

Towards Faithful Model Explanation in NLP: A Survey

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End-to-end neural NLP architectures are notoriously difficult to understand, which gives rise to numerous efforts towards model explainability in recent years. An essential principle of model explanation is Faithfulness, i.e., an explanation should accurately represent the reasoning process behind the model’s prediction. This survey first discusses the definition and evaluation of Faithfulness, as well as its significance for explainability. We then introduce the recent advances in faithful explanation by grouping approaches into five categories: similarity methods, analysis of model-internal structures, backpropagation-based methods, counterfactual intervention, and self-explanatory models. Each category will be illustrated with its representative studies, advantages, and shortcomings. Finally, we discuss all the above methods in terms of their common virtues and limitations, and reflect on future work directions towards faithful explainability. For researchers interested in studying interpretability, this survey will offer an accessible and comprehensive overview of the area, laying the basis for further exploration. For users hoping to better understand their own models, this survey will be an introductory manual helping with choosing the most suitable explanation method(s).

1. Introduction

Since the birth of deep learning, end-to-end Neural Networks (NNs) have achieved enormous success on a wide range of NLP tasks (Wang et al. 2018, 2019). However, they largely remain a black-box to humans, i.e., lacking *explainability*. Recently, numerous methods have been developed to explain how these models work, but there is not yet any unified framework to assess their quality.

In this survey, we review existing model explanation methods through the lens of *Faithfulness*, the extent to which an explanation accurately reflects a model’s reasoning process.

The survey is structured as follows:

- Section 1 introduces the general notion of explainability in NLP and Faithfulness as a central principle of model explanations.
- Section 2 synthesizes existing model explanation methods in pursuit of Faithfulness, by grouping them into five categories: similarity methods, analysis of model-internal structures, backpropagation-based methods, counterfactual intervention, and self-explanatory models.
- Section 3 discusses their common virtues and challenges and identifies future work directions towards improving Faithfulness.
- Section 4 concludes the survey.

1.1 Explainability in NLP

We start by introducing the notion of explainability in NLP, discussing its definition and importance. To prepare for our analysis of model explanation methods in subsequent sections, we will also present a set of properties to categorize different methods, as well as several common design principles.

1.1.1 What Is Explainability.

According to the Cambridge Dictionary, an *explanation* is:

The details or reasons that someone gives to make something clear or easy to understand ([Walter 2008](#)).

In the context of Machine Learning, *explainability* (also referred to as *interpretability*¹) is the extent to which the internal mechanics of a model can be presented in understandable terms to a human ([Lipton 2017](#); [Murdoch et al. 2019](#); [Barredo Arrieta et al. 2020](#)).

Despite this intuitive notion, explainability has no established technical definition in the community, which results in numerous papers “wielding the term in a quasi-scientific way”, essentially referring to different concepts ([Lipton 2017](#); [Doshi-Velez and Kim 2017](#); [Miller 2018](#); [Murdoch et al. 2019](#)). We argue that the confusion mainly lies in the interpretation of two key concepts in the above definition: (a) what are the “internal mechanics”? and (b) who is the “human”?

Internal mechanics. This can refer to either (i) **what knowledge a model encodes** or (ii) **why a model makes certain predictions**. Past work in NLP explainability can be dissected along this dividing line:

(i) The “what” type of work aims to accurately characterize the capacity and deficiency of a model M , in terms of some target knowledge K , which can be linguistic, commonsense, world knowledge, etc. For example, given a Machine Translation (MT) model, does it implicitly capture linguistic knowledge such as the syntactic tree of the input and output sentences? Previous research answers such questions with methods including:

- **probing classifiers** (or auxiliary/diagnostic classifiers): ([Veldhoen, Hupkes, and Zuidema 2016](#); [Adi et al. 2017](#); [Conneau et al. 2018](#)),
- **information-theoretic measurement** ([Voita and Titov 2020](#); [Lovering et al. 2020](#));
- **behavioral tests**: including challenge sets ([Levesque, Davis, and Morgenstern 2012](#); [Gardner et al. 2020](#)), adversarial attacks ([Ebrahimi et al. 2018](#); [Wallace et al. 2019a](#)), and prompting ([Petroni et al. 2019](#); [Choenni, Shutova, and van Rooij 2021](#)));
- **visualization** ([Coenen et al. 2019](#); [Ethayarajh 2019](#); [Karidi et al. 2021](#)).

¹ Despite their subtle distinctions in some previous literature, we use the terms interchangeably.

Orthogonal to the choice of method, previous research also spans various domains of the target knowledge K :

- **Syntax:** Agreement (Linzen, Dupoux, and Goldberg 2016), Negative Polarity Items (Marvin and Linzen 2018), Anaphora (Marvin and Linzen 2018), Dependency Trees (Shi, Padhi, and Knight 2016; Hewitt and Manning 2019; Chi, Hewitt, and Manning 2020);
- **Semantics:** Lexical Semantics (Shwartz and Waterson 2018; Garí Soler and Apidianaki 2021), Semantic Roles (Ettinger, Elgohary, and Resnik 2016), Logic (e.g., Negation (Kassner and Schütze 2020; Dobreva and Keller 2021), Conjunction and Disjunction (Saha, Nie, and Bansal 2020), Quantifiers (Haruta, Mineshima, and Bekki 2020)), Monotonicity (Yanaka et al. 2020), Systematicity (Goodwin, Sinha, and O'Donnell 2020);
- **Pragmatics:** Implicatures and Presupposition (Jeretic et al. 2020; Schuster, Chen, and Degen 2020);
- **World and Commonsense knowledge:** Factual knowledge (Petroni et al. 2019; Kassner and Schütze 2020), Numeracy (Wallace et al. 2019c), Time (Zhou et al. 2019; Thukral, Kukreja, and Kavouras 2021), Space (Mirzaee et al. 2021; Masis and Anderson 2021), Factuality (Rudinger, White, and Van Durme 2018);
- **Combination:** (Conneau et al. 2018; Tenney et al. 2019; Tenney, Das, and Pavlick 2019).

It should be noted that “what is known” does not imply “what is used”. For example, even if the previous MT model does encode the linguistic knowledge about syntax trees, this does not mean that it has necessarily *used* it in translation. Instead, it is possible that the model relies on spurious cues, i.e., still not “doing the right thing”. In fact, researchers have found such evidence for some tasks (Ravichander, Belinkov, and Hovy 2021). This leads us to the “why” question.

(ii) The “why” type of work, by contrast, addresses the *causal* question of what factors (input features, model weights, decision rules, etc.) have led the model M to certain predictions Y . It does not assume that “what is present” equals “what is used”, but tries to establish causality between possible factors and the prediction through various approaches. These approaches will be the focus of this survey, so we omit further discussion here.

Human. This refers to the target audience of the explanation, which can include but is not limited to the model developers, fellow researchers, industry practitioners, or end-users. Depending on the audience, the form and goal of the explanation can be entirely different. We will revisit this in Section 1.1.3 - Target Audience.

Instantiating the initial definition with the two clarified concepts, this survey will cover work on explainability in the following sense: **the extent to which why a model makes certain predictions can be presented in understandable terms to some target audience.**

1.1.2 Why Is Explainability Important.

Compared to classic Machine Learning models, end-to-end NNs are intrinsically more complex in terms of the training scheme, reasoning mechanism, and capabilities (Bommasani et al. 2021). For example, it is easy to interpret a Decision Tree, since every node denotes a decision rule, e.g., does the word “advertisement” appear more than twice? By contrast, it is much more opaque what a node/layer in an NN represents and how it contributes to the prediction. Nevertheless, NNs have become the predominant paradigm in NLP research and are increasingly adopted in real-life applications, thus driving the demand to better understand their behavior.

Concretely, explainability can allow us to:

(a) **Discover artifacts in datasets.** Solving the dataset does not mean learning the task, since there can often be unexpected shortcuts (e.g., statistical cues) in data creation. Models are surprisingly good at exploiting them (as shown by Kaushik and Lipton (2018); McCoy, Pavlick, and Linzen (2019); Geva, Goldberg, and Berant (2019), among many others). For example, only using the *hypothesis*² allows the model to achieve a decent performance on Textual Entailment (Poliak et al. 2018). Explaining what features are used in prediction will help us discover such artifacts and create more reliable datasets.

(b) **Diagnose a model’s strengths and weaknesses, and debug it.** Explainability allows us to find where a model succeeds or fails, and fix it before adversaries could exploit them in real use. For example, a model can secretly rely on unwanted biases about gender, race, or age, but we can diagnose and eliminate them through explanations (Ravfogel et al. 2020). Also, if a model is susceptible to subtle perturbations in the data, it is better to discover and guard this in development prior to deployment (Wallace et al. 2019a).

(c) **Enhance user trust in high-stake applications.** In domains like health, law, finance, and human resources, an end-user may not trust a model if it only provides a prediction but no explanation. For example, if a healthcare center’s chatbot tells the patient that they might have COVID based on their description, it is more convincing if there is supporting evidence, e.g., what symptoms are relevant. In such high-stake scenarios, it is crucial to ensure that models are making safe decisions for the right reasons (Janizek, Sturmels, and Lee 2021).

1.1.3 Properties of Explanations.

Model explanation methods in NLP can be categorized with regard to the following properties:

(a) **Time:** when the explanation happens. An explanation can be **post-hoc**, i.e., it is produced *after* the prediction. Any opaque model is given, and then an external method explains it. Or, an explanation can be **built-in**, i.e., it is produced *at the same time with* the prediction. This means that the model is self-explanatory.

(b) **Model accessibility:** what parts of the model the explanation method has access to. A **black-box** explanation can only see the model’s input and output, while a **white-box** explanation can additionally access the model weights.

(c) **Scope:** where the explanation applies in the dataset. A **local** explanation only explains why a model makes a single prediction (or a small number of predictions

² Given a premise P and a hypothesis H , the textual entailment task is to determine if P entails H (whenever P is true, is H also true?). For example, *he can run fast* entails *he can run*.

Method	Time	Model accessibility	Scope	Unit of explanation	Form of explanation
Similarity methods	post-hoc	white-box	local	examples, concepts	importance scores
Analysis of model-internal structures	post-hoc	white-box	local, global	features, interactions	visualization, importance scores
Backpropagation-based methods	post-hoc	white-box	local	features, interactions	visualization, importance scores
Counterfactual intervention	post-hoc	black-box, white-box	local, global	features, examples, concepts	importance scores
Self-explanatory models	built-in	white-box	local, global	features, examples, concepts	importance scores, natural language, causal graphs

Table 1: Comparison of different model explanation methods in terms of their properties. Different colors denote different values of a property. See Section 1.1.3 for details.

in its local vicinity), whereas a **global** explanation provides insights into the general reasoning mechanisms for the entire data distribution.

(d) **Unit of explanation:** what the explanation is in terms of. A prediction can be explained in terms of **input features** (Elazar et al. 2021), **examples** (Wallace, Feng, and Boyd-Graber 2018), **concepts**³ (Rajagopal et al. 2021), **feature interactions** (Hao et al. 2021), or a **combination** of them (Jacovi et al. 2021).

(e) **Form of explanation:** how the explanation is presented. Typical forms include **visualization** (Li et al. 2016), **importance scores** (Arras et al. 2016), **natural language** (Kumar and Talukdar 2020), or **causal graphs** (Dalvi et al. 2021).

(f) **Target audience:** who is the explanation provided for. As mentioned in Section 1.1.1, different audience groups can have distinct goals when requiring model explanations. **Model developers** may want to debug the model; **fellow researchers** may want to find how the model can be extended/improved; **industry practitioners** may want to assess if the model complies with practical regulations, e.g., it cannot use gender bias; and **end-users** may want to verify that they can safely rely on the model’s decisions.

As a preview, Table 1 compares the model explanation approaches to be discussed in terms of these properties.⁴ Note that many existing taxonomies do not explicitly state which properties are taken into account, thus often producing confusing terms. For instance, certain taxonomies juxtapose *example-based*, *local*, and *global* as three classes of explanations, but they are not even concerning the same property. As another example,

³ Prior work has different definitions of “concepts”, including but not limited to phrases (Rajagopal et al. 2021) and high-level features (Jacovi et al. 2021).

⁴ Note that the target audience is not included in the table, since it largely depends on the task and the specific instance of the method.

the term *saliency methods* has been used to refer to Backpropagation-based methods in our taxonomy. In fact, *saliency* only describes the form and the unit of explanation – importance scores of features. Then, technically speaking, all methods in Table 1 have instances that can be called a *saliency method*. Therefore, we aim to outline all properties for comparison and specify their values for each method in our taxonomy.

