Post-hoc Interpretability for Neural NLP: A Survey

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Neural networks for NLP are becoming increasingly complex and widespread, and there is a growing concern if these models are responsible to use. Explaining models helps to address the safety and ethical concerns and is essential for accountability. Interpretability serves to provide these explanations in terms that are understandable to humans. Additionally, post-hoc methods provide explanations after a model is learned and are generally model-agnostic. This survey provides a categorization of how recent post-hoc interpretability methods communicate explanations to humans, it discusses each method in-depth, and how they are validated, as the latter is often a common concern.

CCS Concepts: • **Computing methodologies** → **Natural language processing**; **Neural networks**.

Additional Key Words and Phrases: Interpretability, Transparency, Post-hoc explanations.

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1 INTRODUCTION

Large neural NLP models, most notably BERT-like models [14, 26, 57], have become highly widespread, both in research and industry applications [109]. This increase of model complexity is motivated by a general correlation between model size and test performance [14, 43]. Due to their immense complexity, these models are generally considered black-box models. A growing concern is therefore if it is responsible to deploy these models.

Concerns such as safety, ethics, and accountability are particularly important when machine learning is used for high-stakes decisions, such as healthcare, criminal justice, finance, etc. [84], including NLP-focused applications such as translation, dialog systems, resume screening, search, etc. [28]. For many of these applications, neural models have been shown to exhibit unwanted biases and similar ethical issues [11, 14, 32, 61, 68, 84].

Doshi-Velez and Kim [27] argue, among others [55], that these ethical and safety issues stem from an "incompleteness in the problem formalization". While these issues can be partially prevented with robustness and fairness metrics, it is often not possible to consider all failure modes. Therefore, quality assessment should also be done through model explanations. Furthermore, when models do fail in critical applications, explanations must be provided to facilitate the accountability process. Providing these explanations is the purpose of interpretability.

Doshi-Velez and Kim [27] define *interpretability* as the "ability to explain or to present in understandable terms to a human". However, what constitutes as an "understandable" explanation is an interdisciplinary question. An important work from social science by Miller [64], argues that *effective explanations* must be selective in the sense one must select "one or two causes from a sometimes infinite number of causes". Such observation necessitates organizing interpretability methods by how and what they selectively communicate.

This survey presents such an organization in Table 1, where each row represents a communication approach. For example, the first row describes *input feature* explanations that communicate what

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tokens are most relevant for a prediction. In general, each row is ordered by how abstract the communication approach is, although this is an approximation. Organizing by the method of communication is discussed further in Section 1.1.

	less information					more information
	post-hoc					intrinsic
	black-box	dataset	gradient	embeddings	white-box	model specific
local explanation						
input features	SHAP § 6.4	LIME § 6.3, Anchors § 6.5	Gradient § 6.1, IG § 6.2			Attention
adversarial examples	SEA$^{\mathcal{M}}$ § 7.2		HotFlip § 7.1			
similar examples		Influence Functions$^{\mathcal{H}}$ § 8.1		Representer Pointers† § 8.2		Prototype Networks
counter-factuals	Polyjuice$^{\mathcal{M},\mathcal{D}}$ § 9.1	MiCE$^{\mathcal{M}}$ § 9.2				
natural language	CAGE$^{\mathcal{M},\mathcal{D}}$ § 10.1					GEF$^{\mathcal{D}}$, NILE$^{\mathcal{D}}$
class explanation						
concepts					NIE$^{\mathcal{D}}$ § 11.1	
global explanation						
vocabulary				Project § 12.1, Rotate § 12.2		
ensemble	SP-LIME § 13.1					
linguistic information	Behavioral Probes$^{\mathcal{D}}$ § 14.1			Structural Probes$^{\mathcal{D}}$ § 14.2	Structural Probes$^{\mathcal{D}}$ § 14.2	Auxiliary Task$^{\mathcal{D}}$
rules	SEAR$^{\mathcal{M}}$ § 15.1					

lower abstraction / *higher abstraction* (left vertical axis)

Table 1. Overview of *post-hoc* interpretability methods, where § indicates the section the method is discussed. Rows describe how the explanation is communicated, while columns describe what information is used to produce the explanation. The order of both rows and columns indicates level of abstraction and amount of information, respectively. However, this order is only approximate.

Furthermore, because this survey focuses on *post-hoc* methods, the *intrinsic* section of this table is incomplete and mearly meant to provide a few comparative examples. The specifc *intrinsic* methods shown are: *Attention* [6], *GEF* [56], *NILE* [50]. *Prototype Networks* and *Auxiliary Task* refer to types of models.

$^{\mathcal{M}}$: Depends on a supplementary model. $^{\mathcal{H}}$: Depends on the second-order derivative. $^{\mathcal{D}}$: Depends on a supplementary dataset. †: Depends only on the dataset and white-box access.

Each interpretability method uses different kinds of information to produce its explanation, in Table 1 this is indicated by the columns. The columns are ordered by an increasing level of information. *Black-box* means the method only evaluates the model, this is the least amount of information, while *white-box* refers to knowing everything about the model. Again, this is an inexact ranking but serves as a useful tool to contrast the different methods.

Table 1 frames the overall structure of this survey. Where each method section from 6 to 15 covers a row of Table 1. However, first we cover motivation (section 2), how to validate interpretability (section 4), and a motivating example (section 3). The method sections can be read somewhat independently, but will refer back to these general topics.

Furthermore, the survey limits itself to *post-hoc* interpretability methods. These are methods that provide their explanation after a model is trained and are often model-agnostic. This is in contrast to *intrinsic* methods, where the model architecture itself helps to provide the explanation. These terms are described further in Section 1.2.

1.1 Organizing by method of communication

As a categorization of communication strategies, it's standard in the interpretability literature to distinguish between methods that explain a single observation, called *local explanations*, and methods that explain the entire model called *global explanations* [1, 12, 17, 19, 27, 65]. In this survey, we also consider an additional category of methods that explains an entire output-class, which we call *class explanations*.

To subdivide these categories further, Table 1 orders each communication strategy by their abstraction level. As an example, see Figure 1, where an *input features* explanation highlights the input tokens that are most responsible for a prediction; because this must refer to specific tokens, its ability to provide abstract explanations is limited. For a highly abstract explanation, consider the *natural language* category which explains a prediction using a sentence and can therefore use abstract concepts in its explanation.

		y	explanation
x	the year 's best and most unpredictable comedy	pos	*input feature*
	unpredictable comedies are funny	–	*natural language*

Fig. 1. Fictive visualization of an *input features* explanation which highlights tokens and a *natural language* explanation, applied on a sentiment classification task [104]. y = pos means the gold label is *positive* sentiment.

Communication methods that have a higher abstraction level are typically easier to understand, but the trade-off is that they may reflect the model's behavior less. Because the purpose of interpretability is to communicate the model to a human, this trade-off is necessary [64, 84]. Which communication strategy should be used must be decided by considering the applications and to whom the explanation is communicated to.

Table 1 does have some limitations. Firstly, ordering explanation methods by their abstraction level is an approximation, and while *global explanations* are generally more abstract than *local explanations* this is not always true. For example, the explanation "simply print all weights" (not included in Table 1), is arguably the lowest possible abstraction level, however it also a *global explanation*.

Secondly, there are explanation categories that are not included, such as *intermediate representations*. This category of explanation depends on models that are *intrinsically* interpretable, which are not the subject of this survey. We elaborate on this in Section 1.2.

1.2 Intrinsic versus post-hoc interpretability

A fundamental motivation for interpretability is accountability. For example, if a predictive mistake happens which caused harm, it is important to explain why this mistake happened [28]. Similarly, for high-stakes decisions, it is important to minimize the risk of model failure by explaining the model before deployment [84]. In other words, it is important to distinguish between when interpretability is applied proactively or retroactively to the model's deployment.

It is standard in the literature to categorize if an interpretability method can be applied retroactively or proactively. Unfortunately, the terminology for this taxonomy is not standardized [17].

This survey focuses on the methods that can be applied retroactively, for which the term *post-hoc* is used. Similarly, we use the term *intrinsic* to refer to models that are interpretable by design. These terms were chosen as the best compromise between established terminology [29, 41, 65] and correctness in terms of their dictionary definition.

Intrinsic *methods.* These inherently depend on models that by design are interpretable. Because of this relation, it is also often referred to as *white-box models* [19, 29, 84]. However, the term *white-box* is slightly misleading, as it is often only a part of the transparent model.

As an example, consider *intermediate representation* explanations, this category depends on a model that is constrained to produce a meaningful *intermediate representation*. In Neural Modular Networks [4, 35] this could be `find-max-num(filter(find()))`, which represents how to extract an answer from a question-paragraph-pair. However, how this representation is produced is not necessarily *intrinsically* interpretable.

Intrinsic methods are attractive because they may be more responsible to use in high-stakes decision processes. However, as Jacovi and Goldberg [41] argue, "a method being *inherently interpretable* is merely a claim that needs to be verified before it can be trusted". Verifying this is often non-trivial, as has repeatedly been shown with *Attention* [6], where multiple papers have found contradicting conclusions regarding interpretability [42, 88, 100, 105].

Post-hoc *methods.* These are the focus of this survey. While many *post-hoc* methods are model-agnostic, this is not a necessary property, and in some cases does only apply to a category of models. Indeed, in this survey, only methods that apply to neural networks are discussed.

Because of the inherent ability to explain the model after training, *post-hoc* methods are valuable in legal proceedings, where models may need to be explained retroactively [28]. Additionally, they fit into existing quality assessment structures, such as those used to regulate banking, where quality assessment is also done after a model has been built [12]. Finally, it is guaranteed that they will not affect model performance.

However, *post-hoc* methods are often criticized for providing false explanations, and it has been questioned if it is reasonable to expect models, that were not designed to be explained, to be explained anyway [84]. The question of how to validate explanations is covered in detail in Section 4. Furthermore, we pay special attention to how each method is validated in the literature throughout the survey.

Comparing. Both *Intrinsic* and *post-hoc* methods have their merits, but often provide different values in terms of *accountability*. Finally, *post-hoc* methods can often be applied also to *intrinsicly* interpretable models. Observing a correlation between methods from these two categories can therefore provide validation of both methods [42].

2 MOTIVATIONS FOR INTERPRETABILITY

The need for interpretability comes primarily from an "incompleteness in the problem formalization" [27], meaning if the model was constrained and optimized to prevent all possible ethical issues, interpretability would be much less relevant. However, because perfect optimization is unlikely, hence *safety* and *ethics* are strong motivations for interpretability.

Additionally, when models misbehave there is a need for explanations, to hold people or companies accountable, hence *acountability* is often a core motivation for interpretability. Finally, explanations are often useful, or sometimes necessary, for gaining *scientific understanding* about models. This section aims to elaborate on what exactly is understood by these terms and how interpretability can address them.

Ethics, in the context of interpretability, is about ensuring that the model's behavior is aligned with common ethical and moral values. Because there does not exist an exact measure for this desideratum, this is ultimately something that should be judged qualitatively by humans, for example by an *ethics review committee*, who will inspect the model explanations.

