted class label, confirming the correctness of `PredictionAttributor`. The performance drop for the lower layer is due to the absence of class-based latent concepts in the lower layers i.e. concepts that comprised more than 90% of the tokens belonging to sentences of one of the classes.

Table 11: Saliency-based method: accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept in the sentiment classification task. The reason of very low values for the lower layers is mainly due to the absence of class-based latent concepts in the lower layers i.e. concepts that comprised more than 90% of the tokens belonging to sentences of one of the classes.

	Sentiment		
Layer	BERT	RoBERTa	XLM-R
Layer 0	6.40	12.08	7.46
Layer 1	7.12	12.46	5.57
Layer 2	7.66	17.29	6.36
Layer 3	7.13	22.00	8.03
Layer 4	12.18	20.08	9.71
Layer 5	13.24	24.25	8.88
Layer 6	11.18	17.26	8.75
Layer 7	12.80	39.87	14.05
Layer 8	4.06	92.84	15.75
Layer 9	31.94	99.59	32.63
Layer 10	99.57	99.69	92.06
Layer 11	99.71	99.48	94.97
Layer 12	99.25	99.27	99.08

Table 12: BERT: Accuracy of `ConceptMapper` in mapping a representation to the correct latent concept. See Table 13, 14 in the Appendix for results on all layers.

Layers		0	2	5	10	12
POS	Top 1	100	100	99.03	92.67	84.19
	Top 2	100	100	99.75	97.89	94.15
	Top 5	100	100	99.94	99.68	99.05
Sentiment	Top 1	100	100	97.19	83.09	68.24
	Top 2	100	100	99.63	92.67	83.24
	Top 5	100	100	99.94	97.75	94.24

F.3 `ConceptMapper`

We evaluate the correctness of `ConceptMapper` in mapping a test representation to the training data latent concepts. `ConceptMapper` trains using representations and their cluster IDs as labels. We randomly split this training data into 90% train and 10% test where the test data serves as the gold annotation of latent concepts. We train `ConceptMapper` using the train instances and measure the accuracy of the test instances. Table 12 summarizes the results of BERT (See App. Tables 13, 14 for all results). Observing Top-1 accuracy, the performance of `ConceptMapper` starts high (100%) for lower layers and drops to 84.19 and 68.24% for the last layer. We found that the latent space becomes dense on the last layer. This is in line with Ethayarajh [2019] who showed that the representations of higher layers are highly anisotropic. This causes concepts to be close in the space. If true, the correct label should be among the top predictions of the mapper. We empirically tested it by considering the top two and top five predictions of the mapper, achieving a performance of up to 99.05% and 94.24% for POS and Sentiment respectively.

We also validate `ConceptMapper` by measuring the accuracy of the test instances for both the sentiment classification and POS tagging tasks based on the BERT, RoBERTa, and XLMR models. The top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for each layer is shown in Table 13 and Table 14. For all models, the performance of the top-5 is above 99% for the POS tagging task and above 90% for the sentiment classification task.

Table 13: Top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for the POS tagging task. The top-5 performance reaches above 99% for all models demonstrating that the correct latent concept is among the top probable latent concepts of `ConceptMapper`.

	POS								
	BERT			**RoBERTa**			**XLM-R**		
Layer	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5
Layer 0	100	100	100	99.91	99.95	99.98	99.99	100	100
Layer 1	100	100	100	99.92	99.94	99.98	100	100	100
Layer 2	100	100	100	99.76	99.92	99.98	99.72	99.98	100
Layer 3	99.85	99.98	100	99.38	99.85	99.98	98.25	99.60	99.98
Layer 4	99.72	99.92	99.97	98.67	99.58	99.87	97.72	99.60	99.98
Layer 5	99.03	99.75	99.94	97.69	99.15	99.73	97.05	99.23	99.91
Layer 6	97.76	99.34	99.83	96.52	98.71	99.59	95.8	98.95	99.76
Layer 7	96.51	98.91	99.68	94.72	98.11	99.57	93.92	98.31	99.80
Layer 8	95.27	98.52	99.79	92.56	97.55	99.52	94.20	98.52	99.80
Layer 9	94.54	98.25	99.70	92.24	97.48	99.55	92.79	97.82	99.73
Layer 10	92.67	97.89	99.68	91.61	97.19	99.55	92.03	97.66	99.60
Layer 11	90.86	97.34	99.64	90.72	96.77	99.58	90.40	97.28	99.67
Layer 12	84.19	94.15	99.05	86.88	95.13	99.15	85.07	94.57	99.08

Table 14: Top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for the sentiment classification task. The top-5 performance reaches above 90% for all models demonstrating that the correct latent concept is among the top probable latent concepts of `ConceptMapper`.