1.1.4 Principles of Explanations.

To motivate principled design and evaluation of model explanations, previous work has identified a set of principles that a good explanation should satisfy. Here is a non-exhaustive synthesis:

(a) **Faithfulness** (also referred to as *fidelity* or *reliability*): *an explanation should accurately reflect the reasoning process behind the model's prediction* (Harrington et al. 1985; Ribeiro, Singh, and Guestrin 2016; Jacovi and Goldberg 2020). This is at the heart of this survey. In our opinion, Faithfulness is the most fundamental requirement for any explanation – after all, what is an explanation if it *lies* about what the model does under the hood? An unfaithful explanation can sound intuitive to humans, but has little to do with how the model makes the prediction. For example, by looking at the attention weights⁵ of a sentiment classification model, it may be intuitive to interpret tokens with higher weights as “more important” to the prediction, whereas empirically it is questionable if such causal relation exists (Jain and Wallace 2019).

(b) **Plausibility** (also referred to as *persuasiveness* or *understandability*): *an explanation should be understandable and convincing to the target audience* (Herman 2019; Jacovi and Goldberg 2020). This implies that Plausibility depends on who the target audience is. For example, a relevance propagation graph across NN layers may be a perfectly plausible explanation for model developers, but not at all plausible to non-expert end-users.

(c) **Input Sensitivity**: the term is used by many papers in different senses, but the commonality is that *an explanation should be sensitive (resp. insensitive) to changes in the input that influence (resp. do not influence) the prediction*. Specifically, it has at least the following sub-principles:

(i) Sundararajan, Taly, and Yan (2017): (for explanations whose unit is features and form is importance scores), if two inputs differ only at one feature and lead to different model predictions, then the explanation should assign non-zero importance to the feature.

(ii) Adebayo et al. (2018): if the input data labels are randomized, the explanation should also change. This is because label randomization does change model predictions, so the explanation should be sensitive.

(iii) Kindermans et al. (2019): if a constant shift is added to every input example in the training data, the explanation should not change. This is because the model is invariant to the constant shift, and thus the explanation should not be sensitive.

(d) **Model Sensitivity**: likewise, the term is used in different senses, but in general, it means that *an explanation should be sensitive (resp. insensitive) to changes in the model that influence (resp. do not influence) the prediction*. Specifically, it requires at least that:

⁵ We will elaborate on attention in Section 2.3.

(i) [Sundararajan, Taly, and Yan \(2017\)](#): an explanation should be insensitive to model implementation details that do not affect the prediction. More specifically, two models are *functionally equivalent* if their outputs are equal for *all* possible inputs, although their implementations might be different. The explanation should always be identical for functionally equivalent models. This is called Implementation Invariance in the paper.

(ii) [Adebayo et al. \(2018\)](#): if the model weights are randomized, the explanation should also change. Similar to (c)(ii), weight randomization does change model predictions, so the explanation should be sensitive.

(e) **Completeness**: *an explanation should comprehensively cover all relevant factors to the prediction* ([Sundararajan, Taly, and Yan 2017](#)). More formally, for explanations in the form of importance scores, the importance of all features should sum up to some kind of “total importance” of the model output.⁶

(f) **Minimality** (also referred to as *compactness*): *an explanation should only include the smallest number of necessary factors* ([Halpern and Pearl 2005; Miller 2018](#)). Intuitively, this is analogous to the Occam’s razor principle, which prefers the simplest theory among all competing ones.

These principles have been proposed and entertained by the community, but not all of them have established technical definition, evaluation, or even a consensus on whether they are necessary as a principle. In fact, we do not agree with all of them, as will be discussed in Section 1.2.4. Therefore, in this survey, we mainly focus on Faithfulness as it is generally considered one of the most central requirements for explanations ([Jain and Wallace 2019; Bastings and Filippova 2020; Jacovi and Goldberg 2020, inter alia](#)), but we will still refer to the other principles when discussing relevant work throughout subsequent sections.

1.2 Faithfulness as a Principle

Now, we will zoom in on Faithfulness as one of the above principles, analyzing what it means, its relation to other principles, why it is important, and how it can be measured.

1.2.1 Definition.

As mentioned before, a faithful explanation should **accurately reflect the reasoning process behind the model’s prediction** ([Harrington et al. 1985; Ribeiro, Singh, and Guestrin 2016; Jacovi and Goldberg 2020](#)). This is only a loose description though. In fact, there is not yet a consistent and formal definition of Faithfulness in the community. Instead, people often define Faithfulness on an ad-hoc basis, in terms of different evaluation metrics. We will detail it in Section 1.2.4.

1.2.2 Relation between Faithfulness and Other Principles.

We elucidate the relation between Faithfulness and several other principles introduced in Section 1.1.4, since they are often implicitly conflated in the literature.

⁶ See Section 2.4.2 – Propagation Methods for more details on “total importance”.

Faithfulness vs. Plausibility. There is an intrinsic tension between Faithfulness and Plausibility. Think about an extreme case: if an “explanation” were just a copy of all model weights, it would be perfectly faithful but not at all plausible to any target audience. Now consider the other extreme: we could first ask the target audience which features they consider the most important when they themselves were predicting the label of the example. We could then simply copy their response as our “explanation” of how our target model works. This “explanation” would be perfectly plausible to the audience since it fully matches the human reasoning process, but not at all faithful since it has nothing to do with how the model works. Therefore, Plausibility does not guarantee Faithfulness, and vice versa.

Moreover, when we observe that an explanation is implausible in human terms, there can be two possibilities: (a) the model itself is not reasoning in the same way as humans do, and (b) the explanation is unfaithful. For instance, if an explanation says that the model is mainly relying on function words like *the*, *a* instead of content words like *awesome*, *great* in sentiment classification, it could be that (a) the model is truly relying on those uninformative words to make predictions, potentially because of spurious correlations in the dataset, or that (b) the model is actually relying on content words, but the explanation does not faithfully reflect the fact. Thus, while a lot of prior work evaluates explanations via user studies, this only touches on Plausibility, but does not tell us anything about Faithfulness.

Faithfulness vs. Sensitivity, Implementation Invariance, Input Invariance, and Completeness. These four principles are sometimes seen as necessary conditions for Faithfulness, though not always explicitly (Sundararajan, Taly, and Yan 2017; Kindermans et al. 2019; Yeh et al. 2019). Practically, they are often used to prove that an explanation is *not* faithful via counterexamples. For example, given an explanation method, researchers run it on a dataset and see if there exists any example(s) where these principles are violated. This is called sanity checks in the literature (Adebayo et al. 2018).

Faithfulness vs. Minimality. There are no known relations between them, either from the literature or from the authors’ point of view.

1.2.3 Importance.

We believe that Faithfulness is one of the most fundamental principles for explainability in any AI system. In NLP specifically, there are two additional pieces of empirical evidence in support of Faithfulness:

(a) **Faithfulness establishes causality.** As mentioned in Section 1.1.1, there are two types of work in NLP explainability: *what knowledge a model encodes* and *why a model makes certain predictions*. The *what* type of work tells us “what is known by the model”, but this is oftentimes implicitly assumed to be also “what is used by the model in making predictions”. However, this assumption is not sound. For example, Ravichander, Belinkov, and Hovy (2021) show that language models encode linguistic features like tense and number, although they are irrelevant to the end task labels. This means that a model can encode more than what eventually gets used. Therefore, findings from the *what* type of work are correlational but not causal. To establish causality, we need faithful explanations of how the model makes predictions.

(b) **An unfaithful explanation can be dangerous.** Consider an explanation that is not faithful but extremely plausible. It will look very appealing to end-users. Thus, even if the model makes wrong predictions in the future, users may still trust them simply because the explanation sounds plausible. For example, Pruthi et al. (2020) show that it is possible to attention weights can be a *deceiving* explanation to end-users. They train

the model to attend minimally to gender-related tokens (e.g. *he* and *she*), therefore *hiding* the fact that the model is relying on gender bias in prediction. Users may still find the model trustworthy from the explanation since it seems free from bias.

1.2.4 Evaluation.

As mentioned in Section 1.2.1, Faithfulness does not have an established formal definition, but is usually defined ad-hoc during evaluation. However, the evaluation metrics are often inconsistent and incomparable with each other, making it difficult to objectively assess progress in this field.

In their seminal opinion piece, [Jacovi and Goldberg \(2020\)](#) outline several design principles of Faithfulness evaluation metrics, three of which are the most important (and most ignored) in our view: (a) “Be explicit in what you evaluate”. Especially, do not conflate Plausibility and Faithfulness. (b) Faithfulness evaluation should not involve human judgment on explanation quality. Humans do not know whether an explanation is faithful; if they did, the explanation would be necessary. (c) Faithfulness evaluation should not involve human-provided gold labels (for the examples to be explained). A faithful explanation method should be able to explain *any* prediction of the model, whether it is correct or not.

With the above principles in mind, we review existing Faithfulness evaluation methods, which broadly fall into six categories: **axiomatic evaluation**, **predictive power evaluation**, **robustness evaluation**, **perturbation-based evaluation**, **white-box evaluation** and **human perception evaluation**.

(a) Axiomatic evaluation treats certain principles (also called *axioms*) from Section 1.1.4 as *necessary conditions* for Faithfulness, and test if an explanation method satisfies them. If it fails any test, then it is unfaithful. However, passing all tests does not guarantee that it is faithful. Thus, axiomatic evaluation is mostly used to disprove Faithfulness via counterexamples.

As mentioned in Section 1.2.2, principles that have been viewed as necessary conditions for Faithfulness include Model Sensitivity, Input Sensitivity, and Completeness.

In particular, under **Model Sensitivity**, [Sundararajan, Taly, and Yan \(2017\)](#) tests Implementation Invariance, which means that two functionally equivalent models (i.e., they have the same outputs for all inputs) should have the same explanation. An **assumption** of this test is that two models are functionally equivalent *only if* they have the same reasoning process ([Jacovi and Goldberg 2020](#)). If this assumption holds, when a method provides different explanations for functionally equivalent models, it is unfaithful. However, we do not agree with this assumption. First, it treats the model as a black-box, only considering its input and output. But the reason why we need explanations is that models should not be black-boxes. Second, there exist functionally equivalent models that rely on entirely different reasoning mechanisms, such as various sorting algorithms. It is counter-intuitive if all of them have the same explanation. Therefore, we do not believe that Implementation Invariance is a necessary condition for Faithfulness.

Other axiomatic tests under Model Sensitivity ([Adebayo et al. 2018](#)), Input sensitivity ([Sundararajan, Taly, and Yan 2017; Adebayo et al. 2018; Kindermans et al. 2019](#)), and Completeness ([Yeh et al. 2019](#)), are considered more sensible as necessary

conditions for Faithfulness by us.⁷

(b) Predictive power evaluation uses the explanation to predict model decisions on unseen examples, and considers a higher accuracy as indicating higher Faithfulness. The **assumption** is that an explanation is unfaithful if it results in different decisions than the model it explains (Jacovi and Goldberg 2020). In practice, there are two ways to derive predictions from the explanation: with (other) **models** or with **humans**. In the former case, either the explanation is an executable model itself, e.g., rule lists (Sushil et al. 2018), or another proxy model is trained with the explanation as input (Li et al. 2020). In the latter case, humans are considered the “proxy model”. They are asked to simulate the model’s decision on new input examples with only access to the explanation (Doshi-Velez and Kim 2017; Ribeiro, Singh, and Guestrin 2018; Chen et al. 2018; Ye, Nair, and Durrett 2021).

In our opinion, the first case (with models) is theoretically reasonable. Nevertheless, in practice, it is still questionable how expressive the proxy model should be. If too expressive, the proxy model can learn the label itself, regardless of the quality of the explanation.

The second case (with humans) is less reasonable from our view. First, it mingles Plausibility with Faithfulness. If humans fail to simulate model predictions, then it could *either* that the explanation is not plausible (to them) *or* that the explanation is unfaithful. Moreover, when simulating the model’s prediction, it is difficult to ensure that humans can eliminate their own judgments of what the gold label should be.

Therefore, we believe that the predictive power evaluation is a sensible test for Faithfulness, but we should be cautious with human involvement.

(c) Robustness evaluation measures if the explanation is stable against subtle changes in the input examples, e.g., images that are indistinguishable from each other.

In its earliest version, robustness requires that similar inputs should have similar explanations (Alvarez-Melis and Jaakkola 2018). However, this does not rule out the possibility that the model itself can be brittle to subtle input perturbations.

Later work remedies this flaw by imposing constraints on model predictions. Now, robustness means that for similar inputs that have similar outputs, the explanations should be similar (Ghorbani, Abid, and Zou 2019; Yeh et al. 2019). The underlying **assumption** is that on similar inputs, the model makes similar predictions *only if* the reasoning process is similar (Jacovi and Goldberg 2020).