For some ethical concerns, such as discrimination, it may be possible to measure and satisfy this ethical concern via fairness metrics and debiasing techniques [32]. However, this often requires a finite list of protected attributes [38], and such a list will likely be incomplete, hence the need for a qualitative assessment [27, 55].

Safety. is about ensuring the model performs within expectations in deployment. As it is nearly impossible to truly test the model, in the end-to-end context that it will be deployed, ensuring *safety* does to some extent involve qualitative assessment [27]. Lipton [55] frames this as *trust*, and suggests one interpretation of this is "that we feel comfortable relinquishing control to it".

While all types of interpretability can help with *safety*, in particular, *adversarial examples* and *counterfactuals* are useful, as they evaluate the model on data outside the test distribution. Lipton [55] frames this in the broader context of *transferability*, which is the model's robustness to adversarial attacks and distributional shifts.

Accountability. relates to explaining the model when it does fail in production. The "right to explanation", regarding the logic involved in the model's prediction, is increasingly being adopted, most notably in the EU via its GDPR legislation. However, also the US and UK have expressed support for such regulation [28]. Additionally, industries such as banking, are already required to audit their models [12].

Accountability is perhaps the core motivation of interpretability, as Miller [64] writes "Interpretability is the degree to which a human can understand the cause of a decision", and it is exactly the causal reasoning that is relevant in *accountability* [28].

Scientific Understanding. addresses a need from researchers and scientists, which is to generate hypotheses and knowledge. As Doshi-Velez and Kim [27] frames it, sometimes the best way to start such a process is to ask for explanations. In model development, explanations can also be useful for *model debugging* [12], which is often facilitated by the same kinds of explanations.

3 MOTIVATING EXAMPLE

Because *post-hoc* methods are often model-agnostic, explaining and discussing them can often become abstract. To make the method sections as concrete and comparable as possible this survey will show fictive examples based on the "Stanford Sentiment Treebank" (SST) dataset [92]. The SST dataset has been modeled using LSTM [104], Self-Attention-based models [26], etc., all of which are popular examples of neural networks.

Note that the methods described in this survey are, in general, not restricted to sequence-to-class problems and can also be applied to sequence-to-sequence, and most other language problems, although it may sometimes require modification of either the method or the visualization tools surrounding the method [59].

		$p(y|\mathbf{x})$	y
x	<u>the</u> <u>year</u> <u>'s</u> best <u>and</u> <u>most</u> unpredictable comedy	0.91	pos
x	<u>we</u> <u>never</u> <u>feel</u> <u>anything</u> <u>for</u> <u>these</u> characters	0.95	neg
x	<u>handsome</u> <u>but</u> <u>unfulfilling</u> <u>suspense</u> <u>drama</u>	0.18	neg

Fig. 2. Three examples from the SST dataset [92]. x is the input, with each token denoted by an <u>underline</u>. y is the gold target label, where pos is *positive* and neg is *negative* sentiment. Finally, $p(y|\mathbf{x})$ is the model's estimate of x belonging to category y. Note that the model predicts the 3rd (last) wrong, indicated with red.

The predictions of Figure 2 can be explained by asking different questions, each of which communicates a different aspect of the model that is covered in the sections of this survey.

local explanations. explain a single observation:

Input Features	*Which tokens are most important for the prediction, Section 6.*
Adversarial Examples	*What would break the model's prediction, Section 7.*
Similar Examples	*What training examples influenced the prediction, Section 8.*
Counterfactuals	*What does the model consider a valid opposite example, Section 9.*
Natural Language	*What would a generated natural language explanation be, Section 10.*

Class explanations. summarize the model, but only with regard to one selected class:

Concepts	*What concepts (e.g. movie genre) can explain a class, Section 11.*

Global explanations. summarize the entire model with regards to a specific aspect:

Vocabulary	*How does the model relate words to each other, Section 12.*
Ensemble	*What examples are representative of the model, Section 13.*
Linguistic information	*What linguistic information does the model use, Section 14.*
Rules	*Which general rules can summarize an aspect of the model, Section 15.*

4 MEASURES OF INTERPRETABILITY

Because interpretability is by definition about explaining the model to humans [27, 64], and these explanations are often qualitative, it is not clear how to quantitatively evaluate and compare interpretability methods. This ambiguity has lead to much discussion. Most notable is the *intrinsically* interpretable method *Attention*, where different measures of interpretability have been published resulting in conflicting findings [42, 88, 105].

In general, there is no consensus on how to measure interpretability. However, validation is still paramount. As such, this section attempts to cover the general categories, themes, and methods that have been proposed. Additionally, each method section, starting from *input features*, in Section 6, will briefly cover how the authors choose to evaluate their method.

To describe the evaluation strategies, we use the terminology defined by Doshi-Velez and Kim [27], which separates the evaluation of interpretability into three categories, *functionally-grounded*, *human-grounded*, and *application-grounded*. This categorization reflects the need to have explanations that are useful to humans (*human-grounded*) and accurately reflect the model (*functionally-grounded*).

Application-grounded. evaluation is when the interpretability method is evaluated in the environment it will be deployed. For example, does the explanations result in higher survial-rates in a medical setting, or higher-grades in a homework-hint system [27, 108]. Importantly, this evaluation should include the baseline where the explanations are provided by humans.

Due to the application-specific and long-term nature of this approach, *application-grounded* evaluation is rarely done in NLP interpretability research. Instead, more synthetic and general evaluation setups can be used, which is what *functionally-grounded* and *human-grounded* evaluation is about. These categories each provide an important but different aspect for validating interpretability and should therefore be used in combination.

Human-grounded. evaluation checks if the explanations are useful to humans. Unlike *application-grounded*, the task is often simpler and can be evaluated immediately. Additionally, expert humans are often not required [27]. In other literature this is known as *plausibility* [41], *simulatability* [55], and *comprehensibility* [81].

Providing explanations that are informative to humans is a non-trivial task, and often involves interdisciplinary knowledge from the human-computer interaction (HCI) and social science fields. Miller [64] provides an excellent overview from the social science perspective, and criticizes current works by saying "most work in explainable artificial intelligence uses only the researchers' intuition of what constitutes a 'good' explanation".

It is therefore critical that interpretability methods are *human-grounded*; common strategies to measure this are:

- Humans have to choose the best model based on an explanation [78].
- Humans have to predict the model's behavior on new data [76].
- Humans have to identify an outlier example called an intruder [18]. This is often used for *vocabulary* explanations [69].

Functionally-grounded. evaluation checks how well the explanation reflects the model. This is more commonly known as *faithfulness* [29, 41, 78, 105] or sometimes *fidelity* [81].

It might seem surprising that an explanation, which is directly produced from the model, would not reflect the model. However, even intrinsically interpretable methods such as *Attention* and *Neural Modular Networks* have been shown to not reflect the model [42, 93].

Interestingly, *human-grounded* interpretability methods can not reflect the model perfectly, because humans require explanations to be selective, meaning the explanation should select "one or two causes from a sometimes infinite number of causes" [64]. Regardless, the explanations must still reflect the model to some extent, which surprisingly is not always the case [41, 84]. Additionally, explanations that provide a similar type of explanation, with similar selectiveness, should compete on proving the explanation that best reflects the model.

For some tasks, measuring if an interpretability method is *functionally-grounded* is trivial. In the case of *adversarial examples*, it is enough to show that the prediction changed and the adversarial example is a paraphrase. In other cases, most notably *input features*, providing a *functionally-grounded* metric can be very challenging [2, 39, 41, 47, 111].

In general, common evaluation strategies are:

- Comparing with an intrinsically interpretable model, such as logistic regression [78].
- Comparing with other post-hoc methods [42].
- Proposing axiomatic desirables [94].
- Benchmarking against random explanations [39].

5   METHODS OF INTERPRETABILITY

The main objective of this survey is to give an overview of *post-hoc* interpretability methods and categorize them by how they communicate. Section 6 to Section 15 will be dedicated towards this goal.

Table 1 represents a table-of-content, relating each section to a communication approach, but also contrasts the different methods by what information they use. In addition, the motivating example in Section 3 gives a brief idea of the different communication approaches.

Each method section from *input features* (section 6) to *rules* (section 15) covers one communication approach, corresponding to one row in Table 1, and can be read somewhat independently. Each section discusses the purpose of the communication approach and covers the most relevant methods. Because interpretability is a large field, this survey chooses methods based on historical progression and diversity regarding what information they use, this is discussed more in *limitations* (section 2).

Furthermore, the method sections will use the terminology[1] covered in *motivation for interpretability* (section 2) and *measures of interpretability* (section 2).

6   INPUT FEATURES

An *Input feature* explanation is a *local explanation*, where the goal is to determine how important an *input feature*, e.g. a token, is for a given prediction. This approach is highly adaptable to different problems, as the input features are always known and are often meaningful to humans. Especially in NLP, the input features will often represent words, sub-words, or characters. Knowing which words are the most important, can be a powerful explanation method. An *input feature* explanation of the input $\mathbf{x}$, is represented as

$$\mathbf{E}(\mathbf{x}, c) : \mathbf{I^d} \to \mathbb{R}^{\mathbf{d}}, \text{ where I is the input domain and } \mathbf{d} \text{ is the input dimensionality.} \qquad (1)$$

Note that, when the output is a score of importance the explanation is called an *importance measure*.

Importantly, *input feature* explanations can only explain one class at a time. Often, the selected class is either the most likely class or the true-label class, in this section the explained class is denoted with c.

6.1   Gradient

One simple *importance measure*, is taking the gradient w.r.t. the input [5, 53].

$$\mathbf{E}_{\text{gradient}}(\mathbf{x}, c) = \nabla_{\mathbf{x}} f(\mathbf{x})_c, \text{ where } f(\mathbf{x}) \text{ is the model logits.} \qquad (2)$$

This essentially measures the change of the output, given an ϵ-change to each input feature. Note, while NLP features are often discrete, it is still possible to take the gradient w.r.t. the one-hot-encoding by treating it as continuous. Although, because the one-hot-encoding has shape $\mathbf{x} \in \mathbf{I}^{V \times T}$, where V is the vocabulary size and T is the input length, it is necessary to reduce the vocabulary dimension, such $\mathbf{E}(\mathbf{x}) \in \mathbf{I}^T$, when visualizing the importance per word, as seen in Figure 3.

The primary argument for the *gradient* method being *functionally-grounded*, is that for a linear model $f(\mathbf{x}) = \mathbf{x}\mathbf{W}$, the explanation would be $\mathbf{W}^\top$ which is clearly a valid explanation [2]. However, this does not guarantee *functionally-groundedness* for non-linear models [53].

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[1]If you are viewing this survey in a PDF reader, each term will *link* to the section where it's defined.