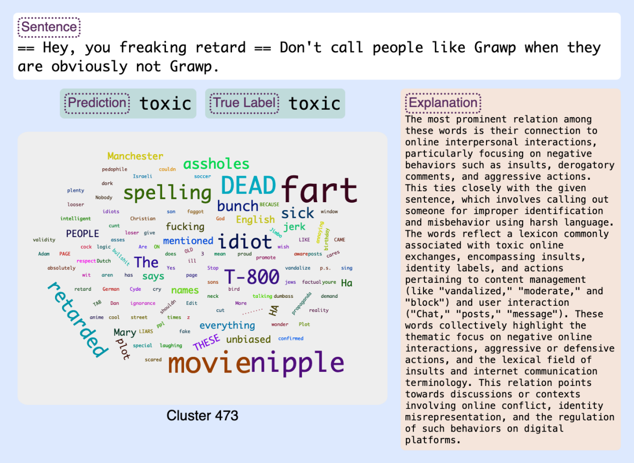
	Sentiment								
	BERT			**RoBERTa**			**XLM-R**		
Layer	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5
0	100	100	100	99.95	100	100	100	100	100
1	100	100	100	99.86	99.98	100	100	100	100
2	100	100	100	99.89	99.98	100	99.9	100	100
3	98.80	100	100	99.44	99.83	99.96	99.57	99.99	100
4	97.84	99.85	99.99	99.28	99.73	99.91	99.4	99.96	100
5	97.19	99.63	99.94	98.4	99.5	99.84	99.12	99.84	99.96
6	96.44	99.30	99.89	97.35	99.15	99.82	98.9	99.84	99.96
7	94.86	98.97	99.90	96.13	98.74	99.63	98.22	99.62	99.9
8	93.26	97.99	99.67	87.42	95.14	98.43	98.13	99.48	99.84
9	90.42	96.97	99.20	75.38	88.14	96.07	96.37	98.77	99.66
10	83.09	92.67	97.75	65.84	81.13	93.46	89.12	95.2	98.61
11	76.84	88.02	96.01	65.91	81.36	93.43	70.99	84.31	94.18
12	68.24	83.24	94.24	70.83	84.54	95.67	55.3	75.08	91.74

G Toxicity Classification Task

G.1 Experimental Setup

We use the Jigsaw Toxicity dataset for the toxicity classification task (Toxicity). This dataset comprises Wikipedia comments labeled by human annotators to identify instances of toxic behavior. We retain only the "toxic" feature as the label for each instance, thereby classifying each instance as `toxic` or `non-toxic`. The dataset has more than 159k, 63k, and 89k instances for train, dev, and test. We randomly select 9k, 800, and 800 splits for train, dev, and test respectively. We use $K = 600$ for `ConceptDiscoverer` and have the same setting for the rest of the module-specific hyperparameters.

G.2 Qualitative Evaluation

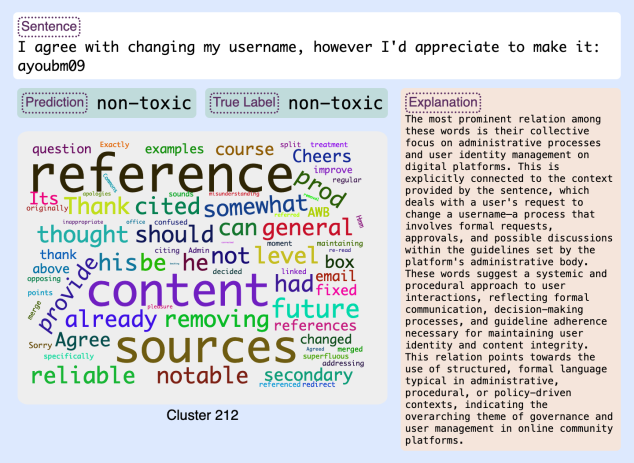


Sentence
== Hey, you freaking retard == Don't call people like Grawp when they are obviously not Grawp.