We identify two problems with this evaluation. First, though the notion of “indistinguishable inputs” makes sense in vision, it is hardly applicable to NLP since the input space is discrete. Second, the above assumption is questionable. Even though the inputs and outputs are similar, the model’s reasoning mechanism can still differ. For example, consider two similar cat images, which differ only in the length of the cat’s fur. We observe that the model predicts `cat` for both images with similar confidence. Now, it is still possible that the model is mainly relying on different features (e.g., body shape in the first image, while fur color in the second) in the two predictions. There is theoretically nothing preventing the model from doing so. Thus, if we observe that an explanation is not robust, we cannot conclude if it is because the explanation is unfaithful *or* the model is truly relying on different features.

⁷ Please refer back to Section 1.1.4 for details.

Therefore, we do not recommend robustness as a good evaluation metric for Faithfulness.

(d) Perturbation-based evaluation perturbs parts of the input according to the explanation, and observes the change in the output. It differs from robustness evaluation in that robustness considers extremely similar inputs and expects that the explanation is similar; but now, we consider inputs that are not necessarily similar, and the expectation of the explanation depends on which parts of the input are perturbed.

Concretely, consider an explanation in the form of feature importance scores. We now remove a fixed portion of features from the input, based on the explanation. If the most important features are first removed, the model prediction is expected to change drastically. Conversely, removing the least important features should result in a smaller change. This type of evaluation has been widely adopted in both vision (Bach et al. 2015; Shrikumar, Greenside, and Kundaje 2017; Chen et al. 2018) and language (Arras et al. 2016; Chen et al. 2018; Serrano and Smith 2019; Jain and Wallace 2019; DeYoung et al. 2020; Atanasova et al. 2020).

One underlying **assumption** is that different parts of the input are *independent* in their contribution to the output (Jacovi and Goldberg 2020). However, features can be correlated. When one feature is removed, we cannot guarantee that other features stay untouched.

Another **assumption** is that the observed performance change does *not* come from nonsensical inputs. When certain features are perturbed, the resulting input becomes out-of-distribution (OOD). Compared to CV, this has more serious consequences in NLP, since removing a word can make the sentence ungrammatical or nonsensical, but removing a pixel almost does not change the semantics of an image. Hooker et al. (2019) addresses the issue in CV by proposing the RemOve And Retrain (ROAR) benchmark. According to a given explanation method, the set of most important features is removed from *both* the training and the testing data. The model is then trained and tested again on the new data, and a larger performance drop indicates higher Faithfulness. In their experiments, image classification models are found to still achieve decent accuracy even after most input features (90%) are removed. This indicates that the performance drop observed in previous evaluation approaches without retraining might indeed come from the distribution shift instead of the lack of important information. However, though ROAR ensures that the training and testing data come from the same distribution, it brings about a new problem – the model itself is not the same.

In short, while perturbation-based evaluation has been widely used, we should be cautious about the assumptions and their consequences, especially since there is still no good fix in NLP.

(e) White-box evaluation rely on known ground-truth explanations, against which a candidate explanation can be compared. The ground-truth explanations come from **transparent tasks** or **transparent models**.

Transparent tasks are typically synthetic tasks where the set of informative features is controlled. For example, reconstructing a simple function (Chen et al. 2018; Hooker et al. 2019), counting and comparing the number of digits (De Cao et al. 2020), or text classification on synthetic hybrid documents (Poerner, Schütze, and Roth 2018). Since the informative features are controlled, any model that performs well on the tasks must have relied on these features. Therefore, the ground-truth explanation is known.

Transparent models are inherently interpretable models, e.g., Logistic Regression or Decision Tree. The ground-truth explanation of important features can be directly

obtained through their weights or prediction structure (Ribeiro, Singh, and Guestrin 2016; Natesan Ramamurthy et al. 2020).

Thus, one can run an explanation method with the transparent task or the transparent model, and compare the resulting explanation with the ground truth. If they are clearly different, then the explanation method is unfaithful.

However, this test is still only a sanity check, constituting a necessary instead of sufficient condition for Faithfulness. Since the synthetic setups are simplified, passing the white-box test still does not guarantee that the explanation method can generalize to real-world scenarios.

(f) **Human perception evaluation** assesses if the explanation matches human perception. For example, if the explanation is a set of feature importance scores, to what extent does it align with human-annotated importance scores?

A lot of previous work report this type of user studies (Feng et al. 2018; DeYoung et al. 2020), without clarifying what principle is evaluated. Essentially, such tests only evaluate Plausibility. For them to also touch on Faithfulness, we need to make the **assumption** that models reason in the same way as humans do. Obviously, this does not always hold; otherwise, we will not need explanations at all. As said at the beginning of Section 1.2.4, Faithfulness evaluation should not involve human judgment on the explanation quality (Jacovi and Goldberg 2020).

Summary. Among existing evaluation approaches, we recommend axiomatic evaluation, predictive power evaluation (with models), perturbation-based evaluation, and white-box evaluation, with caveats specified before. More ideally, more than one of the above evaluations should be done, since some of them only test a necessary condition of Faithfulness.

To complement the list of design principles provided by Jacovi and Goldberg (2020), we additionally propose a few more towards a better evaluation of Faithfulness:

(a) **Define Faithfulness in advance rather than ad-hoc.** Instead of using the same term to refer to different things, a clear definition at the beginning of the evaluation will greatly benefit comparability.

(b) **State the assumptions of the evaluation, where they do not hold, and its implications.** Especially, do not make assumptions about how the model reasons, e.g., “they reason in the same way as humans do”, as this conflates plausibility with Faithfulness.

(c) **Disentangle the capacity of the model and the quality of the explanation.** For example, a non-robust explanation can result from *either* the model relying on inconsistent features *or* the explanation being unfaithful.

2. Attempts at Faithful Explanation

2.1 Overview with Motivating Example

We summarize recent advances in developing faithful explanation methods into five categories: similarity methods, analysis of model-internal structures, backpropagation-based methods, counterfactual intervention, and self-explanatory models. To give the reader a quick overview, we briefly explain the intuition behind each method with a motivating example.

Consider the Sentiment Analysis task, where a model should determine if the sentiment of a given piece of text (e.g., product/movie review) is positive, negative, or neutral. An example input can be:

This movie is great. I love it.

Suppose the model prediction is positive, which matches the ground truth. Our goal, now, is to explain **why the model makes such a prediction**. Here is how each method answers the question on a high level:

Similarity methods provide explanations in terms of previously seen examples, similar to how humans justify their actions by analogy. Specifically, they identify training instances or concepts⁸ that are similar to the current test example in the model’s induced representation space (e.g. *The movie is awesome, The TV show is great*) as an explanation, assuming that the reasoning mechanism for similar examples is intrinsically similar.

Analysis of model-internal structures examines the activation patterns of nodes, layers, or other model-specific mechanisms (e.g., attention ([Bahdanau, Cho, and Bengio 2015](#))), and derives an explanation with techniques like visualization, clustering, correlation analysis, etc. For example, on a visualized heat-map of attention weights, *great* and *love* may have the highest weight among all token positions. This can be interpreted as that these two tokens are contributing the most to the prediction.

Backpropagation-based methods compute the gradient (or some variation of the gradient) of the model prediction with respect to each feature (e.g., input token). Features with the largest absolute gradient value (say, *great* and *love*) are then considered most important to the prediction. The intuition behind is that *theoretically*, even a slight change in those features⁹ could have resulted in a large change in the model output. For example, if *great* becomes *good* and *love* becomes *like*, the model’s confidence of positive will probably not be as high.

Counterfactual intervention perturbs a specific feature (e.g., input token) while controlling for other features and observes the resulting influence in the model prediction. For example, to test if the word *great* is important for the model prediction, we can mask it out or replace it with another word, e.g. *OK*, and see how the model prediction changes. If the probability of the positive class decreases dramatically, then the word *great* has been an important feature.

Self-explanatory models do not rely on a post-hoc explanation but provide explanations as a byproduct of the inference. For example, a self-explanatory model can be trained to predict the sentiment label (e.g., positive) and justify its prediction at the same time, by producing a natural language explanation (e.g., “The words *great* and *love* indicate that the person adores the movie”).

2.2 Similarity Methods

2.2.1 Overview.

Similarity methods provide explanations in terms of training examples. Specifically, to explain the model prediction on a test example, they find its most similar¹⁰ training examples in the learned representation space, as support for the current prediction. This is akin to how humans explain their actions by analogy, e.g., doctors make diagnoses based on past cases and courts make judgments based on precedents.

⁸ cf. Section 1.1.3

⁹ For discrete inputs like tokens, the slight change is defined in terms of similarity metrics in the embedding vector space.

¹⁰ In practice, commonly used similarity metrics include cosine, Euclidean, etc.

2.2.2 Past Work.

[Caruana et al. \(1999\)](#) formalize the earliest approach of this kind, named “case-based explanation”. Based on the learned hidden activations of the trained model, it finds the test example’s k-Nearest Neighbors (kNN) in the training set as an explanation. Note that the similarity is defined in terms of the *model’s learned space* but not the *input feature space*, since otherwise the “explanation” would be model-independent. The authors analyze the theoretical applicability of this approach to Decision Trees and Neural Networks, but did not experiment or evaluate it in practice.

[Wallace, Feng, and Boyd-Graber \(2018\)](#) also use the kNN search algorithm; but instead of a post-hoc explanation, they replace the model’s final softmax¹¹ classifier with a kNN classifier at test time. Concretely, during training, the model architecture is unmodified. Then, each training example is passed through the trained model, and their representations are saved. Now, the inference is done with a modified architecture: a test example is passed through the model and then classified based on the labels of its kNNs in the learned representation space. This approach does not degrade the model performance, according to experimental results with LSTM and CNN models on six text classification tasks. Moreover, it can be combined with other explanation methods of feature importance. However, the resulting explanations are only evaluated on whether the identified features align with human perception of importance on qualitative examples, which is irrelevant to Faithfulness.

[Rajagopal et al. \(2021\)](#) introduce a self-explanatory classification model where one component is called a global interpretable layer. This layer essentially identifies the most similar *concepts* (phrases in this case) in the training data for a given test example. Their approach is mainly evaluated in terms of Plausibility to humans, e.g., how adequate/understandable/trust an explanation is based on their subjective judgment. Only one metric touches on Faithfulness – whether humans can predict model prediction based on the explanation. However, they only report the relative difference in the metric with and without the explanation, instead of absolute scores, which makes it hard to determine how faithful the approach is.

2.2.3 Advantages.

(a) Similarity methods are **intuitive** to humans since the justification by analogy paradigm has long been established.

(b) They are also **easy to implement**, as no re-training or data manipulation is needed. The similarity scores are available by simply passing examples through the trained model to obtain the model’s representation of them.

(c) In addition, they are **highly model-agnostic**, since all kinds of neural networks have a representation space. Thus, any similarity metric (like cosine similarity) can be easily applied.

(d) Finally, human subjects rate similarity-based explanations ([Rajagopal et al. 2021](#)) as more **understandable, adequate and trustworthy** to several other baselines in the family of backpropagation-based methods and counterfactual intervention ([Simonyan, Vedaldi, and Zisserman 2014](#); [Han, Wallace, and Tsvetkov 2020](#)).

¹¹ https://en.wikipedia.org/wiki/Softmax_function

"You mean to imply that I have nothing to eat out of.... On the contrary, I can supply you with everything even if you want to give dinner parties," warmly replied Chichagov, who tried by every word he spoke to prove his own rectitude and therefore imagined Kutuzov to be animated by the same desire.

Kutuzov, shrugging his shoulders, replied with his subtle penetrating smile: "I meant merely to say what I said."

Figure 1: A neuron that “turns on” inside quotes (figure from Karpathy, Johnson, and Fei-Fei (2015)). Blue/red indicates positive/negative activations respectively, and a darker shade indicates larger magnitude.

2.2.4 Disadvantages.

(a) Most similarity methods only provide the user with the **outcome** of the model’s reasoning process (i.e., which examples are similar in the learned space), but do not shed light on *how* the model reasons (i.e., how the space is learned) (Caruana et al. 1999).

(b) Existing work mostly evaluates the resulting explanations with Plausibility-related metrics, including adequacy, relevance, understandability, usefulness, etc., through human judgments. But as mentioned in Section 1.2, Plausibility is not equal to **Faithfulness**. These evaluations only measure whether the explanation aligns with how *humans* reason about an example, but not how models do it. Thus, it is questionable whether similarity methods can truly establish causality between the model prediction and the explanation.

2.3 Analysis of Model-Internal Structures

2.3.1 Overview.

The analysis of model-internal structures, e.g., neurons, layers, and specific mechanisms like convolution or attention, is believed to shed light on the inner workings of NLP models. Common analysis techniques include visualization (e.g., activation heatmaps, information flow), clustering (e.g., neurons with similar functions, inputs with similar activation patterns), and correlation analysis (e.g., between neuron activations and linguistic properties).

2.3.2 Past Work.

We categorize research into this area historically, breaking it into work that happened before and after the advent of the attention mechanism (Bahdanau, Cho, and Bengio 2015). The reason is that attention has become one of the most widely-adopted architectures in NLP systems nowadays and has significantly reshaped this line of work ever since.