										$p(y\|\mathbf{x})$	y	c
x	the	year	's	best	and	most	unpredictable	comedy		0.91	pos	pos
x		we	never	feel	anything	for	these	characters		0.95	neg	neg
x			handsome	but	unfulfilling	suspense	drama			0.18	neg	pos

Fig. 3. Hypothetical visualization of applying $\mathbf{E}_{\text{gradient}}(\mathbf{x})$, where c is the explained class. Note that because the vocabulary dimention is reduced away, typically using the L^2-norm, it is not possible to separate positive influence (red) from negative influence (blue).

6.2 Integrated Gradient (IG)

The *gradient* approach has been further developed, the most notable development is *Integrated Gradient* [94].

Sundararajan et al. [94] primarily motivate *Integrated Gradient* via the desirables they call *sensitivity* and *completeness*. *Sensitivity* means, if there exists a combination of $\mathbf{x}$ and baseline $\mathbf{b}$ (often an empty sequence), where the output of $f(\mathbf{x})$ and $f(\mathbf{b})$ are different, then the feature that changed should get a non-zero attribution. This desirable is not satisfied for the gradient method, for example due to the truncation in $\text{ReLU}(\cdot)$. *Completeness* means, the sum of importance scores assigned to each token should equal the model output relative to the baseline $\mathbf{b}$.

To satify these desirables, Sundararajan et al. [94] develop equation (3) which integrates the gradients between an uninformative baseline $\mathbf{b}$ and the observation $\mathbf{x}$ [94].

$$\mathbf{E}_{\text{integrated-gradient}}(\mathbf{x}, c) = (\mathbf{x} - \mathbf{b}) \odot \frac{1}{k} \sum_{i=1}^{k} \nabla_{\tilde{\mathbf{x}}_i} f(\tilde{\mathbf{x}}_i)_c, \quad \tilde{\mathbf{x}}_i = \mathbf{b} + {}^{i}/k (\mathbf{x} - \mathbf{b}) \tag{3}$$

This approach has been successfully applied to NLP, where the uninformative baseline can be an empty sentence, such as padding tokens [67].

Although Integrated Gradient has become a popular approach, it has recently received criticism in computer vision (CV) community for not being *functionally-grounded* [39]. One reason is that it multiples by the input which is not directly related to the model [2]. Whether or not this is a concern in NLP remains to be seen.

6.3 LIME

Another popular approach is *LIME* [78]. This distinguishes itself from the gradient-based methods by not relying on gradients. Instead, it samples nearby observations $\tilde{\mathbf{x}}$ and uses the model estimate $p(c|\tilde{\mathbf{x}})$ to fit a logistic regression. The parameters $\mathbf{w}$ of the logistic regression then represents the *importance measure*, since larger parameters would mean a greater effect on the output.

$$\mathbf{E}_{\text{LIME}}(\mathbf{x}, c) = \underset{\mathbf{w}}{\arg\min} \frac{1}{k} \sum_{i=1}^{k} \left(p(c|\tilde{\mathbf{x}}_i) \log(q(\tilde{\mathbf{x}}_i)) + (1 - p(c|\tilde{\mathbf{x}}_i)) \log(1 - q(\tilde{\mathbf{x}}_i)) + \lambda \|\mathbf{w}\|_1 \right.$$
$$\text{where } q(\tilde{\mathbf{x}}) = \sigma(\mathbf{w}\tilde{\mathbf{x}}) \tag{4}$$

One major complication of *LIME* is how to sample $\tilde{\mathbf{x}}$, representing the nearby observations. In the original paper [78], they use a Bag-Of-Words (BoW) representation with a cosine distance. While this approach remains possible with a model that works on sequential data, such distance metrics may not effectively match the model's internal space. In more recent work [110], they sample $\tilde{\mathbf{x}}$ by masking words of $\mathbf{x}$. However, this requires a model that supports such masking.

									$p(y\|\mathbf{x})$	y	c
x	the	year	's	best	and	most	unpredictable	comedy	0.91	pos	pos
x		we	never	feel	anything	for	these	characters	0.95	neg	neg
x			handsome	but	unfulfilling	suspense	drama		0.18	neg	pos

Fig. 4. A fictive visualization of LIME, where the weights of the logistic regression determine the *importance measure*. Note that for LIME, it is possible to have negative importance (indicated by blue). Furthermore, some tokens have no importance score, due to the L^1-regularizer.

The advantages of *LIME* are that it only depends on black-box information and the dataset, therefore no gradient calculations are required. Secondly, it uses a LASSO logistic regression, which is a normal logistic regression with an L_1-regularizer. This means that its explanation is selective, as in sparse, which may be essential for providing a human-friendly explanation [64].

Ribeiro et al. [78] show that LIME is *functionally-grounded* by applying LIME on *intrinsically* interpretable models, such as a logistic regression model, and then compare the LIME explanation with the *intrinsic* explanation from the logistic regression. They also show *human-groundedness* by conducting a human trial experiment, where non-experts have to choose the best model, based on the provided explanation, given a "wrong classifer" tranined on a bias dataset and a "correct classifer" trained on a curated dataset.

6.4 Kernel SHAP

A limitation of *LIME* is that the weights in a linear model are not necessarily *intrinsically* interpretable. When there exists multicollinearity (input features are linearly correlated with each other) then the model weights can be scaled arbitrarily creating a false sense of importance.

To avoid the multicollinearity issue, one approach is to compute Shapley values [89] which are derived from game theory. The central idea is to fit a linear model for every permutation of features enabled. For example, if there are two features $\{x_1, x_2\}$, the Shapley values would aggregate the weights from fitting the datasets with features $\{\varnothing\}, \{x_1\}, \{x_2\}, \{x_1, x_2\}$. If there are T features this would require $O(2^T)$ models.

While this method works in theory, it is clearly intractable. Lundberg and Lee [58] present a framework for producing Shapley values in a more tractable manner. The model-agnostic approach they introduce is called *Kernel SHAP*. It combines 3 ideas: it reduces the number of features via a mapping function $h_{\mathbf{x}}(\mathbf{z})$, it uses squared-loss instead of cross-entropy by working on logits, and it weights each observation by how many features there are enabled.

$$\mathbf{E}_{\text{SHAP}}(\mathbf{x}, c) = \underset{\mathbf{w}}{\text{argmin}} \sum_{\mathbf{z} \in \mathbb{Z}^M} \pi(\mathbf{z}) \; (f(h_{\mathbf{x}}(\mathbf{z}))_c - g(\mathbf{z}))^2$$
$$\text{where } g(\mathbf{z}) = \mathbf{w}\mathbf{z} \tag{5}$$
$$\pi(\mathbf{z}) = \frac{M-1}{(M \text{ choose } |\mathbf{z}|)|\mathbf{z}|(M-|\mathbf{z}|)}$$

In (5), $\mathbf{z}$ is a $\{0, 1\}^M$ vector that describes which combined features are enabled. This is then used in $h_{\mathbf{x}}(\mathbf{z})$, which enables those features in $\mathbf{x}$. Furthermore, $\mathbb{Z}^M$ represents all permutations of enabled combined features and $|\mathbf{z}|$ is the number of enabled combined-features. Figure 5, demonstrates a fictive example of how input features can be combined and visualize their shapley values.

		$p(y|\mathbf{x})$	y	c
x	the year 's best and most unpredictable comedy	0.91	pos	pos
x	we never feel anything for these characters	0.95	neg	neg
x	handsome but unfulfilling suspense drama	0.18	neg	pos

Fig. 5. Fictive visualization of *Kernel SHAP*, showing how features can be combined to make *SHAP* more tractable to compute.

Lundberg and Lee [58] show *functionally-groundedness* by using that Shapley values uniquely satisfy a set of desirables and that *SHAP* values are also Shapley values. Furthermore, they show *human-groundedness* by asking humans to manually produce importance measures and correlate them with the *SHAP* values.

SHAP and Shapley values in general are heavily used in the industry [12]. In NLP literature *SHAP* has been used by Wu et al. [110]. This popularity is likely due to their mathematical foundation and the shap library. In particular, the shap library also presents Partition SHAP which claims to reduce the number of model evaluations to M^2, instead of 2^M [2]. One major disadvantage of *SHAP* is it inherently depends on the masked inputs still being valid inputs. For some NLP models, this can be accomplished with a [MASK] token, while for it is not possible in a *post-hoc* setting. For this reason, *SHAP* exists at an intersection between *post-hoc* and *intrinsic* interpretability methods. This intersection is discussed more in Section 18.

6.5 Anchors

A further development of the idea, that sparse explanations are easier to understand, is *Anchors*. Instead of giving an importance score, like in the case of the gradient-based methods or *LIME*, the *Anchors* simply provides a shortlist of words that were most relevant for making the prediction [79]. The authors show *human-groundedness* with a similar user setup as in *LIME* [78].

		$p(y|\mathbf{x})$	y	c
x	the year 's best and most unpredictable comedy	0.91	pos	pos
x	we never feel anything for these characters	0.95	neg	neg
x	handsome but unfulfilling suspense drama	0.18	neg	pos

Fig. 6. Fictive visalization, showing the *anchors* that are responsible for the prediction.

The list-of-words called "anchors" (A) is formalized in (6). Note that $c = \text{argmax}_i\, p(i|\mathbf{x})$ is a requirement for *anchors*, as using $\text{prec}(A) = \mathbb{E}_{\mathcal{D}(\tilde{\mathbf{x}}|A)}\left[\mathbb{1}_{y=\tilde{y}}\right]$ in (6) would cause *anchors* to be unaffected by the model.

---

[2]See documentation https://shap.readthedocs.io/en/latest/example_notebooks/tabular_examples/model_agnostic/Simple%20Boston%20Demo.html

$$\mathbf{E}_{\text{anchors}}(\mathbf{x}) = \underset{A \text{ s.t. } \text{prec}(A) \geq \tau \wedge A(\mathbf{x})=1}{\text{argmax}} \text{cov}(A)$$

$$\text{where } \text{prec}(A) = \mathbb{E}_{\mathcal{D}(\tilde{\mathbf{x}}|A)} \left[\mathbb{1}_{[\text{argmax}_i \, p(i|\mathbf{x}) = \text{argmax}_i \, p(i|\tilde{\mathbf{x}})]} \right]$$

$$\text{cov}(A) = \mathbb{E}_{\mathcal{D}(\tilde{\mathbf{x}})} \left[A(\tilde{\mathbf{x}}) \right] \tag{6}$$

$$A(\mathbf{x}) = \begin{cases} 1 & \text{if the anchors } A \text{ are in } \mathbf{x} \\ 0 & \text{otherwise} \end{cases}$$

This formalization says the anchor words should have the highest coverage (cov(A)), meaning the most sentences in the dataset $D(\tilde{\mathbf{x}})$ contains the anchors A. Furthermore, only consider anchors A that are sufficiently precise (prec(A) $\geq \tau$) and in $\mathbf{x}$. Precision is defined as the ratio of observations $\tilde{\mathbf{x}}$ with anchors A, denoted $\mathcal{D}(\tilde{\mathbf{x}}|A)$, where the predicted label of $\tilde{\mathbf{x}}$ matches the predicted label of $\mathbf{x}$.