Prediction toxic True Label toxic

Explanation
The most prominent relation among these words is their connection to online interpersonal interactions, particularly focusing on negative behaviors such as insults, derogatory comments, and aggressive actions. This ties closely with the given sentence, which involves calling out someone for improper identification and misbehavior using harsh language. The words reflect a lexicon commonly associated with toxic online exchanges, encompassing insults, identity labels, and actions pertaining to content management (like "vandalized," "moderate," and "block") and user interaction ("Chat," "posts," "message"). These words collectively highlight the thematic focus on negative online interactions, aggressive or defensive actions, and the lexical field of insults and internet communication terminology. This relation points towards discussions or contexts involving online conflict, identity misrepresentation, and the regulation of such behaviors on digital platforms.

Figure 11: RoBERTa: A toxic labeled test instance correctly predicted by the model.



Sentence
I agree with changing my username, however I'd appreciate to make it: ayoubm09

Prediction non-toxic True Label non-toxic

Explanation
The most prominent relation among these words is their collective focus on administrative processes and user identity management on digital platforms. This is explicitly connected to the context provided by the sentence, which deals with a user's request to change a username—a process that involves formal requests, approvals, and possible discussions within the guidelines set by the platform's administrative body. These words suggest a systemic and procedural approach to user interactions, reflecting formal communication, decision-making processes, and guideline adherence necessary for maintaining user identity and content integrity. This relation points towards the use of structured, formal language typical in administrative, procedural, or policy-driven contexts, indicating the overarching theme of governance and user management in online community platforms.

Figure 12: RoBERTa: A non-toxic labeled test instance correctly predicted by the model.

G.2.1 Correct prediction with correct gold label

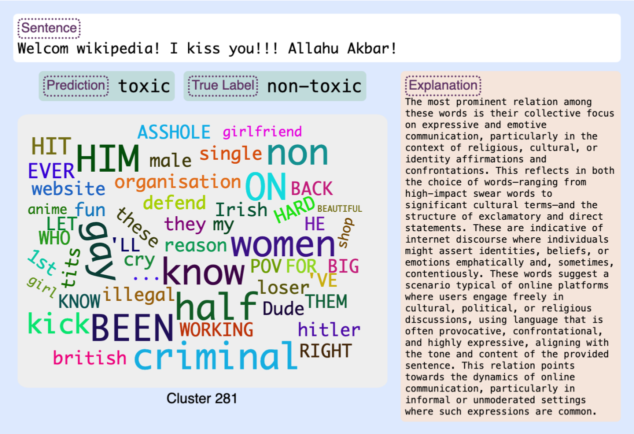
Figure 11 and Figure 12 present the correct prediction case for a toxic and a non-toxic labeled instance. In the toxic label instance, `PlausiFyer`discovers that the words in latent concept have common semantics of negative behaviors and highlights the reason for toxic label due to harsh language. For the non-toxic labeled instance, `PlausiFyer`finds that the relation between the sentence and the list of

Table 15: Number of clusters for each polarity. The total number of clusters is 600.

	Toxicity								
	BERT			RoBERTa			XLM-R		
Layer	non-toxic	toxic	Mix	non-toxic	toxic	Mix	non-toxic	toxic	Mix
Layer 0	15	30	555	22	15	563	19	16	565
Layer 1	13	27	560	17	20	563	16	16	568
Layer 2	11	33	556	18	24	558	16	20	564
Layer 3	16	35	549	17	28	555	16	21	563
Layer 4	18	36	546	20	29	551	15	24	561
Layer 5	12	41	547	28	33	539	14	22	564
Layer 6	15	48	537	37	42	521	23	24	553
Layer 7	18	49	533	324	131	145	114	53	433
Layer 8	23	49	528	332	186	82	267	74	259
Layer 9	43	52	505	373	158	69	334	134	132
Layer 10	116	73	411	425	137	38	328	154	118
Layer 11	298	110	192	449	130	21	423	139	38
Layer 12	374	155	71	502	92	6	449	129	22

words in the latent concept is about the governance theme and user management in online community platforms.

G.2.2 Wrong prediction with correct gold label



Sentence
Welcom wikipedia! I kiss you!!! Allahu Akbar!

Prediction toxic

True Label non-toxic

Explanation
The most prominent relation among these words is their collective focus on expressive and emotive communication, particularly in the context of religious, cultural, or identity affirmations and confrontations. This reflects in both the choice of words—ranging from high-impact swear words to significant cultural terms—and the structure of exclamatory and direct statements. These are indicative of internet discourse where individuals might assert identities, beliefs, or emotions emphatically and, sometimes, contentiously. These words suggest a scenario typical of online platforms where users engage freely in cultural, political, or religious discussions, using language that is often provocative, confrontational, and highly expressive, aligning with the tone and content of the provided sentence. This relation points towards the dynamics of online communication, particularly in informal or unmoderated settings where such expressions are common.