The pre-attention era. The initial success of neural models in NLP sparked interest in finding interpretable functions of individual neurons. (Karpathy, Johnson, and Fei-Fei 2015) examine the activation patterns of neurons in a character-level Long-Short Term Memory (LSTM) language model. They found neurons with specific purposes, e.g., one that activates within quotes, inside if-statements, or toward the end of a line, respectively (Figure 1). Li et al. (2016) visualize LSTM’s representation of compositional structures in language, including negation (e.g., “not + adjective”) and intensification (e.g., “very + adjective”), as shown in Figure 2. Neurons are found to capture basic semantic properties of compositionality, for instance, negated positive adjectives (e.g.

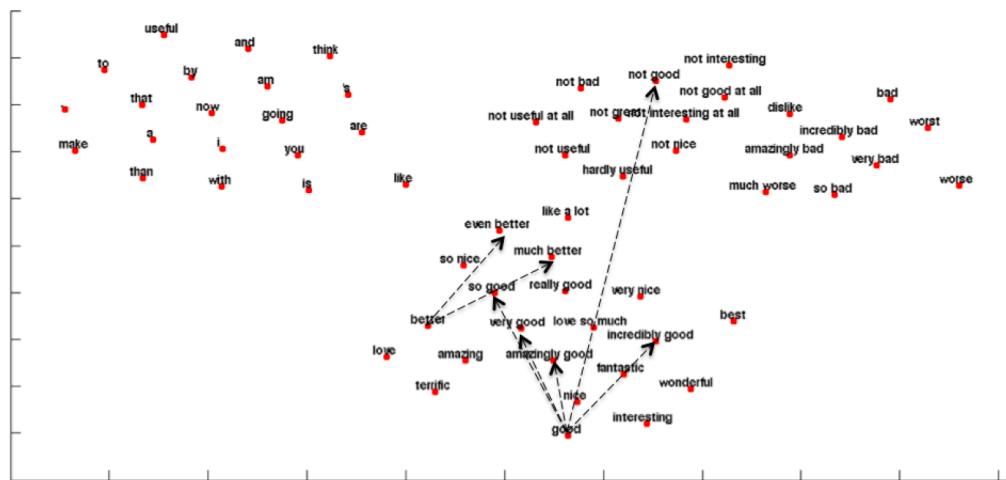


Figure 2: t-SNE visualization on latent representations for modifications and negations (figure from Li et al. (2016)).

“not nice”, “not good”) are clustered together with negative adjectives (e.g. “bad”) in the latent representation space. Also using visualization methods, Strobelt et al. (2018) identifies neurons in LSTM with specific functions, e.g., those that turn on for “a + adjective + noun”. Poerner, Roth, and Schütze (2018) and Hiebert et al. (2018) take the reverse direction: instead of analyzing which neurons fire for a given input pattern, they look for inputs that have similar neuron activations. Preliminary observations show that Gated Recurrent Units (GRU) and LSTM language models can capture certain orthographic and grammatical patterns.

In the meantime, a variety of visualization tools are developed, including RNNvis¹² (Ming et al. 2017), LSTMVis¹³ (Strobelt et al. 2018), Seq2Seq-Vis¹⁴ (Strobelt et al. 2019), etc., allowing researchers to inspect and interact with their own models.

The post-attention era. Since its birth, Transformers (Vaswani et al. 2017) has become the foundation of State-of-the-Art (SOTA) systems on many NLP tasks (Devlin et al. 2019; Liu et al. 2019; Clark, Luong, and Le 2020; Brown et al. 2020; Raffel et al. 2020). The core of Transformers is an attention mechanism, **self-attention**. Simply put, self-attention is a function that takes in a sequence of vectors $X = \langle x_1, x_2, \dots, x_n \rangle$ as input and returns another sequence of vectors $Y = \langle y_1, y_2, \dots, y_n \rangle$ of the same length. Each y_i is a weighted average of all x_i 's, i.e., $y_j = \sum_{i=1}^n a_{ij}x_i$. These weights a_{ij} are called **attention weights**, representing how much the model attends to each input feature when computing the weighted average.¹⁵

12 <https://www.myaooo.com/projects/rnnvis/>

13 <http://lstm.seas.harvard.edu/>

14 <https://seq2seq-vis.io/>

15 The attention weights are computed by a **compatibility function**, which assigns a score to each pair of input features indicating how strongly they should attend to each other. Usually, it is instantiated as a re-scaled dot product. Read more in <https://towardsdatascience.com/deconstructing-bert-part-2-visualizing-the-inner-workings-of-attention-60a16d86b5c1>.

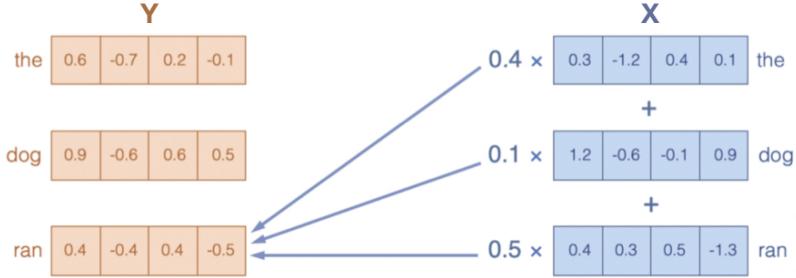


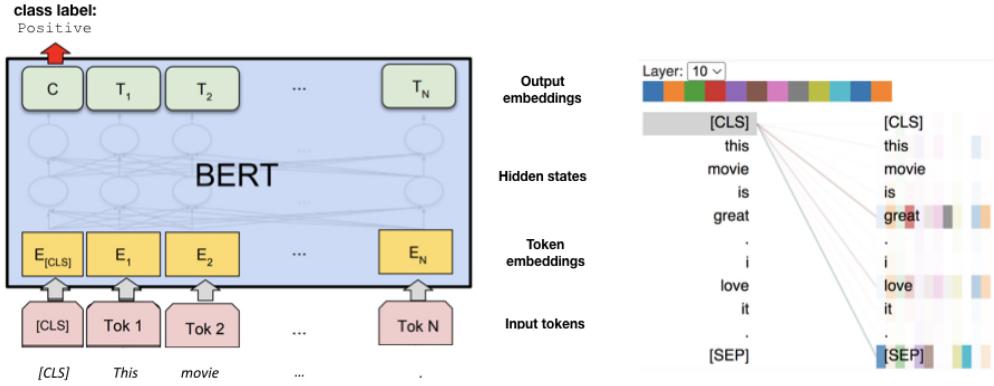
Figure 3: An illustration of the self-attention function (figure from <https://towardsdatascience.com/deconstructing-bert-part-2-visualizing-the-inner-workings-of-attention-60a16d86b5c1>). Each output vector y_j is a weighted average of input vectors X .

In NLP Transformer models, we can think of the initial X as word embeddings, i.e., each x_i is a vector representing a word in the input. Then, each y_i can be viewed as a **composite embedding**. For example, in Figure 3, the embedding for *ran* in Y is a composite of embeddings for *the*, *dog*, and *ran* in X , parameterized by a_{ij} . A Transformer model learns many such attention functions, each called an **attention head**. For example, in BERT (base), there are $12 \text{ layers} \times 12 \text{ heads/layer}$, which makes a total of 144 distinct attention heads. This allows the model to capture a broad range of linguistic phenomena, as we will discuss later.

Given this intuitive structure, it is tempting to interpret attention weights as the *importance* of input tokens to the output. Consider our running example, a sentence for sentiment classification: *This movie is great. I love it.* Figure 4 (left) shows how a BERT-based model makes a prediction: each input token embedding is encoded by a stack of intermediate Transformer layers, the core of which is the 144 attention heads; then, using the embedding of [CLS] (a special token for sentence classification tasks) in the final layer, it predicts the class label *positive*. On the right, it shows the attention weights from [CLS] to all tokens in the penultimate layer. Among all input tokens, *great* and *love* receive the highest averaged weights over all heads. They are often intuitively understood as the most important tokens for the prediction, which aligns with human perception. Such types of understanding have been used (implicitly or explicitly) as evidence for model interpretability in different tasks and domains, such as text classification (Martins and Astudillo 2016), knowledge base induction (Xie et al. 2017), and medical code prediction (Mullenbach et al. 2018).

Meanwhile, as in RNNs, people also discover units that capture interpretable input patterns in Transformer-based language models. By visualizing the activation patterns (Figure 5), Vig (2019) finds individual attention heads in GPT-2 (Radford et al. 2019) and BERT (Devlin et al. 2019) that are responsive to lexical patterns like named entities, subject-verb pairs, prepositions, acronyms, or coreference. Clark et al. (2019) further confirm these findings quantitatively, showing that certain attention heads can predict linguistic dependencies with remarkably high accuracy (e.g., direct objects of verbs, determiners of nouns, objects of prepositions, and coreferents) (Figure 6).

Despite these intuitive findings, researchers started the debate on whether attention constitutes a faithful model explanation. In their work, “Attention is not Explanation”,



(a) A BERT sentiment classification model. The class label is predicted with the embedding of CLS (a special token for sentence classification tasks) in the final layer.

(b) Attention weights from CLS to all tokens. Each color represents an attention head. Lines represent averaged attention weights over all heads, and darker shades stand for higher weights.

Figure 4: A BERT sentiment classification model (left, adapted from (Devlin et al. 2019)) and its attention weights on input tokens (right, created using BertViz(Vig 2019)). Given the input *This movie is great. I love it.*, the model predicts positive using CLS. In the penultimate layer, *great* and *love* are among the tokens with highest attention weight from CLS.

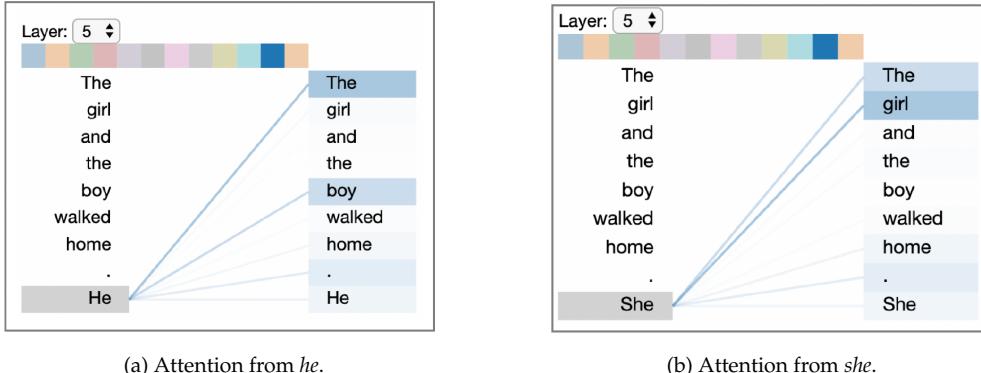


Figure 5: An attention head in GPT-2 that captures coreference (figure from Vig (2019)). The left and the right column stand for the output and the input of the attention function, respectively (i.e., each vector on the left is a weighted combination of all vectors on the right). Darker shades indicate larger attention weights.

Jain and Wallace (2019) contend that attention weights do not correlate with other feature importance measures that measure the feature's contribution to the output (e.g., gradient-based measures, which we will cover in Section 2.4). Also, one can construct an “adversarial attention distribution”, i.e., one that is maximally different from the

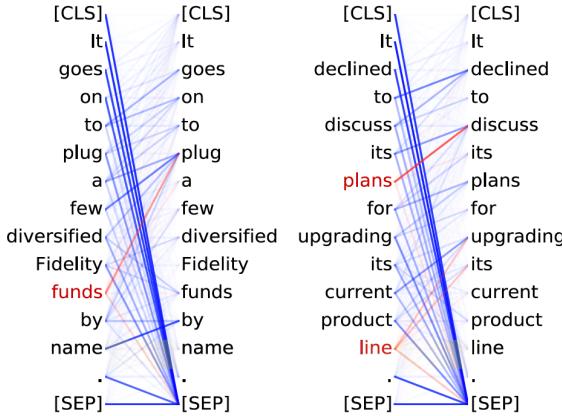


Figure 6: An attention head in BERT where direct objects attend to their verbs, with 86.8% accuracy (figure from Clark et al. (2019)). The direct objects of interest are highlighted in red.

after 15 minutes watching the movie i was asking myself what to do leave the theater sleep or try to keep watching the movie to see if there was anything worth i finally watched the movie what a waste of time maybe i am not a 5 years old kid anymore

original α
 $f(x|\alpha, \theta) = 0.01$

after 15 minutes watching the movie i was asking myself what to do leave the theater sleep or try to keep watching the movie to see if there was anything worth i finally watched the movie what a waste of time maybe i am not a 5 years old kid anymore

adversarial $\tilde{\alpha}$
 $f(x|\tilde{\alpha}, \theta) = 0.01$

Figure 7: A sentiment analysis model’s attention distribution α over words in a negative movie review (figure from Jain and Wallace (2019)). The left shows the observed attention weights (*waste* seems most important), and the right shows an adversarially constructed set of attention weights while controlling for all other parameters θ (*was* seems most important). Despite being quite dissimilar, they yield effectively the same prediction ($f = 0.01$).

original distribution but has little influence on the model output. For example, in Figure 7, a sentiment classification model predicts that a movie review is negative. Original attention weights suggest that *waste* and *asking* appear the most important, but the adversarial distribution shifts the model’s attention onto uninformative words like *myself* and *was*, without changing its prediction.