Solving this optimization problem exactly is infeasible, as the number of anchors is combinatorially large. To approximate it, Ribeiro et al. [79] model prec(A) $\geq \tau$ probabilistically [44] and then use a bottom-up approach, where they add a new word to the k-best anchor candidate in each iteration similar to beam-search.

7 ADVERSARIAL EXAMPLES

An *adversarial example*, is an input that causes a model to produce a wrong prediction, due to limitations of the model. The adversarial example is often produced from an existing example, for which the model produces a correct prediction. Because the *adversarial example* serves as an explanation, in the context of an existing example it is a *local explanation*.

This class of methods is not always about interpretability, it can also be about robustness. For example, in the case of Universal Adversarial Triggers [103], they find an ungrammatical sequence of tokens, that if included in an example, causes the model to always make a wrong prediction, which can for example be used to circumvent a spam filter. Because this has little relation to an actual input, such an adversarial example does not explain the model's support boundary and is therefore unrelated to interpretability. Additionally, some works may use adverserial examples to train their model to be more robust [96].

When *adversarial examples* do inform us about the support boundaries of a given example, then this also informs us of the logic involved and therefore provides interpretability. In fact, this explanation can be similar to the *input feature* methods, discussed in Section 6. Many of those methods, also indicate what words should be changed to alter the prediction. An important difference is that *adversarial* explanations are contrastive, meaning they explain by comparing with another example, while *input features* explain only concerning the original example. Contrastive explanations are, from a social science perspective, generally considered more *human-grounded* [64].

In the following discussions, we refer the original example as $\mathbf{x}$ and the adversarial example as $\tilde{\mathbf{x}}$. The goal is to develop an adversarial method A, that maps from $\mathbf{x}$ to $\tilde{\mathbf{x}}$:

$$A(\mathbf{x}) \rightarrow \tilde{\mathbf{x}} \tag{7}$$

Importantly, to ensure that an *adverserial example* method is *functionally-grounded*, one only needs to assert that $\text{argmax}_i \, p(i|\mathbf{x}) \neq \text{argmax}_i \, p(i|\tilde{\mathbf{x}})$ and that $\mathbf{x}$ and $\tilde{\mathbf{x}}$ are paraphrases. Compared to other explanation types, this is reasonably trivial to measure. See Section 4 for a general discussion on measures of interpretability.

7.1 HotFlip

A great example of the relation between *input feature* explanations and *adversarial examples* is *HotFlip* [30]. Here the effect of changing token v to another token $\tilde{v}$ at position t, on the model loss $\mathcal{L}$, is estimated via using gradients

$$\mathcal{L}(y, \tilde{\mathbf{x}}_{t:v \to \tilde{v}}) - \mathcal{L}(y, \mathbf{x}) \approx \frac{\partial \mathcal{L}(y, \mathbf{x})}{\partial x_{t,\tilde{v}}} - \frac{\partial \mathcal{L}(y, \mathbf{x})}{\partial x_{t,v}}, \qquad (8)$$

where $\tilde{\mathbf{x}}_{t:v \to \tilde{v}}$ is the input $\mathbf{x}$, with the token v at position t changed to $\tilde{v}$. Had a gradient approximation not been used, the alternative would be to exactly compute a forward pass for every possible token swap. Instead, this approximation only requires one backward pass.

To produce an adversarial sentence with multiple tokens changed, the authors use a beam-search approach. A visualization of *HotFlip* can be seen in Figure 7.

$$A_{\text{HotFlip}}(\mathbf{x}) = \underset{\tilde{\mathbf{x}}_{t:v \to \tilde{v}}}{\operatorname{argmax}} \frac{\partial \mathcal{L}(y, \mathbf{x})}{\partial x_{t,\tilde{v}}} - \frac{\partial \mathcal{L}(y, \mathbf{x})}{\partial x_{t,v}} \qquad (9)$$

Fig. 7. Hypothetical visualization of *HotFlip*. The highlight indicates the gradient w.r.t. the input, which HotFlip uses to select which token to change. $\mathbf{x}$ indicates the original sentence, and $\tilde{\mathbf{x}}$ indicates the adversarial sentence.

The *HotFlip* paper [30] primarily investigates character-level models, for which the desire is to build a model that is robust against typos. However, in terms of word-level models, it is necessary to constrain the possible changes, such that the adversarial sentence is a paraphrase. They do this via the word-embeddings, such that the adversarial word and the original word are constrained to have a cosine similarity of at least 0.8.

The *HotFlip* approach has proven effective for other adversarial explanation methods, such as the aforementioned Universal Adversarial Triggers [103].

7.2 Semantically Equivalent Adversaries (SEA)

An alternative approach to produce adversarial examples that are ensured to be paraphrases is to sample from a paraphrasing model $q(\tilde{\mathbf{x}}|\mathbf{x})$. Ribeiro et al. [80] do this by measuring a semantical-equivalency-score $S(\mathbf{x}, \tilde{\mathbf{x}})$, as the relative likelihood of $q(\tilde{\mathbf{x}}|\mathbf{x})$ compared to $q(\mathbf{x}|\mathbf{x})$. It is then possible to maximize the similarity, while still having a different model prediction. The exact method is defined in (10), which also constrains the optimization with a minimum semantical-equivalency-score and ensures the predicted label is different.

$$A_{\text{SEA}}(\mathbf{x}) = \underset{\tilde{\mathbf{x}} \sim q(\tilde{\mathbf{x}}|\mathbf{x})}{\text{argmax}} \, S(\mathbf{x}, \tilde{\mathbf{x}})$$

$$\text{s.t. } S(\mathbf{x}, \tilde{\mathbf{x}}) \geq 0.8$$

$$\underset{i}{\text{argmax}} \, p(i|\mathbf{x}) \neq \underset{i}{\text{argmax}} \, p(i|\tilde{\mathbf{x}}) \tag{10}$$

$$\text{where } S(\mathbf{x}, \tilde{\mathbf{x}}) = \min\left(1, \frac{q(\tilde{\mathbf{x}}|\mathbf{x})}{q(\mathbf{x}|\mathbf{x})}\right)$$

The reason why a relative score is necessary, as opposed to just using $S(\mathbf{x}, \tilde{\mathbf{x}}) = q(\tilde{\mathbf{x}}|\mathbf{x})$, is that for two normal sentences $\mathbf{x}_1$ and $\mathbf{x}_2$ of different length, longer sentences are just inherently less likely. Therefore, to maintain a comparative semantic-equivalency-score normalizing by $q(\mathbf{x}|\mathbf{x})$ is necessary [80].

	$\mathbf{x}$	$p(y\|\mathbf{x})$	y	$S(\mathbf{x}, \tilde{\mathbf{x}})$
$\mathbf{x}$	the year 's best and most unpredictable comedy	0.91	pos	–
$\tilde{\mathbf{x}}$	the best and most unpredictable comedy this year	0.13	–	0.87
$\mathbf{x}$	we never feel anything for these characters	0.95	neg	–
$\tilde{\mathbf{x}}$	we never empathize for these characters	0.11	–	0.93

Fig. 8. Hypothetical results of using *SEA* [80]. Note that unlike *HotFlip*, *SEA* can change and delete multiple tokens simultaneously as it samples from a paraphrasing model. Again, $\mathbf{x}$ indicates the original sentence, $\tilde{\mathbf{x}}$ indicates the adversarial sentence, and $S(\mathbf{x}, \tilde{\mathbf{x}})$ is the semantic-equivalency-score which must be at least 0.8.

8 SIMILAR EXAMPLES

For a given *input example*, a *similar examples* explanation finds examples from the training dataset, that in terms of the model's understanding, looks like the *input example*. Because this explanation method centers around a specific *input example*, it is a *local explanation*.

Merely defining an auxiliary distance function between observations does not depend on the model, this can therefore not explain the model. It is therefore critical that a *similar examples* explanation directly inform about how the model predicted the *input example*.

Similar examples explanations can be quite useful, particularly for discovering dataset artifacts, as some of the *similar examples* may have nothing to do with the *input example*, except for the artifacts.

8.1 Influence functions

Influence functions is a classical technique from robust statistics [23]. However, in robust statistics, there are strong assumptions regarding convexity, low-dimensionality, and differentiability. Recent efforts in deep learning remove the low-dimensionality constraint and to some extent the convexity constraint [48].

The central idea in *influence functions*, is to estimate the effect on the loss $\mathcal{L}$, of removing the observation $\tilde{\mathbf{x}}$ from the dataset. The most influential examples are those where the loss changes the most. Let $\tilde{\theta}$ be the model parameters if $\tilde{\mathbf{x}}$ had not been included in the training dataset, then the loss difference can be estimated using

$$\mathcal{L}(y, \mathbf{x}; \tilde{\theta}) - \mathcal{L}(y, \mathbf{x}; \theta) \approx \frac{1}{n} \nabla_\theta \mathcal{L}(y, \mathbf{x}; \theta)^\top H_\theta^{-1} \nabla_\theta \mathcal{L}(\tilde{y}, \tilde{\mathbf{x}}; \theta). \tag{11}$$

Importantly, the Hessian H_θ needs to be positive-definite, which can only be guaranteed for convex models. The authors Koh and Liang [48] avoids this issue, by adding a diagonal to the Hessian, until it is positive-definite. Additionally, they solve the computational issue of computing a Hessian, by formulating (11) as a Hessian-vector product. Such formulation can be solved in $O(np)$ time, where n is the number of observations and p is the number of parameters, hence a computational complexity identical to one training epoch.

One limitation of *influence functions*, as can be seen in Figure 9, is that although the *similar examples* can quantifiably be said to influence the prediction of the *input example*, via the learning phase, the explanation does not provide a direct indication of what exactly about the *similar examples* that was important. Additionally, computing the *influence functions* is not always numerically stable [112], because (11) uses the gradient $\nabla_\theta \mathcal{L}(\tilde{y}, \tilde{\mathbf{x}}; \theta)$ which is optimized to be close to zero.

	$\mathbf{x}$	$p(y\lvert\mathbf{x})$	y	Δ
$\mathbf{x}$	<u>the</u> <u>year</u> 's <u>best</u> <u>and</u> <u>most</u> <u>unpredictable</u> <u>comedy</u>	0.91	pos	–
$\tilde{\mathbf{x}}$	<u>a</u> <u>delightfully</u> <u>unpredictable</u> , <u>hilarious</u> <u>comedy</u>	0.95	pos	3.82
$\tilde{\mathbf{x}}$	<u>loud</u> <u>and</u> <u>thoroughly</u> <u>obnoxious</u> <u>comedy</u>	0.98	neg	−1.51

Fig. 9. Fictive result showing the *similar examples* $\tilde{\mathbf{x}}$, in relation to the *input example* $\mathbf{x}$, showing both examples with positive and negative influence. Δ is the approximated loss difference, estimated using *influence functions* (11).

Koh and Liang [48] looked at support-vector-machines, which are known to be convex, and convolutional neural networks which are generally non-convex. Han et al. [36] then extended the analysis of *influence functions* to BERT [26]. This is a crucial step, as BERT may be much further from convexity than CNNs, thus cause the *influence functions* to be less *functionally-grounded*.