Figure 13: RoBERTa: A non-toxic labeled instance that is incorrectly predicted as toxic.

Figure 13 shows a non-toxic labeled instance that is incorrectly predicted as toxic. The sentence contains non-toxic content and has cultural/religious terms expressing positive emotion. However, the model predicts this sentence with a toxic label. The latent concept provides helpful evidence that it contains many toxic words such as "ASSHOLE", "idiot", "bitch", and "Niggers". Also, the `PlausiFyer`provides additional information that both the sentence and the latent concept contain the context of religion and culture. We hypothesize that the model captures the correlations between the toxic content or label and the religion/culture concept in the training. Thus, the model has a bias in the prediction with the religion/culture-related content to the toxic label.

G.3 Module Specific Evaluation

G.3.1 `ConceptDiscoverer`

We also form latent concepts of each layer using `ConceptDiscoverer` and annotate them with the procedure mentioned in F. In the toxicity classification task, we discovered that 88%, 99%, and 96%

of the latent concepts of BERT, RoBERTa, and XLMR were made up of either toxic majority or non-toxic majority sentences (see Table 15). Similar to the sentiment, we noticed that the 12th layer has a higher number of class-based clusters of Roberta and XLMR.

G.3.2 `PredictionAttributor`

For toxicity, we found over 98% accuracy in mapping the salient representation to the correct latent concept for the last layer (see Tables 16). This high accuracy indicates that `PredictionAttributor` performs effectively and accurately in the toxicity task.

Table 16: Saliency-based method: accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept in the toxicity classification task. The reason of very low values for the lower layers is mainly due to the absence of class-based latent concepts in the lower layers i.e. concepts that comprised more than 90% of the tokens belonging to sentences of one of the classes.

	Toxicity		
Layer	BERT	RoBERTa	XLM-R
Layer 0	10.54	13.45	6.57
Layer 1	8.98	19.14	8.45
Layer 2	10.92	19.92	10.56
Layer 3	49.90	22.95	13.90
Layer 4	50.07	34.30	15.12
Layer 5	11.30	31.50	23.89
Layer 6	66.21	35.42	34.47
Layer 7	67.11	91.84	59.38
Layer 8	63.74	97.84	77.43
Layer 9	84.41	98.79	94.44
Layer 10	94.92	99.30	97.52
Layer 11	94.73	99.49	97.39
Layer 12	98.93	99.72	99.61

G.3.3 `ConceptMapper`

Table 17 presents the performance of `ConceptMapper` for toxicity. The accuracy of the first layer is high (around 100%) and drops as the layer increases for all models. In the last layer, the accuracy of the top prediction arrives at 67.01%, 81.43%, and 64.19% for BERT, RoBERTa, and XLMR. We also consider the top two and top five predictions of the mapper. The performances of the top two and the top five predictions are more than 81% and 93% for these three models. Especially, the mapper based on the RoBERTa model has the best performance, achieving 81.43%, 93.72%, and 98.21% for the top one, two, and five predictions respectively.

Table 17: Top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for the toxicity classification task. The top-5 performance reaches above 90% for all models demonstrating that the correct latent concept is among the top probable latent concepts of `ConceptMapper`.

	Toxicity								
	BERT			**RoBERTa**			**XLM-R**		
Layer	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5
0	100	100	100	99.96	99.99	100	100	100	100
1	100	100	100	99.92	100	100	100	100	100
2	99.99	100	100	99.94	100	100	99.75	100	100
3	99.07	99.88	100	99.34	99.80	99.92	99.46	99.95	100
4	98.49	99.78	99.99	96.87	98.96	99.78	98.81	99.83	100
5	98.25	99.72	99.94	93.10	97.63	99.26	97.72	99.42	99.89
6	97.22	99.51	99.88	87.72	95.05	98.50	94.83	98.45	99.61
7	95.00	98.57	99.68	73.50	87.21	95.70	86.96	95.37	98.72
8	91.87	97.41	99.18	67.62	83.09	94.38	79.62	91.37	97.62
9	85.66	93.80	98.01	66.75	82.80	94.38	73.73	88.57	96.76
10	76.22	87.90	95.89	64.87	81.37	93.07	66.10	82.36	93.39
11	70.53	84.31	94.31	77.91	91.09	98.10	68.30	84.49	95.28
12	67.01	81.71	93.65	81.43	93.72	98.21	64.19	81.96	94.26

H NLI Task

H.1 Experimental Setup

We use the MNLI dataset for the NLI task. This task classifies each sentence pair into three classes: `entailment`, `contradiction`, and `neutral`. The MNLI dataset contains 393k, 19.65k, and 19.65k splits for train, dev, and test. We randomly select 9k and 1.2k for train and dev splits. We use $K = 400$ for `ConceptDiscoverer` and set the same numbers for the other hyperparameters.