As a direct response, Wiegrefe and Pinter (2019) offer several counter-arguments: (a) Existence does not entail exclusivity. Theoretically, attention weights provided an explanation, but not the only explanation. In practice, most tasks considered in Jain and Wallace (2019) are binary classification, which leaves a vast amount of freedom in model parameters. Therefore, it should not be surprising if adversarial attention distributions can be found. (b) Adversarial distributions are not adversarial **weights**. The adversarial

attention distributions are artificially constructed by humans, but not learned by models through training. In other words, any trained model would probably not **naturally** attend most to uninformative words like *myself* and *was*. In fact, even when the authors try to guide the model’s attention towards such uninformative words using specially designed training objectives, they seldom converge to these adversarial distributions. (c) Though attention correlates poorly with other feature importance measures, it fares well on human evaluation. (This is, however, orthogonal to Faithfulness.)

[Pruthi et al. \(2020\)](#) again refutes argument (b), showing that with a simple training objective, they successfully guide the model to learn intended adversarial attention distributions. For example, when predicting the occupation of a person in the text, the model is trained to assign minimal attention weights to gender indicator tokens (e.g. “he” and “she”), while it is still *using* this signal in predictions. This implies that attention weights can be deceiving, i.e., a human user might find the model trustworthy since it is seemingly not relying on gender biases, yet it still does under the hood.

In favor of the use of attention as explanations, other researchers argue that existing criticisms mainly target single sequence tasks (e.g., Sentiment Analysis), but sequence-to-sequence tasks (e.g., Machine Translation (MT)) may be a more suitable use case because of the interaction between the two sequences. Similar to previous findings in single sequence tasks, attention heads in MT also capture semantic and syntactic dependencies ([Voita et al. 2018; Raganato and Tiedemann 2018; Voita et al. 2019](#)). However, regarding the contribution to the output, it is found that modifying or pruning the **encoder-decoder** attention heads *does* influence MT model predictions substantially ([Voita et al. 2019; Vashisht et al. 2019](#)), different than the case of single sequence tasks in [Jain and Wallace \(2019\)](#). Other attention heads, such as the encoder- or decoder- only ones, are less influential ([Voita et al. 2019; Raganato, Scherrer, and Tiedemann 2020](#)). In addition, in terms of the correlation with other feature importance measures, [Ferrando and Costa-jussà \(2021\)](#) qualitatively show that the L^2 -norm of attention vectors does correlate with gradient-based feature contributions.

Summarizing the debate, [Bastings and Filippova \(2020\)](#) still argue against attention and in favor of saliency methods¹⁶ as faithful explanations. However, they acknowledge that understanding the *role* of the attention mechanism is still interesting (e.g., what linguistic information it captures; which heads can be pruned without performance loss).

To make attention more faithful to model predictions, recent studies have started exploring ways to remedy the flaws of the interpretation. [Tutek and Snajder \(2020\)](#) argue that a problem with the current interpretation is that attention weights are assigned to **hidden states** (in intermediate layers) instead of **input representations** (in the initial layer), but we nevertheless interpret attention weights as the importance of the corresponding input feature. In fact, hidden states may have already mixed in information from other input features. To fix this, the authors introduce two regularization techniques: weight tying, which minimizes the distance between hidden states and their corresponding input representation; and an auxiliary Masked Language Modeling (MLM) task, which decodes input representations from their corresponding hidden state. Both techniques aim to make hidden states more representative of input representations. Experiments show that they effectively increase the influence of modifying the attention distribution on model predictions. [Hao et al. \(2021\)](#) explore an alternative path by combining attention with backpropagation-based methods, which

¹⁶ including backpropagation-based methods and counterfactual intervention in later sections of the survey.

we will revisit in Section 2.4. Their proposed Attention Attribution approach greatly eliminates uninformative connections in the vanilla attention weights¹⁷ and strengthens connections that contribute to the final prediction. With the new attention distribution, the authors are able to prune attention heads without much contribution, construct reasoning dependency graphs, and generate adversarial examples to attack models.

Readers who are interested in visualizing attention can look into the following tools: BertViz¹⁸ (Vig 2019) and LIT¹⁹ (Tenney et al. 2020).

2.3.3 Advantages.

- (a) The visualization of model-internal structures is **intuitive and readable** to humans, especially end-users.
- (b) There are many **interactive** tools, which help the user form hypotheses about their data and models and dynamically adjust them through minimal testing.
- (c) The attention mechanism can capture the **interaction** between features, whereas many other methods can only capture the sole influence of features themselves.
- (d) Model weights are **easily accessible and computationally efficient**, compared to other methods.

2.3.4 Disadvantages.

- (a) Vanilla attention weights may not necessarily represent **causal contribution**, as mentioned in the debate.
- (b) We often interpret attention weights on **hidden states** as the importance of input representations; however, a hidden state may not represent its corresponding input token because of contextual information.
- (c) Attention weights reflect how much the model attends to each input position **at one time step**, but not taking the whole computation path into account.

2.4 Backpropagation-based Methods

2.4.1 Overview.

By the name “backpropagation-based methods”, we refer to two specific lines of work: *gradient methods* and *propagation methods*.

They both attempt to identify the contribution of input features via a *backward pass* through the model, propagating the *importance* (or *relevance*, used interchangeably in the literature) scores from the output layer to the input layer.

The key difference is that **gradient methods follow standard backpropagation rules**. In other words, they directly compute the *gradient* (or some variant of it) of the output w.r.t the input features via the chain rule, assuming features with larger gradient values are more influential to the model prediction. By contrast, **propagation methods define custom backpropagation rules** for each layer and compute the relevance scores layer by layer until reaching the input. This is believed to better capture the redistribution of relevance through different layer types.

¹⁷ For example, a lot of tokens attend most to [SEP], a special token to mark the sentence boundary.

¹⁸ <https://github.com/jessevig/bertviz>

¹⁹ <https://pair-code.github.io/lit/>

Method	Computation of $r_i(x)$
Simple Gradients	$\frac{\partial M(x)}{\partial x_i}$, $\ \frac{\partial M(x)}{\partial x_i}\ _1$, or $\ \frac{\partial M(x)}{\partial x_i}\ _2$
Gradient \times Input	$x_i \odot \frac{\partial M(x)}{\partial x_i}$
Integrated Gradients	$(x_i - \bar{x}_i) \odot \int_{\alpha=0}^1 \frac{\partial M(\bar{x} + \alpha(x - \bar{x}))}{\partial x_i} d\alpha$ approximated by $(x_i - \bar{x}_i) \odot \sum_{\alpha=0}^1 \frac{\partial M(\bar{x} + \alpha(x - \bar{x}))}{\partial x_i}$
SmoothGrad	$\frac{1}{m} \sum_1^m \hat{r}_i(x)(x + \mathcal{N}(0, \sigma^2))$ where $\hat{r}_i(x)$ is any other relevance computation

Table 2: Summary of different **gradient methods** in terms of how they compute $r_i(x)$, the relevance of feature x_i . See Section 2.4.2 – Gradient methods for details on notations.

Most ideas in this family have been first proposed in Computer Vision (CV) and then adapted to NLP. In the following subsection, we will explain their origin and then adaptation.

To synthesize existing work, we will use the following notations throughout the remaining parts of the section: An example x (e.g., an image or a sentence) has features $x_i, i \in \{1, 2, \dots, n\}$ (e.g., a pixel or a token). A model M takes x as input and predicts $y = M(x)$ as output. Our goal is to explain the relevance of each feature x_i to y , denoted by $r_i(x)$. For some specific methods, we also define a *baseline input* \bar{x} (e.g., an all-black image, or a sentence with all-zero token embeddings) against which x is compared. We will define each subsequent method using these notations.

2.4.2 Past Work.

We describe first gradient methods and then propagation methods.

Gradient methods. As their name suggests, gradient methods treat the gradient (or some variant of it) of the model output w.r.t each input feature as its relative importance. Typically, the feature can be a pixel in vision and a token in language. Intuitively, the gradient represents how much difference a tiny change in the input will make to the output. This idea comes from linear models (e.g., Logistic Regression), where each feature has a linear coefficient as their importance to the output. In the case of non-linear models, a natural analog of such coefficients would be gradients, as they characterize the marginal effect of a feature change on the output.

Using the notation in Section 2.4.1, the core difference of existing gradient methods lies in how they calculate $r_i(x)$, the relevance of feature x_i , which is summarized in Table 2. Figure 8 shows a visual comparison of them.

The most straightforward idea is to take the gradient itself (referred to as **Simple Gradients** or **Vanilla Gradients**), $\frac{\partial M(x)}{\partial x_i}$, as the feature relevance (Baehrens et al. 2010; Simonyan, Vedaldi, and Zisserman 2014). The *sign* of the gradient represents whether the feature is contributing positively or negatively to the output, e.g., increasing or decreasing the probability of a certain class in a classification task. The *magnitude* of

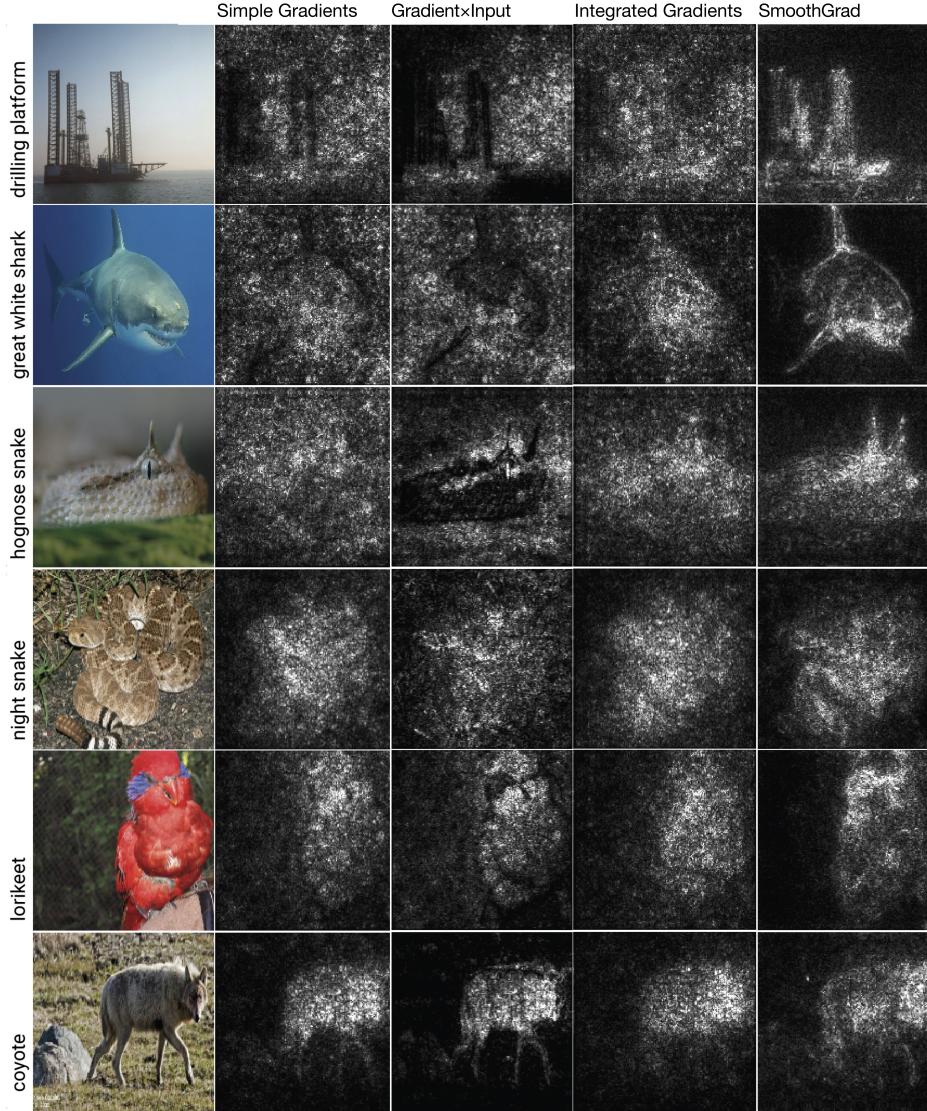


Figure 8: A visualization of different gradient methods on qualitative image classification examples (figure adapted from (Smilkov et al. 2017)). Brighter shades indicates higher relevance for the prediction.

the gradient stands for the extent to which the feature influences the output. Typically, this is measured by the L^1 -norm or L^2 -norm of the gradient. Simple Gradients are easy to implement and intuitive to understand. However, they have two apparent problems. **First**, a function can be *saturated*. Consider common neuron activation functions like sigmoid ($y = \frac{1}{1+e^{-x}}$) and tanh ($y = \frac{e^x - e^{-x}}{e^x + e^{-x}}$), shown in Figure 9. When $x \rightarrow \pm\infty$, we have $\frac{dy}{dx} \rightarrow 0$. In other words, when the input feature value is large enough, it has a very small gradient locally, while it may have a large contribution to the output y globally.