Han et al. [36] validates for *functionally-groundedness* by removing the 10% most influential training examples from the dataset and then retrain the model. The results show a significant decrease in the model's performance on the test split, compared to removing the 10% least influential examples and 10% random examples, validating that the influential examples are important.

It is worth noting that Koh and Liang [48] measured *human-groundedness* by a simulated user-study where 10% of training observations were given a wrong label. *Influence functions* were then used to select a fraction of the dataset, which the simulated user then inspected and corrected labels on. The idea being, wrongly labeled observations should affect the loss more than correctly labeled observations, hence *influence functions* will tend to find wrongly labeled observations. However, Han et al. [36] did not repeat this experiment.

Performance considerations. A criticism of influence functions has been that it is computationally expensive. Although $\nabla_\theta \mathcal{L}(y, \mathbf{x}; \theta)^\top H_\theta^{-1}$ can be cached for each test example, it is still too computationally intensive for real-time inspection of the model. Additionally, having to compute the weight-gradient $\nabla_\theta \mathcal{L}(\tilde{y}, \tilde{\mathbf{x}}; \theta)$ and inner-product for every training observation, does not scale sufficiently. To this end, Guo et al. [34] propose to only use a subset of training data, using a KNN clustering. Additionally, they show that the hyperparameters when computing $\nabla_\theta \mathcal{L}(y, \mathbf{x}; \theta)^\top H_\theta^{-1}$ can be tuned to reduce the computation to less than half.

8.2 Representer Point Selection

An alternative to *influence functions*, is the Representer theorem [87]. The central idea is that the logits of a test example $\mathbf{x}$, can be expressed as a decomposition of all training samples $f(\mathbf{x}) =$

$\sum_{i=1}^{n} \boldsymbol{\alpha}_i \kappa(\mathbf{x}, \tilde{\mathbf{x}}_i)$. The original Representer theorem [87] works on *reproducing kernel Hilbert spaces*, which is not applicable for deep learning. However, recent work has applied the idea to neural networks [112].

Let $\boldsymbol{\theta}_L$ be the weight matrix of the final layer, such that the logits $f(\mathbf{x}) = \boldsymbol{\theta}_L \mathbf{z}_{L-1}(\mathbf{x})$, then if the regularized loss $\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(\tilde{y}_i, \tilde{\mathbf{x}}_i; \theta) + \lambda \|\boldsymbol{\theta}_L\|^2$, is a stationary point and $\lambda > 0$, then

$$f(\mathbf{x}) = \sum_{i=1}^{n} \boldsymbol{\alpha}_i \mathbf{z}_{L-1}(\tilde{\mathbf{x}}_i)^\top \mathbf{z}_{L-1}(\mathbf{x}), \text{ where } \boldsymbol{\alpha}_i = \frac{1}{2\lambda \cdot n} \frac{\partial \mathcal{L}(\tilde{y}_i, \tilde{\mathbf{x}}_i; \theta)}{\partial \mathbf{z}_{L-1}(\mathbf{x}_i)} . \tag{12}$$

To understand the importance of each training observation $\tilde{\mathbf{x}}_i$, regarding the prediction of class c for the test example $\mathbf{x}$, one just looks at the c'th element of each term $\boldsymbol{\alpha}_i \mathbf{z}_{L-1}(\tilde{\mathbf{x}}_i)^\top \mathbf{z}_{L-1}(\mathbf{x})$. This appraoch is more numerically stable than *influence functions* [112], but has the downside of only depending on intermediate representation of the final layer, while *influence functions* employs the entire model.

Because *Representer Point Selection* does depend on a specific model setup, where the last layer is regularized, this could be considered an *intrinsic* method. However, Yeh et al. [112] shows that the stationary solution can be achieved *post-hoc*, meaning after learning, with minimal impact on the model predictions. They do this via the optimization problem

$$\boldsymbol{\theta}_L = \underset{\boldsymbol{W}}{\arg\min} \left(\frac{1}{n} \sum_{i=1}^{n} \mathcal{L}(p(\cdot|\tilde{\mathbf{x}}_i; \theta), \boldsymbol{W} \mathbf{z}_{L-1}(\tilde{\mathbf{x}}_i; \theta)) + \lambda \|\boldsymbol{W}\|^2 \right), \tag{13}$$

where θ is the original model parameters, $\boldsymbol{\theta}_L$ are the new parameters for the last layer, and $\mathcal{L}$ is the full cross-entropy loss. Because this is a fairly low-dimensional problem, fine-tuning this can be done with an L-BFGS optimizer or similar [112].

	x	$p(y|\mathbf{x})$	y	$\boldsymbol{\alpha}_{i,y}$
x	the year 's best and most unpredictable comedy	0.91	pos	–
$\tilde{\mathbf{x}}$	a delightfully unpredictable , hilarious comedy	0.95	pos	1.02
$\tilde{\mathbf{x}}$	a singularly off-putting romantic comedy	0.98	neg	−0.43

Fig. 10. Hypothetical results from using *Representer Point Selection* to find the similar examples $\tilde{\mathbf{x}}$ of the original example $\mathbf{x}$.

Yeh et al. [112] shows this approach is *human-grounded*, via a simulated user study where the simulated user has to correct false labels in the training datasets. They do this by randomly label samples wrong, then use the absolute representer values $|\boldsymbol{\alpha}_{i,c}|$ to identify which observations were the most important for the prediction. This is then compared with *influence functions*, which provide a similar metric. Their results show that *Representer Point Selection* and *influence functions* can identify wrong labels equally well, but that the observations which *Representer Point Selection* selects affects the models performance more.

9   COUNTERFACTUALS

Counterfactual explanations are essentially answering the question "how would the input need to change for the prediction to be different?". Furthermore, these *counterfactual examples* should be a minimal-edit from the original example and fluent. However, all of these properties can also be said of *adversarial explanations*, and indeed some works confuse these terms. The critical difference

is that *adversarial examples* should be paraphrases of the original example, while *counterfactual examples* should be semantically opposite [83].

Another common confusion is with *counterfactual datasets*, also known as *Contrast Sets*. These datasets are used in robustness research and could consist of *counterfactual examples*. However, these datasets are generated without using a model [31, 45], and can therefore not be used to explain the model. *Contrast Sets* are however important for ensuring a robust model.

In social sciences, *counterfactual explanations* are considered highly useful for a person's ability to understand causal connections. Miller [64] explains that "why" questions are often answered by comparing *facts* with *foils*, where the term *foils* is the social sciences term for *counterfactual examples*.

9.1 Polyjuice

Polyjuice by Wu et al. [110] is primarily a *counterfactual dataset* generator, and the generation is therefore detached from the model. However, by strategically filtering these generated examples such that the model's prediction is changed the most, they condition the *counterfactual* generation on the model, thereby making a *post-hoc* explanation.

The generation is done by fine-tuning a GPT-2 model [74] on existing *counterfactual datasets* [31, 45, 60, 85, 106, 114]. For each pair of original and counterfactual example, they produce a training prompt, see (14) for the exact structure. What the conditoning code is and what is replaced in (14) is determined by the existing *counterfactual datasets*.

$$
\begin{aligned}
prompt = \text{``} &\underbrace{\text{It is great for kids}}_{\text{original sentence}} \text{<GENERATE>} \\
&\underbrace{\text{[negation]}}_{\text{conditioning code}} \underbrace{\text{It is [BLANK] great for [BLANK]}}_{\text{masked counterfactual}} \\
&\text{<REPLACE>} \underbrace{\text{not [ANSWER] children [ANSWER]}}_{\text{masking answers}} \text{<EOS>''}
\end{aligned}
\tag{14}
$$

For *counterfactual* generation, they specify the original sentence and optionally the condition code, and then let the model generate the *counterfactuals*. These *counterfactuals* are independent of the model. To make them dependent on the model, they filter the *counterfactuals* and select those examples that change the prediction the most. One important detail is that they adjust the prediction change with an *importance measure* (*SHAP*), such that the *counterfactual examples* that could have been generated by an *importance measure* are valued less. An example of this explanation can be seen in Figure 11.

	x							$p(y\mid\mathbf{x})$	y
x	the	year	's	best	and	most	unpredictable comedy	0.91	pos
x̃	the	year	's	worst	and	least	unpredictable comedy	0.11	–
x		we	never	feel	anything	for	these characters	0.95	neg
x̃			we	feel	everything	for	these characters	0.02	–

Fig. 11. Hypothetical results of *Polyjuice*, showing how some words were either replaced or removed to produce *counterfactual examples*.

To validate *Polyjuice*, for a *human-grounded* experiment, they show that humans were unable to predict the model's behavior for the *counterfactual examples*, thereby concluding that their method highlights potential robustness issues. Whether *Polyjuice* is *functionally-grounded* is somewhat questionable, because the model is not a part of the generation process itself, it is merely used as a filtering step.

9.2 MiCE

Like *Polyjuice* [110], *MiCE* [83] also uses an auxiliary model to generate *counterfactuals*. However, unlike *Polyjuice*, *MiCE* does not depend on auxiliary datasets and the counterfactual generation is more tied to the model being explained, rather than just using the model's predictions to filter the *counterfactual examples*.

The counterfactual generator is a T5 model [75], a sequence-to-sequence model, which is fine-tuned by input-output-pairs, where the input consists of the gold label and the masked sentence, while the output is the masking answer, see (15) for an example.

$$
\begin{aligned}
&input = \text{``}\underbrace{\texttt{label: positive}}_{\text{gold label}}\texttt{, input: }\underbrace{\texttt{This movie is [BLANK]!}}_{\text{masked sentence}}\text{''}\\
&target = \text{``}\texttt{[CLR] }\underbrace{\texttt{really great}}_{\text{masking answer}}\texttt{ [EOS]}\text{''}
\end{aligned}
\tag{15}
$$

The *MiCE* approach to selecting which tokens to mask is to use an *importance measure*, specifically *the gradient w.r.t. the input*, and then mask the top x% most important consecutive tokens.

For generating counterfactuals, *MiCE* again masks tokens based on the *importance measure*, but then also inverts the gold label used for the T5-input (15). This way the model will attempt to infill the mask, such the sentence will have an opposite semantic meaning. This process is then repeated via a beam-search algorithm which stops when the model prediction changes, an example of this can be seen in Figure 12.

	x	$p(y\|\mathbf{x})$	y
x	the year 's best and most unpredictable comedy	0.91	pos
	the year 's worst and most unpredictable comedy	0.59	–
$\tilde{\mathbf{x}}$	the year 's worst and most predictable comedy	0.04	–
x	we never feel anything for these characters	0.95	neg
	we can feel anything for these characters	0.73	–
$\tilde{\mathbf{x}}$	we can feel anything for these animals	0.01	–

Fig. 12. Hypothetical visualization of how *MiCE* progressively creates a counterfactual $\tilde{\mathbf{x}}$ from an original sentence **x**. The highlight shows the *gradient* $\nabla_{\mathbf{x}} f(\mathbf{x})_y$, which *MiCE* uses to know what tokens to replace.