H.2 Qualitative Evaluation

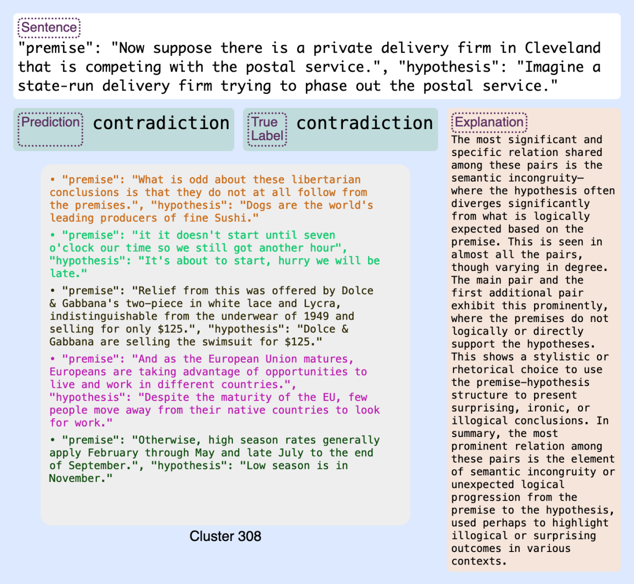
Figure 14 shows a correct prediction instance with a “contradiction” label. `PlausiFyer` detects that all premise-hypothesis pairs are “semantic incongruity”, which means that the premise sentence does not have a matched logic with the hypothesis sentence. This indicates that the model learns the knowledge of the “contradiction" label in the training.

However, due to the complexity of the task, it is difficult for humans to understand or find the relationship between the latent concept and the prediction of the input sentence. Especially, if we have the word cloud as the latent concept-based explanation, it may not be helpful for humans to interpret the model prediction. `PlausiFyer` simplifies the interpretation in such cases.

H.3 Module Specific Evaluation

H.3.1 `ConceptDiscoverer`

In the MNLI task, we found more “mixed” latent concepts than class-based latent concepts related to other tasks. There are 0%, 82%, and 58% discovered label dominant latent concepts by BERT, RoBERTa, and XLMR (see Table 18). We speculate that tasks that involve multiple sentences as input are more complex and abstract, thereby it is difficult to have clear distinct concepts. This observation also varies depending on the model. For instance, we did not detect any class-based latent concepts of the BERT model. However, we achieve good performance in discovering the latent concept when using the RoBERTa model.



Sentence

"premise": "Now suppose there is a private delivery firm in Cleveland that is competing with the postal service.", "hypothesis": "Imagine a state-run delivery firm trying to phase out the postal service."

Prediction contradiction

True Label contradiction

- "premise": "What is odd about these libertarian conclusions is that they do not at all follow from the premises.", "hypothesis": "Dogs are the world's leading producers of fine Sushi."
- "premise": "it it doesn't start until seven o'clock our time so we still got another hour", "hypothesis": "It's about to start, hurry we will be late."
- "premise": "Relief from this was offered by Dolce & Gabbana's two-piece in white lace and Lycra, indistinguishable from the underwear of 1949 and selling for only $125.", "hypothesis": "Dolce & Gabbana are selling the swimsuit for $125."
- "premise": "And as the European Union matures, Europeans are taking advantage of opportunities to live and work in different countries.", "hypothesis": "Despite the maturity of the EU, few people move away from their native countries to look for work."
- "premise": "Otherwise, high season rates generally apply February through May and late July to the end of September.", "hypothesis": "Low season is in November."

Cluster 308

Explanation

The most significant and specific relation shared among these pairs is the semantic incongruity—where the hypothesis often diverges significantly from what is logically expected based on the premise. This is seen in almost all the pairs, though varying in degree. The main pair and the first additional pair exhibit this prominently, where the premises do not logically or directly support the hypotheses. This shows a stylistic or rhetorical choice to use the premise–hypothesis structure to present surprising, ironic, or illogical conclusions. In summary, the most prominent relation among these pairs is the element of semantic incongruity or unexpected logical progression from the premise to the hypothesis, used perhaps to highlight illogical or surprising outcomes in various contexts.