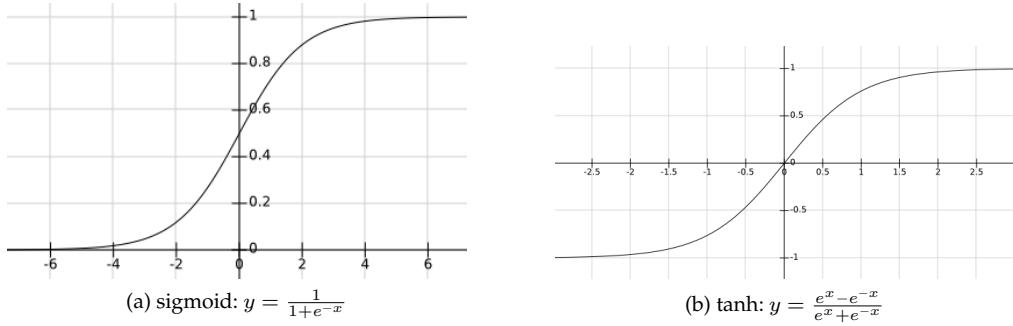


Figure 9: The sigmoid function and the tanh function. Both are “saturated” (i.e., the gradient is near-zero) when the input is small or large enough.

Second, gradient only measures the *responsiveness* of the output w.r.t. the feature (how much the output changes in response to an infinitesimal change in the feature), but not the *contribution* of the feature (how much the current feature value contributes to the output value) (Bastings and Filippova 2020). Say, in an image classification model, you can think of a gradient as an explanation of *how to make an image more (or less) a cat*, but not *what makes the image a cat*. More formally, taking a simple linear model $y = \sum_{i=1}^n w_i x_i$ as an example, the gradient w_i measures the responsiveness while $w_i x_i$ measures the contribution. If w_i is small but x_i is very large, the proportion of $w_i x_i$ in y can still be large. This cannot be captured by the gradient alone.

As a natural solution to the second issue, the **Gradient \times Input** method (Denil, Demiraj, and de Freitas 2015) is proposed. It computes the relevance score of a feature as the dot product of the input feature and the gradient, $x_i \odot \frac{\partial M(x)}{\partial x_i}$, analogous to $w_i x_i$ in a linear model. Intuitively, this incorporates the feature value itself. In CV, the method empirically reduces noise in feature relevance visualizations, e.g., making the edges sharper. However, it is unclear *how much* of the reduction comes from the sharpness in the input image, and how much comes from the model’s behavior. Also, Gradient \times Input fails the Sensitivity test (cf. Section 1.1.4), i.e., if two inputs differ only at feature x_i and lead to different predictions, then x_i should have non-zero relevance. A simple counterexample is when the differing feature x_i in these two inputs both have a zero gradient. Thus, the dot product is also both zero, which fails to capture their difference.

To address the saturation and sensitivity issues, Sundararajan, Taly, and Yan (2017) introduce the **Integrated Gradients** method. It estimates the global relevance of a feature by comparing the input with a *baseline input* \bar{x} . Typically, the baseline is chosen as an all-black image for vision and a sentence with all-zero token embeddings for language. With the original x and the baseline \bar{x} , the algorithm consists of four stages: first, it interpolates input points between x and \bar{x} , formally

$$x^\alpha = \bar{x} + \alpha(x - \bar{x}),$$

where $\alpha \in [0, 1]$; second, for each interpolated x^α , it computes the gradient of model output w.r.t to the target feature, or

$$\frac{\partial M(x^\alpha)}{\partial x_i}, \text{ 20}$$

third, the gradients are integrated, yielding

$$\int_{\alpha=0}^1 \frac{\partial M(x^\alpha)}{\partial x_i} d\alpha,$$

which is approximated by

$$\sum_{\alpha=0}^1 \frac{\partial M(x^\alpha)}{\partial x_i}$$

in practice; finally, the integral is re-scaled to remain in the same space as the original input, resulting in the final relevance score

$$r_i(x) = (x_i - \bar{x}_i) \odot \sum_{\alpha=0}^1 \frac{\partial M(x^\alpha)}{\partial x_i}.$$

Integrated Gradients satisfy the Sensitivity principle, as opposed to Gradient×Input. However, it is empirically observed to be visually noisy in CV, often resulting in blurry or unintelligible feature relevance maps (Smilkov et al. 2017).²¹

To this end, **SmoothGrad** is introduced (Smilkov et al. 2017), attempting to “remove noise by adding noise”. It hypothesizes that the Integrated Gradients method is visually noisy because the gradient can fluctuate rapidly with only subtle changes in the input. For example, one of the most commonly used activation functions, ReLU ($y = \max(0, x)$), is not continuously differentiable (at $x = 0$, the gradient does not exist). Such local fluctuations may lead to the apparent visual diffusion in relevance maps. Therefore, SmoothGrad proposes to create a few noisy copies of the original input, compute relevance maps for each copy with any existing method, and finally average all maps to obtain a less noisy map. Formally, the final relevance score is defined as

$$r_i(x) = \frac{1}{m} \sum_1^m \hat{r}_i(x)(x + \mathcal{N}(0, \sigma^2)),$$

where m is the number of noisy copies, $\mathcal{N}(0, \sigma^2)$ is Gaussian noise with mean 0 and standard deviation σ , and $\hat{r}_i(x)$ is any other relevance computation. This method proves effective in visually denoising the relevance maps. However, it is only qualitatively evaluated in terms of human readability; no Faithfulness is assessed.

In NLP, both Simple Gradients and Integrated Gradients have been adopted, but mostly targeting sequence classification tasks. Li et al. (2016) use Simple Gradients to

²¹ Of course, it is questionable if this noise comes from the deficiency of the explanation method or the model reasoning mechanism itself.

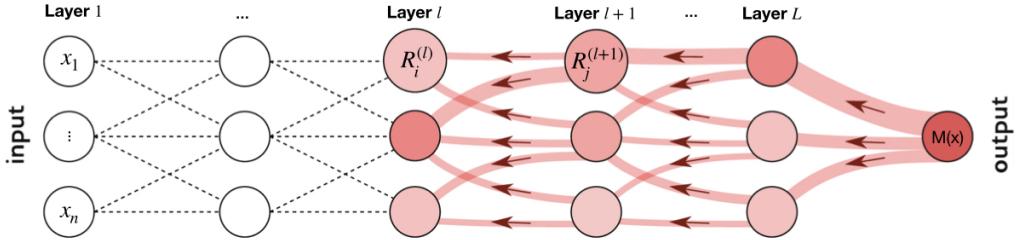


Figure 10: A schematic visualization of propagation methods. This figure is adapted from (Montavon et al. 2019).

explain token importance in RNN models on sentiment classification. More recently, targeting Transformer models, Hao et al. (2021) and Janizek, Sturmels, and Lee (2021) adapt Integrated Gradients to capture token interactions on paraphrase detection, natural language inference, as well as sentiment classification.

Propagation methods. While gradient methods follow standard backpropagation rules, propagation methods define a custom backward pass, using purposely designed local propagation rules for different layer types to emphasize individual neurons’ contribution to the output.

We now formalize the process using a feed-forward network as an example, as shown in Figure 10. As before, let x represent the input and $M(x)$ represent the output of model M after a forward pass. Denote any layer in M by l ($l = 1, 2, \dots, L$), the dimension of which is d_l . Define $R_i^{(l)}$ as the relevance score of any neuron i in layer l . Our goal is to find $R_i^{(1)}$, the relevance of any input feature x_i . In other words, $r_i(x) = R_i^{(1)}$.

Unlike gradient methods, propagation methods do not have a closed-form expression for $r_i(x)$. Instead, they start with the output $M(x)$, which is considered the top-level relevance, $R_i^{(L)}$. Next, $R_i^{(L)}$ is propagated from layer L to $L - 1$ based on layer-specific rules, such that each neuron in $L - 1$ receives a proportion of it. This process then proceeds layer by layer. Between any two adjacent layers l and $l + 1$, a generic function $D()$ determines how $R_j^{(l+1)}$ (the relevance of any neuron j in $l + 1$) is *recursively distributed* to $R_i^{(l)}$ (the relevance of any neuron i in l), where i and j are connected. Formally,

$$R_i^{(l)} = \begin{cases} M(x), & \text{for } l = L; \\ D(R_j^{(l+1)}), & \text{for } 1 \leq l < L. \end{cases} \quad (1)$$

The recursion terminates once reaching $l = 1$. All subsequently introduced propagation methods follow the same procedure above, while differing in the definition of $D()$, summarized in Table 3. Unfortunately, there is no unified visualized comparison of all these methods yet. We will illustrate each method individually and provide visualizations when possible.

Among the earliest methods in this family, **DeconvNet** (Zeiler and Fergus 2014) and **Guided BackPropagation (GBP)** (Springenberg et al. 2015) both design custom rules for ReLU units ($y = \max(0, x)$) in particular, since it is arguably the most commonly used

Method	Definition of $D()$
Simple Gradients	$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \mathbb{1}_{\sum_{i=0}^{d_l} a_i w_{ij} > 0} \cdot R_j^{(l+1)}$
DeconvNet	$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \mathbb{1}_{R_j^{(l+1)} > 0} \cdot R_j^{(l+1)}$
Guided BackPropagation	$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \mathbb{1}_{\sum_{i=0}^{d_l} a_i w_{ij} > 0} \cdot \mathbb{1}_{R_j^{(l+1)} > 0} \cdot R_j^{(l+1)}$
Layerwise Relevance Propagation	$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{c_{ij}}{\sum_{i=0}^{d_l} c_{ij}} R_j^{(l+1)}$
DeepLift	$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{a_i w_{ij} - \bar{a}_i w_{ij}}{\sum_{i=0}^{d_l} (a_i w_{ij} - \bar{a}_i w_{ij})} R_j^{(l+1)}$
Deep-Taylor Decomposition	$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{\partial R_j^{(l+1)}}{\partial a_i} _{\{\bar{a}_i\}^{(j)}} (a_i - \bar{a}_i^{(j)})$

Table 3: Summary of different propagation methods in terms of how they define the recursive function $D()$, as in $R_i^{(l)} = D(R_j^{(l+1)})$.²³ Simple Gradients from gradient methods is included for comparison. See Section 2.4.2 – Propagation methods for details on notations.

non-linear activation at that time. Formally, suppose a ReLU unit j in $l + 1$ is connected to a set of neurons $i = 0, 1, \dots, d_l$ in l . Let a_i denote the activation of any neuron i . Then we have $a_j = \max(\sum_{i=0}^{d_l} a_i w_{ij}, 0)$ by the definition of ReLU, where w_{ij} is the weight connecting i and j .²² According to the standard backpropagation rule used by Simple Gradients, only positive inputs in the forward pass ($\sum_{i=0}^{d_l} a_i w_{ij} > 0$) will have non-zero gradients in the backward pass. In other words,

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \mathbb{1}_{\sum_{i=0}^{d_l} a_i w_{ij} > 0} \cdot R_j^{(l+1)},$$

where $\mathbb{1}$ is the indicator function.²⁴ It is believed that this rule is not ideal for relevance redistribution. By contrast, DeconvNet proposes to zero out the redistributed relevance only if the incoming relevance $R_j^{(l+1)}$ is non-positive, regardless of the input $\sum_{i=0}^{d_l} a_i w_{ij}$:

²² To conveniently incorporate the bias term b , we let $a_0 = 1$ and $w_{0j} = b$.

²³ Since $D()$ is layer-specific, we only show one or more representative rules for each method here: the ReLU unit propagation rule for Simple Gradients, DeconvNet, and GBP; the general-form rule for LRP; the Rescale rule for DeepLift; and the general-form rule for Deep-Taylor Expansion.