Because *MiCE* uses the model prediction to stop the beam-search, it will inherently be somewhat *functionally-grounded*. However, it may be that using the *gradient* as the *importance measure*, is not *functionally-grounded*. Ross et al. [83] validates that using the *gradient* is *functionally-grounded*, by looking at the number of edits and fluency of *MiCE* and compares it to a version of *MiCE* where random tokens are masked. They find that using the *gradient* significantly improves both fluency and reduces the number of edits it takes to change a prediction.

10 NATURAL LANGUAGE

A common concern for many of the explanation methods presented in this survey is that they are difficult to understand for people without specialized knowledge. It is therefore attractive to directly generate an explanation in the form of *natural language*, which can be understood by simply reading the explanation for a given example. Because these utterances explain just a single example, they are a *local explanation*.

Much research in the area of *natural language* explanations uses the explanations to improve the predictive performance of the model itself. The idea is that by enforcing the model to reason about its behavior, the model can generalize better [16, 50–52, 56, 76]. These approaches are however in the category of *intrinsic* methods. While those methods are often quite general, they are not discussed in this survey which focuses on *post-hoc* methods.

These *post-hoc* methods are referred to as *rationalization* methods, in the sense that they attempt to explain after a prediction has been made [76]. Note that the term is a misnomer, as rationalizations in the dictionary sense[3] can also be false.

10.1 Rationalizing Commonsense Auto-Generated Explanations (CAGE)

Rajani et al. [76] provide explanations to the Common sense Question Answering (CQA) dataset, which is a multiple-choice question answering dataset [95]. The explanations are independent of the model and are provided via Amazon Mechanical Turk. To provide rationalization explanations, they then fine-tune the GPT model [73], using the question, answers, and explanation. See (16) for an example of the exact prompt construction.

$$
\begin{aligned}
input = \text{``}\underbrace{\text{What could people do that involves talking?}}_{\text{question}} \underbrace{\text{confession}}_{\text{choice 1}}, \underbrace{\text{carnival}}_{\text{choice 2}} \\
, \text{or} \underbrace{\text{state park}}_{\text{choice 3}}? \underbrace{\text{confession}}_{\text{answer}} \text{because} \text{''} \\
target = \text{``}\underbrace{\text{confession is the only vocal action.}}_{\text{rational explanation}}\text{''}
\end{aligned} \tag{16}
$$

For simpler tasks, such as "Stanford Sentiment Treebank" [104], the prompt could simply be "`[input]. [answer] because [explanation]`", see Figure 13 for hypothetical explanations using such a setup.

	x	$p(y\|\mathbf{x})$	y
x	the year 's best and most unpredictable comedy	0.91	pos
	unpredictable comedies are funny	–	–
x	we never feel anything for these characters	0.95	neg
	it is important to feel for characters	–	–

Fig. 13. Hypothetical explanations from using *CAGE* to produce rationalizations for the prediction.

They find that rationalization explanations provide nearly identical explanations as reasoning explanations (those where the answer is not known by the explanation model). The method is

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[3]"the action of attempting to explain or justify behaviour or an attitude with logical reasons, even if these are not appropriate." – Oxford Defintion of *rationalization*.

validated to be *human-grounded*, by tasking humans to use the explanation to predict the model behavior, again they find identical performance.

It is questionable how *functionally-grounded CAGE* is, as its only connection to the model is during inference of an explanation, where the answer is produced by the model. Because there are no other connections to the explained model, the GPT model may not truly depend on the answer, indeed their comparative experiments with reasoning explanations (where the answer is not given) show that the explanations are similar.

11 CONCEPTS

A *concept explanation* attempts to explain the model, in terms of an abstraction of the input, called a *concept*. A classical example in computer vision, is to explain how the concept of stripes affects the classification of a zebra. Understanding this relationship is important, as a computer vision model could classify a zebra based on a horse-like shape and a savana background. Such relation may yield a high accuracy score but is logically wrong.

The term *concept* is much more common in computer vision [33, 46, 66] than in NLP. Instead, the subject is often framed more concretely as bias-detection, in NLP. For example, Vig et al. [101] uses the concept of occupation-words like *nurse*, and relates it to the classification of the words *he* and *she*.

Regardless of the field, in both NLP and CV, only a single class or small subset of classes are analyzed. For this reason, *concept explanation* belong in its own category of *class explanations*. However, in the future, we will likely see more types of *class explanations*.

11.1 Natural Indirect Effect (NIE)

Consider a language model with the prompt $\mathbf{x}$ = "The nurse said that". To measure if the gender-stereotype of "nurse" is female, it is natural to compare $p(\text{she}|\mathbf{x})$ with $p(\text{he}|\mathbf{x})$, or alternatively $p(\text{they}|\mathbf{x})$. Generalized, Vig et al. [101] express this as

$$\text{bias-effect}(\mathbf{x}) = \frac{p(\textit{anti-stereotypical}|\mathbf{x})}{p(\textit{stereotypical}|\mathbf{x})} . \tag{17}$$

Vig et al. [101] then provide insight into which parts of the model are responsible for the bias. They do this by measuring the *Natural Indirect Effect* (NIE) from causal mediation analysis.

Given a model $f(\mathbf{x})$, mediation analysis is used to understand how a latent representation $z(\mathbf{x})$ (called the mediator) affects the final model output. This latent representation can either be a single neuron or several neurons, like an attention head. The *Natural Indirect Effect* measures the effect that goes though this mediator.

To measure causality, an *intervention* on the concept measured must be made. As intervention, Vig et al. [101] replace "nurse" with "man", or "woman" for oppositely biased occupations. They call this replace operation `set-gender`.

Then to measure the effect of the mediator Vig et al. [101] introduce

$$\text{mediation-effect}_{m,z,\bar{m}}(\mathbf{x}) = \frac{\text{bias-effect}_{z(\bar{m}(\mathbf{x}))}(m(\mathbf{x}))}{\text{bias-effect}(\mathbf{x})}, \tag{18}$$

where bias-effect$_{z(\bar{m}(\mathbf{x}))}(\cdot)$ uses a modified model with the mediator values for $z(\bar{m}(\mathbf{x}))$ fixed. With this definition, the *Natural Indirect Effect* follows from causal mediation analysis literature [70].

$$\begin{aligned}
\text{NIE}_z = \mathbb{E}_{\mathbf{x}\in\mathcal{D}}\big[\, &\text{mediation-effect}_{\texttt{identity},z,\texttt{set-gender}}(\mathbf{x}) \\
&- \text{mediation-effect}_{\texttt{identity},z,\texttt{identity}}(\mathbf{x})\big]
\end{aligned} \tag{19}$$

Vig et al. [101] apply *Natural Indirect Effect* to a small GPT-2 model, where the mediator is an attention head. By doing this, Vig et al. [101] can identify which attention heads are most responsible for the gender bias, when considering the occupation concept. Hypothetical results, but results similar to those presented in Vig et al. [101], are presented in Figure 14.
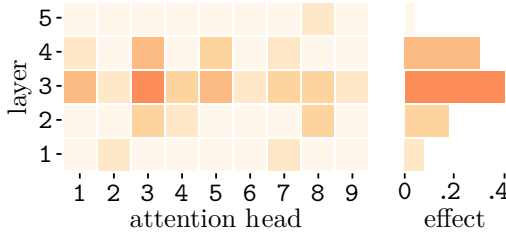

Fig. 14. Visualization of hypothetical *Natural Indirect Effect* (NIE) results, similar to Vig et al. [101]. Such visualization can reveal which attention-head are responsible for gender bias, in a small GPT-2 model. A stronger color indicates a higher NIE, meaning more responsible for the bias.

12 VOCABULARY

Vocabulary explanations, attempts to explain the whole model in relation to each word in the vocabulary, and is therefore a *global explanation*.

In the sentiment classification context, a useful insight could be if positive and negative words are clustered together respectively. Furthermore, perhaps there are words in those clusters which can not be considered of either positive or negative sentiment. Such a finding could indicate a bias in the dataset.

Methods for producing *vocabulary explanations* are almost exclusively using the embedding matrix of the neural network. Because an embedding matrix is often used and because neural NLP models often use pre-trained word embeddings, most research on *vocabulary explanations* is applied to the pre-trained word embeddings [63, 72]. However, in general, these explanation methods can also be applied to the word embeddings after training.

12.1 Projection

A common visual explanation is to project embeddings to two or three dimensions. This is particularly attractive, as word embeddings are of a fixed number of dimensions, and can therefore draw from the very rich literature on projection visualizations of tabular data, most notable is perhaps Principal Component Analysis [71].

t-SNE. Another popular and more recent method is t-SNE [99], which has been applied to word embeddings [53]. This method has in particular been attractive as it allows for non-linear transformations, while still keeping points that are close in the word embedding space, also close in the visualization space. t-SNE does this by representing the two spaces with two distance-distributions, it then minimizes the KL-divergence by moving the points in the visualization space.

Note that Li et al. [53] does not go further to validate t-SNE in the context of word embeddings, except to highlight that words of similar semantic meaning are close together, we provide a similar example in Figure 15.

Supervised projection. A problem with using PCA and t-SNE, is that they are unsupervised. Hence, while they might find a projection that offers high contrast, this projection might not correlate
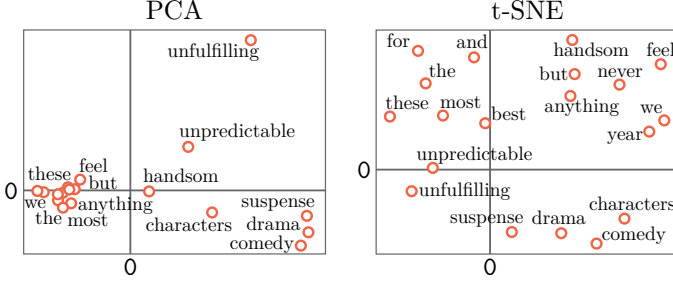
Fig. 15. PCA [71] and t-SNE [99] projection of GloVe [72] embeddings for the words in the semantic classification examples, as shown in Section 3 and elsewhere in this survey.

with what is of interest. An attractive alternative is therefore to define the projection, such that it reveals the subject of interest.

Bolukbasi et al. [13] are interested in how gender-biased a word is. They explore gender-bias, by projecting each word onto a gender-specific vector and a gender-neutral vector. Such vectors can either be defined as the directional vector between "he" and "she", or alternative. Bolukbasi et al. [13] also use multiple gender-specific pairs such as "daughter-son" and "herself-himself", and then use their first Principal Component as a common projection vector.

12.2 Rotation

The category of, for example, all positive sentiment words may have similar word embeddings. However, it is unlikely that a particular basis dimension describes positive sentiment itself. A useful interpretability method, is therefore to rotate the embedding space such the basis-dimensions in the new rotated embedding space represents significant concepts. This is distinct from *projection* methods because there is no loss of information as only a rotation is applied.