Figure 14: MNLI: A contradiction labeled instance that is correctly predicted.

Table 18: Number of clusters for each polarity: '0' for entailment label, '1' for neutral label, and '2' for contradiction label. The total number of clusters is 400.

	MNLI											
	BERT				**RoBERTa**				**XLM-R**			
Layer	0	1	2	Mix	0	1	2	Mix	0	1	2	Mix
Layer 0	0	6	0	394	0	2	0	398	0	7	0	393
Layer 1	0	4	0	396	0	2	0	398	0	4	0	396
Layer 2	0	3	0	397	0	1	0	399	0	3	0	397
Layer 3	0	4	0	396	0	2	0	398	0	5	0	395
Layer 4	0	4	0	396	0	1	0	399	0	4	0	396
Layer 5	0	4	0	396	0	0	0	400	0	4	0	396
Layer 6	0	6	0	394	0	1	0	399	0	4	0	396
Layer 7	0	4	0	396	0	3	0	397	0	2	0	398
Layer 8	0	1	0	399	1	11	6	382	0	1	0	399
Layer 9	0	1	0	399	27	38	24	311	4	6	6	384
Layer 10	0	0	0	400	38	48	34	280	24	41	18	317
Layer 11	0	1	0	399	51	76	50	223	40	67	51	242
Layer 12	0	0	0	400	92	155	81	72	64	86	82	168

H.3.2 `PredictionAttributor`

We found that both RoBERTa and XLMR models have over 90% accuracy for the salient representation mapping for the last layer (see Tables 19). To some extent, this accuracy indicates that `PredictionAttributor` have good performance in the MNLI task based on the RoBERTa and XLMR model. Unlike other tasks, we have extremely low accuracy with the BERT model. We assume that the BERT model may not be able to capture the task knowledge due to the task complexity.

H.3.3 `ConceptMapper`

Similar to other tasks, the performance of `ConceptMapper` has very high accuracy (around 100%) at the first layer for all models. Then, the accuracy is decreased to 72.07%, 77.56%, and 64.19% for the top prediction of BERT, RoBERTa, and XLMR. The accuracy of the top two and two five predictions

Table 19: Saliency-based method: accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept in the MNLI task. The reason of very low values for the lower layers is mainly due to the absence of class-based latent concepts in the lower layers i.e. concepts that comprised more than 90% of the tokens belonging to sentences of one of the classes.

MNLI			
Layer	BERT	RoBERTa	XLM-R
Layer 0	0.027	0.41	0.56
Layer 1	0.083	0.67	0.43
Layer 2	0.04	0	0.23
Layer 3	0	0.05	0.35
Layer 4	0.10	0	0.08
Layer 5	0.10	0	0.12
Layer 6	0.05	0	0.12
Layer 7	0	0	0.13
Layer 8	0	21.61	0
Layer 9	0	83.90	14.29
Layer 10	0	91.78	55.93
Layer 11	0	92.63	89.73
Layer 12	0	95.22	90.58

Table 20: Top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for the MNLI task. The top-5 performance reaches above 90% for all models demonstrating that the correct latent concept is among the top probable latent concepts of `ConceptMapper`.

MNLI									
	BERT			**RoBERTa**			**XLM-R**		
Layer	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5	Top-1	Top-2	Top-5
0	100	100	100	99.97	100	100	100	100	100
1	100	100	100	99.91	99.99	100	100	100	100
2	100	100	100	99.92	99.99	100	99.75	100	100
3	99.25	100	100	99.70	99.92	99.96	99.46	99.95	100
4	99.22	99.97	99.98	99.15	99.65	99.88	98.81	99.83	100
5	99.04	99.95	99.99	97.07	96.98	99.26	97.72	99.42	99.89
6	97.07	99.45	99.90	91.91	95.05	98.50	94.83	98.45	99.61
7	96.81	99.35	99.85	96.99	87.21	95.70	86.96	95.37	98.72
8	94.15	98.18	99.55	94.75	83.09	94.38	79.62	91.37	97.62
9	90.08	96.52	98.90	91.52	82.80	94.38	73.73	88.57	96.76
10	81.31	90.97	97.20	84.79	81.37	93.07	66.10	82.36	93.39
11	79.05	89.62	96.51	81.79	91.09	98.10	68.30	84.49	95.28
12	72.07	89.27	99.45	77.56	93.72	98.21	64.19	81.96	94.26

are above 81% and 94%. The Roberta model still has the best performance than the others, which has 77.56%, 93.72%, and 98.21% accuracy for the top one, two, and five predictions (Table 20).