²⁴ https://en.wikipedia.org/wiki/Indicator_function

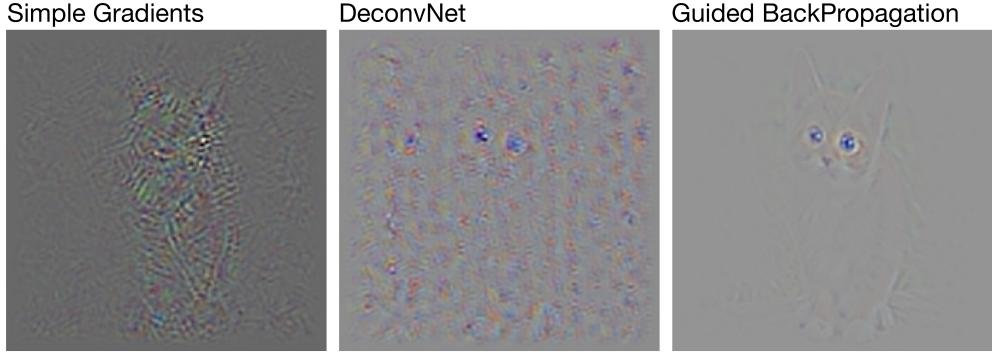


Figure 11: A visualization of DeconvNet and Guided BackPropagation, in comparison with Simple Gradients, on an example cat image (figure adapted from (Springenberg et al. 2015)).

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \mathbb{1}_{R_j^{(l+1)} > 0} \cdot R_j^{(l+1)}.$$

On the other hand, Guided BackPropagation combines the two rules above, zeroing out the redistributed relevance if *either* the incoming relevance or the input is non-positive:

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \mathbb{1}_{\sum_{i=0}^{d_l} a_i w_{ij} > 0} \cdot \mathbb{1}_{R_j^{(l+1)} > 0} \cdot R_j^{(l+1)}.$$

Compared with Simple Gradients, both DeconvNet and Guided BackPropagation produce cleaner feature relevance visualizations as perceived by humans (see Figure 11 for an example). However, they share several shortcomings. **First**, they cannot handle the Sensitivity test (cf. Section 1.1.4) and the saturation issue (Sundararajan, Taly, and Yan 2017; Shrikumar, Greenside, and Kundaje 2017), like certain gradient methods mentioned before. **Second**, because of zeroing out negative inputs and/or negative incoming relevance, both methods cannot highlight features that contribute *negatively* to the output (Shrikumar, Greenside, and Kundaje 2017). For example, the presence of floppy ears might lower the model’s confidence that the image is a cat (instead, it is more likely a dog). **Third**, in terms of Faithfulness, it is shown that both methods are essentially doing (partial) input recovery, which is unrelated to the network’s decision (Nie, Zhang, and Patel 2018). Whichever prediction class is chosen (e.g., cat, dog, ...), the feature attribution is almost invariant. Even with a network of random weights, Guided BackPropagation can still generate human-readable visualizations. Thus, it is suspected that the visualization has little to do with the model’s reasoning process.

While the previous two methods only treat ReLU specifically, **Layerwise Relevance Propagation (LRP)** then comes out as a more generalized solution (Bach et al. 2015). Instead of handcrafting rules directly, it first proposes a high-level *Relevance Conservation*

tion constraint, i.e., the total incoming relevance into a neuron should equal the total outgoing relevance from it. In other words, for all neurons $i = 1, 2, \dots, d_l$ in layer l and all neurons $j = 1, 2, \dots, d_{l'}$ in another layer l' , we have

$$\sum_{i=0}^{d_l} R_j^{(l)} = \sum_{j=0}^{d_{l'}} R_j^{(l')}. \quad (2)$$

Any propagation rule conforming to this constraint can be called an instance of LRP. The original paper proposes several such rules, among which we introduce three. All of them are in the following form:

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{c_{ij}}{\sum_{i=0}^{d_l} c_{ij}} R_j^{(l+1)}. \quad (3)$$

where c_{ij} denotes the contribution of neuron i to neuron j , and is defined by each rule differently. It can be verified that Equation 3 satisfies the Relevance Conservation constraint. Concretely, the three rules are:

(a) the Basic rule, which intuitively takes the product of the activation and the weight as the contribution from i to j :

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{a_i w_{ij}}{\sum_{i=0}^{d_l} a_i w_{ij}} R_j^{(l+1)}; \quad (4)$$

(b) the Epsilon rule, which adds a small term in the denominator to alleviate numerical instability:

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{a_i w_{ij}}{\epsilon + \sum_{i=0}^{d_l} a_i w_{ij}} R_j^{(l+1)}; \quad (5)$$

as ϵ increases, the relevance becomes sparser;

(c) the Gamma rule, which favors positive contributions by up-weighting them separately:

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{a_i (w_{ij} + \gamma w_{ij}^+)}{\sum_{i=0}^{d_l} a_i (w_{ij} + \gamma w_{ij}^+)} R_j^{(l+1)}; \quad (6)$$

where w_{ij}^+ are the positive terms in all w_{ij} 's. As γ increases, negative contributions gradually disappear.

Other LRP rules are omitted because of space, e.g., the Gamma-Beta rule, which treats positive and negative contributions individually.

LRP has several advantages. **First**, unlike gradient methods, differentiability or smoothness properties of neuron activations are not required for LRP. **Second**, Bach

et al. (2015) demonstrate its Faithfulness through a pixel flipping evaluation in digit classification. Essentially, they flip a fixed percentage of pixels in the input image according to relevance scores assigned by LRP, and observe how the prediction changes. Results show that flipping pixels with the highest *positive* scores first rapidly decrease the predicted probability of the target class, while flipping those with *close-to-zero* scores first influence the prediction minimally. More interestingly, if we flip pixels with *negative* relevance scores with regard to an *alternative* class, the prediction can be re-directed toward that class. For example, if the input image is a 3, we can fill in white pixels on the left side of the 3, since they are the ones speaking against an 8 (the alternative class) according to LRP. By this means, we can make the image more like an 8 to the model. All the above results suggest that LRP can indeed reflect the model’s reasoning process to some extent, but no comparison is provided with other explanation methods.

Other criticisms of LRP include: **first**, it still suffers from the saturation problem (Shrikumar et al. 2017); **second**, it violates Implementation Invariance (cf. Section 1.1.4) (Shrikumar, Greenside, and Kundaje 2017); **third**, there is no principled way to decide which rule to choose for which type of layer. The authors offer intuitive heuristics, but fail to support them with rigorous evidence.

In NLP, LRP has been applied/extended to CNNs and RNNs on sentence classification tasks, including topic and sentiment classification (Arras et al. 2016, 2017), to explain which tokens are most important to the prediction. Regarding Faithfulness, similar to pixel flipping in vision, the evaluation here is “word deletion”: a fixed number of tokens are deleted from the input (i.e., setting their corresponding vector to zero) according to the relevance score assigned by an explanation (LRP, Simple Gradients, and a random baseline), and then we track the impact on the classification performance. It is observed that for *correctly* classified inputs, when deleting the *most relevant* tokens first, LRP leads to the most rapid classification performance drop; but for *incorrectly* classified inputs, when deleting the *most irrelevant* tokens first, LRP can most effectively boost the performance. This indicates that LRP does provide informative insights into the model’s reasoning mechanism.

To address LRP’s failure with saturation and the Sensitivity test, two *reference-based* methods, **DeepLift** (Shrikumar, Greenside, and Kundaje 2017) and **Deep-Taylor Decomposition (DTD)** (Montavon et al. 2017), are then introduced. Analogous to Integrated Gradients, they aim to measure the global (instead of local) contribution of input features by finding a reference point (or baseline) \bar{x} to compare with the input x . Ideally, the baseline \bar{x} should represent some “neutral” input, i.e., satisfying $M(\bar{x}) = 0$, so we can attribute all positive contribution to the presence of x . In practice, it needs to be chosen with domain-specific knowledge.

Concretely, **DeepLift** (Shrikumar, Greenside, and Kundaje 2017) first chooses the baseline input \bar{x} , and then computes its corresponding baseline output $M(\bar{x})$, ideally 0. Then, it explains $M(x) - M(\bar{x})$, the difference between the original and the baseline output, in terms of $x - \bar{x}$, the difference between the original and the baseline input. Therefore, it defines the total relevance as $R_i(L) = M(x) - M(\bar{x})$, different from the $R_i(L) = M(x)$ case in previous methods. Then, for the recursive function $D()$, it has several rules, e.g., the Rescale rule and the Reveal-Cancel RULE. We introduce the first here:

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{a_i w_{ij} - \bar{a}_i w_{ij}}{\sum_{i=0}^{d_l} (a_i w_{ij} - \bar{a}_i w_{ij})} R_j^{(l+1)}. \quad (7)$$

This is analogous to the Basic rule in LRP, except for the baseline term. As for advantages, by using a baseline, DeepLift tackles the saturation and the Sensitivity issues. More importantly, When evaluated on a similar pixel flipping test for Faithfulness, DeepLift proves the most effective in manipulating the prediction toward the target class, compared to Integrated Gradients, Gradient \times Input, Simple Gradients, and Guided BackPropagation. However, a downside is that DeepLift still violates Implementation Invariance (Sundararajan, Taly, and Yan 2017).

Deep-Taylor Decomposition (DTD) (Montavon et al. 2017) starts from a more theoretical perspective, treating the explanation as an *approximation* of the upper-level relevance $R_j^{(l+1)}$ through Taylor decomposition.²⁵ Given a function $f(x)$, its first-order Taylor decomposition at $x = \bar{x}$ is

$$f(x) = f(\bar{x}) + \left(\frac{\partial f}{\partial x} \Big|_{x=\bar{x}} \right)^T \cdot (x - \bar{x}) + \epsilon \quad (8)$$

where ϵ is the higher-order residual. When applied to model explanation, we can think $R_j^{(l+1)}$ as $f(x)$, essentially decomposing the upper-level relevance on the activation $\{a_i\}$ of lower-layer neurons $\{i\}$ to which j is connected. If the decomposition is at the baseline $\{\bar{a}_i\}^{(j)}$,²⁶ which has zero relevance, we have

$$R_j^{(l+1)} = \sum_{i=0}^{d_l} \left(\frac{\partial R_j^{(l+1)}}{\partial a_i} \Big|_{\bar{a}_i^{(j)}} \right)^T \cdot (a_i - \bar{a}_i^{(j)}) + \epsilon_j. \quad (9)$$

Then, to determine the relevance for neuron i , we sum up all incoming relevance from all connected j 's in the upper level:

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} R_j^{(l+1)}. \quad (10)$$

Combining the two Equations above, we have

$$R_i^{(l)} = \sum_{j=0}^{d_{l+1}} \frac{\partial R_j^{(l+1)}}{\partial a_i} \Big|_{\{\bar{a}_i\}^{(j)}} (a_i - \bar{a}_i^{(j)}) \quad (11)$$

which is the definition of $D()$.

The choice of the baseline $\{\bar{a}_i\}$ is non-trivial, since it should not only have zero relevance, but also lie in the vicinity of $\{a_i\}$ for the Taylor decomposition to hold. In practice, this is often chosen based on the specific network type.

²⁵ Simply put, Taylor decomposition is a way to locally approximate a potentially non-polynomial function with a polynomial function. See more details at https://en.wikipedia.org/wiki/Taylor_series.

²⁶ The choice of baseline is specific to each neuron j , thus the superscript.

Interestingly, DTD can be viewed as a generalization of several previous methods. For instance, Simple Gradients is proved to be an instance of DTD not at a deliberately chosen baseline \bar{x} , but at a point infinitesimally close to the input x in the direction of the maximum gradient. Also, LRP can also be considered a sequence of DTD performed at each neuron. Each LRP rule is equivalent to DTD with a different baseline point (Montavon et al. 2019).

In terms of evaluation, only qualitative results on human Plausibility are reported, while Faithfulness is unverified.

In NLP, Chefer, Gur, and Wolf (2021) extend DTD to explain the decision of Transformer models on sentiment classification. However, the explanations are evaluated against the ground truth, i.e., human-annotated token relevance, therefore unrelated to Faithfulness either.

Tools. Readers interested in using backpropagation-based methods should consider the following packages: AllenNLP Interpret²⁷ (Wallace et al. 2019b), Captum²⁸ (Kokhlikyan et al. 2020), RNNbow²⁹ (Cashman et al. 2018), and DeepExplain³⁰.

2.4.3 Advantages.

- (a) Backpropagation-based methods generate a spectrum of feature relevance scores, which is easily **readable** for all kinds of target users.
- (b) They are relatively **easy to compute**: gradient methods require only a few calls to the model’s backward() function; propagation methods involve a custom implementation of backward(), but also allow precise control of the relevance redistribution process.
- (c) In terms of **Faithfulness**, gradients (and variants) are intrinsically tied to the influence of input features on the prediction. Empirically, recently proposed methods (e.g., Layerwise Relevance Propagation, DeepLift, Deep-Taylor Decomposition) are shown to be more faithful than previous baselines through input deletion experiments, as mentioned before.
- (d) Unlike the analysis of model-internal structures (e.g., attention weights), backpropagation-based methods take the **entire computation path** into account, instead of only a snapshot at a single point.