Park et al. [69] perform such rotation using *Exploratory Factor Analysis (EFA)* [24]. The idea is to formalize a class of rotation matrices, called the *Crawford-Ferguson Rotation Family* [25]. The parameters of this rotation formulation are then optimized, to make the rotated embedding matrix only have a few large values in each row or column. As an hypothetical example see Table 2.

Basis-dimension	top-3 words
1	handsome, feel, unpredictable
2	most, best, anything
3	suspense, drama, comedy

Table 2. Fictive example of the top-3 words for each basis-dimension in the rotated word embeddings.

Park et al. [69] validate this method to be *human-grounded* by using the *word intrusion* test. The classical word Intrusion test [18] provides 6 words to a human annotator, 5 of which should be semantically related, the 6th is the intruder which is semantically different. The human annotator then has to identify the intruder word. Importantly, semantic relatedness is in this case defined as the top-5 words of a given basis-dimension in the rotated embedding matrix.

Unfortunately, rather than having humans detect the intruder, Park et al. [69] use a distance ratio, related to the cosine-distance, as the detector. This is problematic, as distance is directly

related to how the semantically related words were chosen. In this case the intruder should have been identified either by a human or an oracle model.

13 ENSEMBLE

Ensemble explanations attempts to provide a *global explanation* by combining multiple *local explanations*. This is done such that each *local explaination* represents the different modes of the model.

Ensemble explanations is a very broad category of explanations, as for every type of *local explanation* method there is, an *ensemble* explanation could in principle be constructed. However, in practice very few *ensemble* methods have been proposed, and most of them apply only to tabular data [40, 77, 86]. This is because when non-tabular data is used, it more challenging to compare the selected explanations to ensure they represent different modes. Even *SP-LIME* [78] which does apply to NLP tasks, uses a Bag-of-Word representation as a tabular proxy.

13.1 Submodular Pick LIME (SP-LIME)

SP-LIME by Ribeiro et al. [78] attempts to select B observations (a budget), such that they represent the most important features based on their *LIME* explanation.

More specifically *SP-LIME* calculates the importance of each feature v, by summing the absolute importance for all observations in the dataset, this total importance is $\mathbf{I}_v$ in (20). The objective is then to maximize the sum of $\mathbf{I}_v$ given a subset of features, by strategically selecting B observations. Note that selecting multiple observations which represent the same features will not improve the objective. The specific objective is formalized in (20), which Ribeiro et al. [78] optimize greedily.

$$\mathbf{G}_{\text{SP-LIME}} = \underset{\tilde{\mathcal{D}} \text{ s.t. } |\tilde{\mathcal{D}}| \leq B}{\text{argmax}} \sum_{v=1}^{V} \mathbb{1}_{\left[\exists \tilde{\mathbf{x}}_i \in \tilde{\mathcal{D}} : \left| \mathbf{E}_{\text{LIME}}\left(\tilde{\mathbf{x}}_i, \text{argmax}_i \, p(i|\tilde{\mathbf{x}}_i) \right)_v \right| > 0 \right]} \mathbf{I}_v$$

$$\text{where } \tilde{\mathcal{D}} \subseteq \mathcal{D} \tag{20}$$

$$\mathbf{I}_v = \sum_{\tilde{\mathbf{x}}_i \in \mathcal{D}} \left| \mathbf{E}_{\text{LIME}}\left(\tilde{\mathbf{x}}_i, \underset{i}{\text{argmax}} \, p(i|\tilde{\mathbf{x}}_i) \right)_v \right|$$
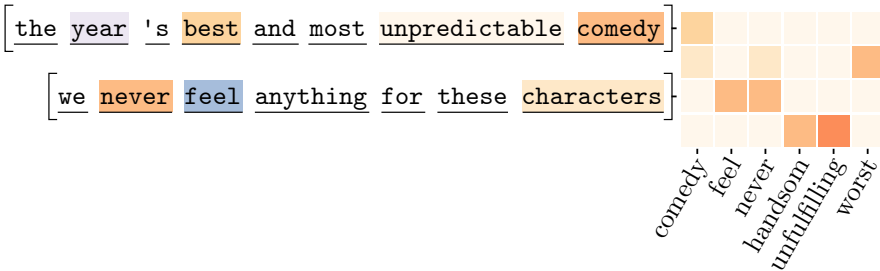

Fig. 16. Visualization of *SP-LIME* in a hypothetical setting. The matrix shows how each selected observation represents the different modes of the model. The left-side shows two out of the four selected example and their *LIME* explanation.

A major challenge with *SP-LIME* is that it requires computing a *LIME* explanation for every observation. Because each *LIME* explanation involves optimizing a logistic regression this can be quite expensive. To reduce the number of observations that need to be explained, Sangroya et al.

[86] proposed using *Formal Concept Analysis* to strategically select which observations to explain. However, this approach has not yet been applied to NLP.

Ribeiro et al. [78] validate *SP-LIME* to be *human-grounded* by asking humans to select the best classifier, where a "wrong classifier" is trained on a biased dataset and a "correct classifier" is trained on a curated dataset. Ribeiro et al. [78] then compare *SP-LIME* with a random baseline, which simply selects random observations. From this experiment, they find that 89% of humans can select the best classifier using *SP-LIME*, where as only 75% can select the best classifier based on the random baseline.

14 LINGUISTIC INFORMATION

To validate that a natural language model does something reasonable, a popular approach is to attempt to align the model with the large body of linguistic theory that has been developed for hundreds of years. Because these methods summarize the model, they are a case of *global explanation*.

Methods in this category either probe by strategically modifying the input to observe the model's reaction or show alignment between a latent representation and some linguistic representation. The former is called *behavioral probes* or *behavioral analysis*, the latter is called *structural probes* or *structural analysis*.

One especially noteworthy subcategory of *Structural Probes* is *BERTology*, which specifically focuses on explaining the BERT-like models [14, 26, 57]. BERT's popularity and effectiveness have resulted in countless papers in this category [20, 21, 62, 82, 97], hence the name *BERTology*. Some of the works use the attention of BERT and are therefore *intrinsic* explanations, while others simply probe the intermediate representations and are therefore *post-hoc* explanations.

There already exist well-written survey papers on *Linguistic Information* explanations. In particular, Belinkov et al. [9] cover *behavioral probes* and *structural probes*, Rogers et al. [82] discuss *BERTology*, and Belinkov and Glass [10] cover *structural probing* in detail. In this section, we will therefore not go in-depth, but simply provide enough context to understand the field and importantly mention some of the criticisms, that we believe have not been sufficiently highlighted by other surveys.

14.1 Behavioral Probes

The research being done in *behavioral probes*, also called *behavioral analysis*, is not just for interpretability but also to measure the robustness and generalization ability of the model. For this reason, many *challenge datasets* are in the category of *behavioral analysis*. These datasets are meant to test the model's generalization capabilities, often by containing many observations of underrepresented modes in the training datasets. However, the model's performance on *challenge datasets* does not necessarily provide interpretability.

One of the initial papers providing interpretability via *behavioral probes* is that by Linzen et al. [54]. They probe a language model's ability to reason about subject-verb agreement correctly. A recent work, by Sinha et al. [91], find that destroying syntax by shuffling words does not significantly affect a model trained on an NLI task, indicating that the model does not achieve natural language understanding.

As mentioned, this area of research is quite large and Belinkov et al. [9] cover *behavioral probes* in detail. Therefore, we just briefly discuss the work by McCoy et al. [60], which provide a particularly useful example on how *behavioral probes* can be used to provide interpretability.

McCoy et al. [60] look at Natural Language Inference (NLI), a task where a premise (for example, "The judge was paid by the actor") and a hypothesis (for example, "The actor paid the judge") are provided, and the model should inform if these sentences are in agreement (called *entailment*). The

other options are *contradiction* and *neutral*. McCoy et al. [60] hypothesise that models may not actually learn to understand the sentences but merely use heuristics to identify *entailment*.

They propose 3 heuristics based on the linguistic properties: lexical overlap, subsequence, and constituent. An example of lexical overlap is the premise "**The doctor** was **paid** by **the actor**" and hypothesis "The doctor paid the actor". The proposed heuristic is that this observation would be classified as *entailment* by the model due to lexical overlap, even though this is not the correct classification.

To test for these heuristics, McCoy et al. [60] developed a dataset, called HANS, which contains examples with these linguistic properties but do not have *entailment*. The results (table 3) validates the hypothesis that the model relies on these heuristics rather than a true understanding of the content. Had just an average score across all heuristics been provided, this would just be a robustness measure. However, by providing meta-information on which pattern each observation follows, the accuracy scores provide interpretability on where the model fails.

	Lexical Overlap	Subsequence	Constituent	Average
BERT [26]	17%	5%	17%	–
Human (Mechanical Turk)	–	–	–	77%

Table 3. Performance on the HANS dataset provided by McCoy et al. [60]. Unfortunately, McCoy et al. [60] do not provide enough information to make a direct comparision possible. For comparison, BERT has 83% accuracy on MNLI [107], which was used for training.

In terms of *functionally-groundedness*, McCoy et al. [60] perform no explicit evaluation. However, given that *behavioral probes* merely evaluate the model, *functionally-groundedness* is generally not a concern. Furthermore, while McCoy et al. [60] do evaluate with humans, this is not a *human-grounded* evaluation. Because they only use humans to evaluate the dataset, not if the explanation itself is suitable to humans.

14.2 Structural Probes

Probing methods primarily use a simple neural network, often just a logistic regression, to learn a mapping from an intermediate representation to a linguistic representation, such as the Part-Of-Speech (POS).

One of the early papers, by Shi et al. [90], analyzed the sentence-embeddings of a sequence-to-sequence LSTM, by looking at POS (part-of-speech), TSS (top-level syntactic sequence), SPC (the smallest phrase constituent for each word), tense (past or non-past), and voice (active or passive). Similarly, Adi et al. [3] used a multi-layer-perceptron (MLP) to analyze sentence-embeddings for sentence-length, word-presence, and word-order. More recently Conneau et al. [22] have been using similar linguistic tasks and MLP probes but have extended previous analyses to multiple models and training methods.

Analog to these papers, a few methods use cluster algorithms instead of logistic regression [15]. Additionally, some methods only look at *word embeddings* [49]. The list of papers is very long, we suggest looking at the survey paper by Belinkov and Glass [10].

BERTology. As an instructive example of probing in BERTology, the paper by Tenney et al. [97] is briefly described. Note that this is just one example of a vast number of papers. Rogers et al. [82] offer a much more comprehensive survey on BERTology.