I LLama2

I.1 Experimental Setup

We also tried the Eraser Movie sentiment classification and Jigsaw Toxicity classification tasks with the Llama2 model. We applied the "Llama-2-7b-chat-hf" version of the Llama2 model. We used the last token of the input prompt as the `[CLS]` token. We only used these `[CLS]` tokens as the latent concept explanation. For `ConceptDiscoverer`, we set $K = 400$ for the sentiment and set $K = 200$ for the toxicity.

Table 21: Number of clusters for each polarity. The total number of clusters is 400.

	Sentiment		
	Llama-2-7b-chat-hf		
Layer	Negative	Positive	Mix
Layer 0	27	372	1
Layer 4	18	12	370
Layer 8	21	21	358
Layer 12	73	47	279
Layer 16	154	90	155
Layer 20	163	102	134
Layer 24	173	108	118
Layer 28	159	106	134
Layer 32	164	103	132

Table 22: Saliency-based method: accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept in the sentiment classification task using Llama2 model.

	Sentiment
Layer	Llama-2-7b-chat-hf
Layer 0	2.88
Layer 4	0.93
Layer 8	1.94
Layer 12	22.11
Layer 16	64.18
Layer 20	70.63
Layer 24	75.64
Layer 28	71.30
Layer 32	71.02

I.2 Sentiment Classification Task

I.2.1 `ConceptDiscoverer`

Compared to the BERT, RoBERTa, and XLMR models (Table 8), the Llama2 model has fewer class-based clusters at the last layer(See Table 21). There are around 67% class-based clusters detected at the last layer for the Llama2 model. The BERT, RoBERTa, and XLMR models have 78%, 95%, and 94% class-based clusters at the last layer.

I.2.2 `PredictionAttributor`

With the Llama2 model, the accuracy in mapping the salient word representation to the correct latent concept for the last layer is approximately 70% (See Table 22). Although this accuracy indicates that the Llama2 model performs well, it is notably lower than the accuracy achieved by the `PredictionAttributor` model based on BERT, RoBERTa, and XLMR models, which has significantly high performance (Table 11).

I.2.3 `ConceptMapper`

We found that, like the performance of using the other three models, the performance of `ConceptMapper` using the Llama2 model exhibits a high Top-1 accuracy (97.55%) in the lower layers, and decreases to 66.47% for the last layer(Table 23). Additionally, the top two and five predictions of the mapper achieve accuracies of 82.84% and 94.88%, respectively. The accuracy of `ConceptMapper` using the Llama2 model is relatively lower compared to its accuracy using BERT, RoBERTa, and XLM-RoBERTa(Table 14).

Table 23: Top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for the sentiment classification task using the Llama2 model.

Sentiment			
	Llama-2-7b-chat-hf		
Layer	Top-1	Top-2	Top-5
0	97.55	97.55	97.55
4	19.90	31.36	47.08
8	49.46	68.06	86.37
12	60.85	77.43	92.36
16	61.86	80.97	95.03
20	64.02	80.61	94.23
24	63.95	82.26	94.23
28	65.83	81.25	94.52
32	66.47	82.84	94.88

I.3 Toxicity Classification Task

I.3.1 `ConceptDiscoverer`

We found that 83% of the latent concepts of Llama2 are the class label-based at the last layer(Table 24). The BERT, RoBERTa, and XLMR models have a relatively higher number of class label-based clusters(Table 15).

I.3.2 `PredictionAttributor`

The accuracy of the Llama2 model in our experiments is significantly lower compared to BERT, RoBERTa, and XLMR (Table 25). The performance of the other three models achieves accuracy values exceeding 90% (Table 16). The lower accuracy is due to several reasons. Llama2 is a generative model and it is hard to restrict its output to a single class. While we optimized the prompt for this purpose, we classified responses as label 0 (non-toxic) only if they contained "non-toxic", "NON-TOXIC", or "Non-toxic". Similarly, we classified responses as 1 (toxic) if they contained variations of the term "toxic". Moreover, many responses of the model did not provide a classification result due to inappropriate or disrespectful content of input instances that was blocked by the safety filter. Consequently, there are many sentences were skipped, which may account for the lower accuracy of Llama2 compared to the other models.

I.3.3 `ConceptMapper`

The top-1 performance of `ConceptMapper` based on the Llama2 model achieves 74.44% for the last layer(Table 26). This performance is better than the one based on the BERT and XLM-Roberta (Table 17). RoBERTa still delivers the best performance.

Table 24: Number of clusters for each polarity. The total number of clusters is 200.

	Toxicity		
	Llama-2-7b-chat-hf		
Layer	Non-toxic	toxic	Mix
Layer 0	84	108	1
Layer 4	35	13	150
Layer 8	27	5	168
Layer 12	43	22	135
Layer 16	61	21	117
Layer 20	62	25	113
Layer 24	69	25	106
Layer 28	67	26	107
Layer 32	69	21	109

Table 25: Saliency-based method: accuracy of `PredictionAttributor` in mapping a representation to the correct latent concept in the toxicity classification task using Llama2 model.

	Toxicity
Layer	Llama-2-7b-chat-hf
Layer 0	2.26
Layer 4	7.20
Layer 8	6.59
Layer 12	32.10
Layer 16	42.91
Layer 20	45.83
Layer 24	46.93
Layer 28	46.43
Layer 32	44.28

Table 26: Top 1, 2, and 5 accuracy of `ConceptMapper` in mapping a representation to the correct latent concept for the toxicity classification task using the Llama2 model.

	Toxicity		
	Llama-2-7b-chat-hf		
Layer	Top-1	Top-2	Top-5
0	96.97	96.97	97.09
4	42.38	62.00	83.86
8	67.83	85.20	97.20
12	70.40	89.24	98.21
16	73.09	87.44	98.77
20	74.22	90.25	98.99
24	71.19	88.68	98.88
28	72.65	90.13	98.76
32	74.44	91.82	99.10

J Limitations

We discussed the limitations of LACOAT as follows:

- While hierarchical clustering is better than nearest neighbor in discovering latent concepts as established by Dalvi et al. [2022], it has computational limitations and it can not be easily extended to a corpus of say 1M tokens. However, the assumptions that are taken in the experimental setup e.g. considering the maximum 20 occurrences of a word (supported by Dalvi et al. [2022]) work well in practice in terms of limiting the number of tokens and covering all facets of a majority of the words. Moreover, the majority of the real-world tasks have limited task-specific data and LACOAT can effectively be applied in such cases. In a contemporary work, Hawasly et al. [2024] recently targeted this limitation by exploring alternative algorithms such as leaders and k-means, demonstrating that these are viable, cheaper alternatives to the expensive agglomerative hierarchical clustering. Future explorations are needed to evaluate the correctness of the resulting clusters. For instance, k-means assume clusters to be spherical and similar assumption is enforced with the fixed distance threshold used in leaders. This limits their usefulness to identify clusters with irregular boundaries.
- The concept discoverer is also constrained by a very small dataset. We conducted experiments to discover latent concepts with varying data sizes. The results indicate that when the data size is below 1000 instances, the discovered latent concepts tend to be sparse and lack coherence to form a clear concept.
- The computational cost of LACOAT is higher than that of the IG method alone. While ConceptDiscoverer runs once per dataset as a pre-processing step, minimizing its impact on runtime during model inference, it still adds additional demand. Moreover, ConceptMapper is a linear classifier with an inference time of $O(d * c)$, where d is the number of features and c is the number of clusters. All other processes, aside from the IG part, have a linear cost.
- For tasks requiring reasoning over multiple sentences, we observe that sometimes the LACOAT explanation's are not clearly indicative of the reason of a prediction which might be based on some syntactic and semantic similarity between multiple input sentences. A possible solution to this is to consider hierarchical relationship between latent concepts in contrast to considering a flat structure among latent concepts. The underlying setup of ConceptDiscoverer supports this. However, comparing hierarchical structures requires further investigation beyond the scope of current work which provides a strong evidence towards faithful and human friendly explanations using training data latent space.
- The human friendly explanations generated by PlausiFyer are prone to errors due to the inherent limitations of generative models such as positional bias [Zheng et al., 2023, Khan et al., 2024], verbosity bias [Huang et al., 2024], sensitivity to prompt style which hinders reproducibility. For instance, in this work, we observed that if we provide the predicted label to PlausiFyer, it generates an explanation describing the relationship between input, latent concept and label irrespective of whether the label is correct or not. A possible solution is to use multiple LLMs [Verga et al., 2024, Wang et al., 2023, Badshah and Sajjad, 2024] and LLMs agents [Chen et al., 2024, Tan et al., 2024] that reasons over diverse explanations and reach to a better precise explanation of a latent concept.