Tenney et al. [97] probe a BERT model [26] by computing a learned weighted-sum $\mathbf{z}_i(\mathbf{x})$ for each intermediate representation $\mathbf{h}_{l,i}(\mathbf{x})$ of the token i, as described in (21).

$$\mathbf{z}_i(\mathbf{x}) = \gamma \sum_{l=1}^{L} s_l \mathbf{h}_{l,i}(\mathbf{x}) \tag{21}$$

$$\text{where } \mathbf{s} = \text{softmax}(\mathbf{w})$$

The weighted-sum $\mathbf{z}_i(\mathbf{x})$ is then used by a classifier [98], and the weights s_l, parameterized by $\mathbf{w}$, describe how important each layer l is. The results can be seen in Figure 17.
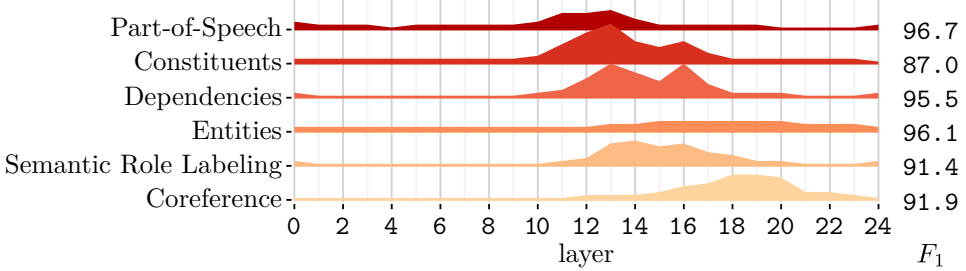
Fig. 17. Results by Tenney et al. [97] which shows how much each BERT [26] layer is used for each linguistic task. The F_1 score for each task is also presented.

Criticisms. A growing concern in the field of probing methods is that given a sufficiently high-dimensional embedding, complex probe, and large auxiliary dataset, the probe can learn everything from anything. If this concern is valid, it would mean that the probing methods do not provide *faithful explanations* [8].

Recent work attempts to overcome this concern by developing baselines. Zhang and Bowman [113] suggest learning a probe from an untrained model, as a baseline. In that paper, they find probes can indeed achieve high accuracy from an untrained model unless the auxiliary dataset size is decreased dramatically. Similarly, Hewitt and Liang [37] use randomized datasets as a baseline, called a control task. For example, for POS they assign a random POS-tag to each word, following the same empirical distribution of the non-randomized dataset. They find that equally high accuracy can be achieved on the randomized dataset unless the probe is made extraordinarily small.

Information-Theoretic Probing. The solutions presented by Zhang and Bowman [113] and Hewitt and Liang [37] are useful. However, limiting the probe and dataset size could make it impossible to find complex hidden structures in the embeddings.

Voita and Titov [102] attempt to overcome the criticism by a more principled approach, using information theory. More specifically, they measure the required complexity of the probe as a communication effort, called *Minimum Description Length* (MDL), and compare the MDL with a control task similar to Hewitt and Liang [37]. They find, similar to Hewitt and Liang [37], that the probes achieve similar accuracy on the probe dataset as on the control task. However, the control task is much harder to communicate (the MDL is higher), indicating that the probe is much more complex, compared to training on the probe dataset.

15 RULES

Rule explanations attempt to explain the model by a simple set of rules, therefore they are an example of *global explanations*.

Reducing highly complex models like neural networks to a simple set of rules is likely impossible. Therefore, methods that attempt this simplify the objectivity by only explaining one particular aspect of the model.

Due to the challenges of producing rules, there is little research attempting it. In Computer Vision, Mu and Andreas [66] is a fairly popularized paper that generates rules for image classification by discovering which attributes cause what predictions. For NLP, we will discuss *SEAR* [80] which is one of the few approaches available.

15.1 Semantically Equivalent Adversaries Rules (SEAR)

SEAR is an extension of the *Semantically Equivalent Adversaries* (SEA) method [80], where they developed a sampling algorithm for finding adversarial examples. Hence, the rule-generation objective is simplified, as only rules that describe what breaks the model needs to be generated.

		$p(y\|\mathbf{x})$	y	Flips
x	the year 's best and most unpredictable comedy	0.91	pos	–
x̃	the best and most unpredictable comedy this year	0.13	–	–
rule	DET year 's ➝ this year	–	–	1%
x	we never feel anything for these characters	0.95	neg	–
x̃	we never empathize for these characters	0.11	–	–
rule	feel ➝ empatize	–	–	4%

Fig. 18. Hypothetical example showing rules which commonly break the model. The flip-rate describes how often these rules break the model. **x** represents the original sentence and x̃ represents an adversarial example.

They propose rules by simply observing individual word changes found by the *SEA* method, and then compute statistics on the bi-grams of the changed word and the Part of Speech of the adjacent word, Figure 18 shows examples of this. If the proposed rule has a high success-rate (called filp-rate), in terms of providing a semantically equivalent adversarial sample, it is considered a rule.

Ribeiro et al. [80] validate this approach by asking experts to produce rules, and then compare the success-rate of human-generated rules and *SEAR*-generated rules. They find that the rules generated by *SEAR* have a higher success-rate.

16 LIMITATIONS

While it is the goal of this survey to provide an overview and categorization of current post-hoc interpretability for neural NLP models, we also recognize that that the field is too vast to include all works in this survey. To decide what works to include, the overall has been to focus on diversity in terms of communication approach and information used. Essentially, to make Table 1 as comprehensive as possible.

Communication approaches like *input features* and *lingustic information* have a particularly large amount of literature, which we did not discuss, as that would outweigh other communication approaches. For these two approaches we focus on highlighting the progression of the field.

Beyond this overarching limitation, the following two limitations are worth discussing.

Quantitative comparisons. Ideally, this survey would include quantitative comparisons of the methods. However, there currently does not exist an unified and principled benchmark yet. Producing a principal benchmark is in itself extreamly difficult and out of scope for this survey, in

Section 18 we discuss further where this difficulty comes from. Performing quantitative comparisons would therefore best be left for future work on interpretability benchmarks.

Visual examples. Because communication is essential to this survey, visual examples of how the method communicates have been provided throughout this survey. These examples are however fictive and optimistic, showing often the best case for each explanation method. However, in practice, accurate and highly useful explanations can only be produced for some examples for *local explanations*, or some datasets in the case of *class and global explanations*. Furthermore, the visualizations are not necessarily the most effective visualizations but are instead what we believe to be the most canonical visualizations.

How an explanation method should be visualized is its own field of study and should draw from human-computer interface literature. This is something that was not covered in this survey.

17   FINDINGS

This survey covers a large range of methods. In particular, we discuss how each method communicates and is evaluated. However, some discussion is not specific to any motivation, measure, or method for interpretability. Therefore, this section covers a few valuable findings which should be discussed from a holistic perspective.

Terminology. Because interpretability is an emerging field, terminology still varies significantly from paper to paper. In particular, the terminology regarding measures of interpretability vary. For example, *human-groundedness* is often confused with *functionally-groundedness*, and for each measure category there are many synonyms such as *plausibility*, *simulatability*, and *comprehensibility* for *human-groundedness*. Additionally, the terms for the communication types are sometimes confused. Especially, *adversarial examples* and *counterfactuals* are occasionally interchanged.

This survey does not seek to unify the terminology, but we hope it will at least serve as a source to understand which terms mean the same and which terms are different.

Synergy. Methods from different communication approaches can benefit each other. For example, both the *adverserial examples* method *HotFlip* and the *counterfactual* method *MiCE* uses the *gradient w.r.t. the input* method from the *input feature* explanation literature. Recognizing these connections allows for flexibility in explanation methods. In the aforementioned example, other *input feature* explanations could have been used as well. Additionally, criticisms on the faithfulness of *input feature* methods could affect its dependents.

Helpful complex models. Models like GPT and T5 are immensely complex and thereby contribute to the interpretability challenge. However, importantly these models are not exclusively bad from an interpretability perspective, as they are also used to provide fluent explanations. For example, in *counterfactual* explanations *Polyjuice* uses the GPT-2 model and *MiCE* uses the T5 model. Similarly, in *natural language* explanations *CAGE* uses GPT. As such, these complex models can not be said to be exclusively counterproductive to interpretability.

18   FUTURE DIRECTIONS AND CHALLENGES

Interpretability for NLP is a fast-growing research field, with many methods being proposed each year. This survey provides an overview and categorization of many of these methods. In particular, we present Table 1 as a way to frame existing research. It is also the hope that Table 1 will help frame future research. In this section, we provide our opinions on what the most relevant challenges and future directions are in interpretability.

Measuring Interpretability. How interpretability is measured varies significantly. Throughout this paper, we have briefly documented how each method measures interpretability. A general observation is that each method paper often introduces its own measures of *functionally-groundedness* or *human-groundedness*. Even when established standards exist, such as the *word intrusion test* [18], they get modified. This trend reduces comparability and risks invalidating the measure itself.

It is important to recognize that measuring interpretability is, in some cases, inherently difficult. For example, in the case of measuring the *functionally-groundedness* of *input feature* explanations, it is inherently impossible to provide gold labels for what is a correct explanation, because if humans could provide gold labels we wouldn't need the explanation in the first place. This fundamentally leaves only proxy measures and axioms of *functionally-groundedness*. However, this doesn't mean highly principled proxy measures can't be developed [39].

For this reason, we are encouraging researchers and reviewers to value principled papers on measuring interpretability. Even if those measures don't become established standards, a dedicated focus on measuring interpretability is a necessity for the integrity of the interpretability field.

Class explanations. There is a large number of papers on explanation methods. However, *class explanations* remain an underrepresented middle ground between *local* and *global explanations*.

The specific communication approach chosen should reflect its application, and for this reason, no explanation type can be said to be superior. However, it's important to recognize that *local explanations* can only provide anecdotal evidence and *global explanations* can be too abstract to ground what is explained. As such *class explanations* have their value, as they are not specific enough to be anecdotal. Simultaneously, they are grounded in the class they explain, making them easier to reason about. For this reason, we would encourage that *class explanation* gain equal representation in interpretability research.

Combining post-hoc with intrinsic methods. *Post-hoc* and *intrinsic* methods are in literature, including this paper, represented as distinct. However, there are important middle grounds.

As mentioned in the introduction, most *intrinsic* methods are not purely intrinsic. They often have an intermediate representation, which can be intrinsically interpretable. However, producing this representation is often done with a black-box model. For this reason, *post-hoc* explanations are needed if the entire model is to be understood.

Beyond this direction, there are works where the training objective and procedure helps to provide better *post-hoc* explanations. This survey briefly argues that the *Kernel SHAP* method exists in this middle ground, as it depends on input-masking being part of the training procedure. In computer vision, Bansal et al. [7] show that adding noise to the input images creates better *input feature* explanations. In general, we hope to see more work in this direction.

19 CONCLUSION

This survey presents an overview of *post-hoc* interpretability methods for neural networks in NLP. The main content of this surveyis on the interpretability methods themself and how they communicate their explanation of the model. This content is categorized through Table 1.

Throughout the survey, we also refer back to *measures of interpretability* (section 4) to describe how each paper evaluates its proposed method. Measuring interpretability is an often undervalued aspect of interpretability with little standardization of the benchmarks. However, by briefly mentioning each method of measurement, we hope that this will lead to less fragmentation.

Finally, we discuss interesting findings and future directions, which we consider particularly important. Overall, we hope that Table 1, the discussions of each communication approach and their methods, and the final discussion sections help frame future research and provide broad insight to those who apply interpretability.

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