2.4.4 Disadvantages.

- (a) Most existing work target **low-level features** only, e.g., pixels in vision and input tokens in language. It is non-intuitive how to compute any sort of gradient w.r.t. higher-level features like case, gender, part-of-speech, semantic role, syntax dependency, coreference, discourse relations, and so on.
- (b) It is questionable if such methods are applicable to **non-classification tasks**, especially when there is no single output of the model, e.g., text generation or structured prediction.
- (c) As mentioned before, certain methods **violate axiomatic principles** of explainability, e.g., Sensitivity and Input Invariance(Sundararajan, Taly, and Yan 2017).

²⁷ <https://allenai.github.io/allennlp-website/interpret>

²⁸ <https://captum.ai/>

²⁹ https://www.eecs.tufts.edu/~dcashm01/rnn_vis/d3_code/

³⁰ <https://github.com/marcoancona/DeepExplain>

(d) The explanation can be **unstable**, i.e., minimally different inputs can lead to drastically different relevance maps (Ghorbani, Abid, and Zou 2019; Feng et al. 2018).

(e) In terms of **Faithfulness**, most methods do not report empirical evaluation results, with only the aforementioned exceptions. Moreover, subsequent researchers find many systematic deficiencies of them in ad-hoc evaluations: (i) as mentioned before, Guided BackPropagation and DeconvNet are shown to be only doing input recovery, ignorant of the model’s behavior (Nie, Zhang, and Patel 2018). (ii) certain explanations (including Simple Gradients, Integrated Gradients, and SmoothGrad) can be adversarially manipulated, i.e., one can construct entirely different gradient distributions with little influence on the prediction (Wang et al. 2020). (iii) certain methods are sensitive to meaningless changes, e.g., adding a constant shift to all data points. This has no impact on the model behavior, but sometimes influences explanations substantially for methods like Gradient \times Input as well as Integrated Gradients and Deep-Taylor Decomposition under certain conditions.(Kindermans et al. 2019) (iv) certain methods are *not* sensitive to meaningful changes, e.g., randomizing the model weights or the data. In such cases, a faithful explanation is expected to change, while in practice this is not the case for methods including Guided BackPropagation and Grad-CAM (Adebayo et al. 2018).

2.5 Counterfactual Intervention

2.5.1 Overview.

The notion of counterfactual reasoning stems from the causality literature in social science: “given two occurring events A and B , A is said to cause B if, under some hypothetical counterfactual case that A did not occur, B would not have occurred” (Roese and Olson 1995; Winship and Morgan 1999; Lipton 2017). In the context of machine learning, counterfactual intervention methods explain the causal effect between a feature and the prediction by erasing or perturbing the feature and observing the change in the prediction. A larger change indicates stronger causality.

2.5.2 Past Work.

One axis along which we can categorize existing studies is *what they intervene in*: **inputs** or **model representations**. The former manipulates the input and passes it through the original model; however, the latter directly manipulates the model-internal structures, e.g., neurons or layers. The rest of this section will elaborate on the two categories.

Intervening in inputs. Input intervention can in turn be categorized along two dimensions: the *target* and the *operation*. The target refers to “what is affected by the intervention”, normally input **features** (e.g., tokens) or **examples** (e.g., input sentences). The operation is the specific intervention method, which can be **erasure** (masking out the target) or **perturbation** (changing the value of the target).

We will first classify existing work based on the target, and then on the operation:

(a) **Feature-targeted intervention.** Earliest work mostly relies on **erasure**, since it is relatively straightforward to implement.

One intuitive idea is **leave-one-out**, which erases a single feature at a time and assesses the resulting change in the prediction. Naturally, the feature can be input words (Li, Monroe, and Jurafsky 2017) or input word vector dimensions (Kádár, Chrupała, and Alishahi 2017; Li, Monroe, and Jurafsky 2017). In these studies, only Plausibility is examined based on human perception of qualitative examples, and no evaluation of Faithfulness is reported. Also crucially, leave-one-out captures the linear contribution of single features, but cannot handle higher-order feature interactions. For example,

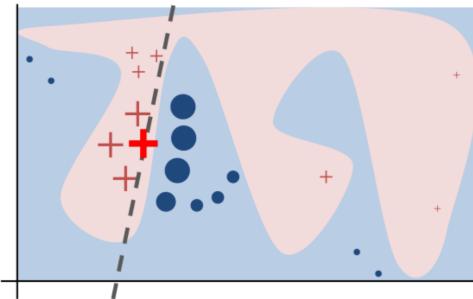


Figure 12: An illustration of the LIME (figure from Ribeiro, Singh, and Guestrin (2016)). The complicated decision boundary of the black-box model (light blue/pink) is locally approximated by a interpretable linear model (dashed line), in the proximity of the current prediction to the explained (bold red cross).

the word *not* may have contrasting contribution toward the sentiment of a sentence, depending on whether it is composed with *good* or *bad*.

To address this issue, researchers propose explanation methods that erase **subsets of features** instead of individual ones. Some studies (Li, Monroe, and Jurafsky 2017) aim to find the minimum subset of input tokens to **erase** such that the model’s decision is **flipped**. Interestingly, others (Ribeiro, Singh, and Guestrin 2018) look for the contrary – the minimum subset of input tokens to **keep** such that the model’s decision is **unchanged** (this is called “Anchors”). No matter which objective is taken, finding the exact desired subset of tokens is intractable, and thus both studies rely on approximated search. As a more efficient alternative, De Cao et al. (2020) propose DiffMask, a method that trains a classifier on top of input representations to decide which subset of tokens to mask. In terms of Faithfulness, Anchors is evaluated with human predictive power: compared to a popular baseline, LIME (Ribeiro, Singh, and Guestrin 2016), it allows users to more accurately predict model decisions on unseen examples. DiffMask proves more faithful than several other baselines including Integrated Gradients (Sundararajan, Taly, and Yan 2017), but only on synthetic tasks.

Based on the idea of feature erasure, a novel family of methods on **surrogate models** come out. The intuition is to locally approximate a black-box model with a white-box surrogate model as an explanation of the current prediction. LIME (Ribeiro, Singh, and Guestrin 2016), or Local Interpretable Model-agnostic Explanations, is a representative method of this type. Suppose the black-box model to be explained has a complicated decision boundary, as shown in Figure 12. Our goal is to provide a local explanation for the current prediction. LIME first samples instances in the neighborhood of the current example by masking out different subsets of its features. Next, it obtains the model prediction on these instances and weighs them by their proximity to the current example (represented by size in Figure 12). Then, it approximates the model’s local decision boundary by learning an interpretable model, e.g., a sparse linear regression, on the input features, which constitutes the explanation. Another widely adopted method, SHAP (Lundberg and Lee 2017), or SHapley Additive exPlanations, can be thought of as using additive surrogate models as an explanation. Originated from the game theory, Shapley values (Shapley 1953) are initially used to determine how to fairly distribute the “payout” among the “players”. In machine learning, it is adapted to explain the

contribution of input features (players) to the prediction (payout). Consider, again, our running example:

This movie is great. I love it.

We can think of this input sentence x as containing a set of binary features x_i , i.e., the presence of a token. Now, the Shapley value represents the contribution of each feature x_i to the prediction. For example, suppose that x_i denotes the presence of *great*. To compute its Shapley value, we need to

- (i) sample a subset of input features including x_i to form a new example x' , e.g., *movie great*, and obtain the model prediction $M(x')$;
- (ii) remove x_i from x' to form another example x'' , e.g., *movie*, and again obtain the new model prediction $M(x'')$;
- (iii) compute the marginal contribution of x_i as the difference between (ii) and (i), i.e., $M(x') - M(x'')$; and
- (iv) repeat the previous steps for all subsets containing x_i .

Finally, the Shapley value is the mean marginal contribution of x_i . When the number of features is large, the above process is computationally expensive. Therefore, the SHAP paper introduces an efficient approximation, which obviates re-sampling a combinatorial number of subsets. In terms of Faithfulness, LIME is evaluated with white-box tests: when used to explain models that are themselves interpretable (e.g., Logistic Regression or Decision Tree), LIME successfully recovers 90% of important features. On the other hand, Shapley values are theoretically shown to be locally faithful, but there is no empirical evidence on whether this property is maintained after the SHAP approximation. Subsequent work also finds other limitations: (i) The choice of neighborhood is critical for such surrogate-model-based methods (Laugel et al. 2018); (ii) Linear surrogate models have limited expressivity. For example, if the decision boundary is a circle and the example is inside the circle, it is impossible to derive a locally faithful linear approximation.

Beyond simply erasing feature subsets, recent work also starts to explicitly model the strength of different **feature interactions**. For example, the Archipelago method (Tsang, Rambhatla, and Liu 2020) measures the contribution of the interaction between a pair of features by erasing *all other* features and recomputing the prediction. It is shown to be faithful on synthetic tasks such as function reconstruction. However, on realistic tasks like sentiment classification, only Plausibility is evaluated.

A major problem with feature erasure is that it results in out-of-distribution (OOD) inputs. For example, when a word is masked out, the resulting sentence often becomes ungrammatical or nonsensical. Exploiting this weakness, Slack et al. (2020) design a method to fool popular erasure-based methods. Suppose a task (e.g., loan application decision) involves sensitive features (e.g., gender or race), and the job of the explanation method is to examine if a model is relying on these features. To fool a given explanation method, the authors design an adversarial pipelined model with two modules. The first module is a classifier to determine if an input example is before or after the erasure. This classification is fairly easy because of the stark differences between the two distributions. Depending on the classification output, the second module makes a prediction on the original task using different reasoning mechanisms: if the input example is in-distribution, then the module will rely on sensitive features entirely; otherwise, it will behave innocuously, only making use of insensitive features. In other words, this pipelined model is indeed biased on all in-distribution examples. However, any explanation method that works by sampling neighboring examples by feature

erasure (e.g., LIME and SHAP) will report that the model is unbiased, because they are designed to capture the model’s behavior within the neighborhood.

This leads us to the other operation – **perturbation** – as another type of feature-targeted intervention. Compared to simple erasure, perturbing the value of the target feature is less likely to result in OOD inputs. For instance, consider again our running example *This movie is great. I love it.* To study the importance of *great* to the prediction, one can replace it with some other word (e.g., *good*, *OK*) instead of just deleting it altogether, and observe the probability change of *positive*.

The outcome of such perturbations is often called *counterfactual examples*, which resemble *adversarial examples* in the robustness literature. They differ in at least three aspects though: (i) the goal of the former is to explain the model’s reasoning mechanism, while that of the latter is to examine model robustness; (ii) the former should be meaningfully different in the perturbed feature (e.g., *This movie is great* → *This movie is not so great*), while the latter should be similar to, or even indistinguishable from, the original example (e.g., *This movie is great* → *This movie is GREAT*); (iii) the former can lead to changes in the label, whereas the latter do not (Kaushik, Hovy, and Lipton 2020). Prior work has explored different ways to create counterfactual examples, manual (Kaushik, Hovy, and Lipton 2020) or automatic (Wu et al. 2021). However, no evaluation of Faithfulness has been reported.

(b) **Example-targeted intervention** In addition to features, counterfactual intervention can directly happen on the level of examples. A representative method of this type is called **influence functions** (Koh and Liang 2017), which is designed to explain which training examples are most influential in the prediction of a test example. This may remind us of similarity methods in Section 2.2 (Caruana et al. 1999). Although both methods share the same goal, they rely on different mechanisms. Similarity methods identify the most influential training examples via similarity search, whereas influence functions are based on counterfactual reasoning – if a training example were absent or slightly changed, how would the prediction change?

Since it is impractical to retrain the model after **erasing/perturbing** every single training example, influence functions provide an approximation by directly recomputing the loss function. Essentially, erasing a training example is equivalent to upweighting it by $-\frac{1}{n}$, and modifying it is the same as moving $\frac{1}{n}$ mass from it to the new example. Therefore, one can approximate the new model parameters resulting from the erasure/perturbation of a training example without having to retrain the model. After the invention in vision (Koh and Liang 2017), influence functions have been adapted to NLP (Han, Wallace, and Tsvetkov 2020). Although they are claimed to be “inherently faithful”, this is not well-supported empirically. Crucially, the approximation relies on the assumption that the loss function is convex. Koh and Liang (2017) examines the assumption in vision, showing that influence functions can still be a good approximation even when the assumption does not hold (specifically, on CNNs for image classification). In NLP, though, only a qualitative sanity check is performed (on BERT for text classification), and no baseline is provided. In fact, Basu, Pope, and Feizi (2020) further discover that influence functions can become fragile in the age of deep neural networks. The approximation accuracy can vary significantly depending on a variety of factors: “the network architecture, its depth and width, the extent of model parameterization and regularization techniques, and the examined test points”. The findings call for increased caution on the consequences of the assumption as models become more complex.

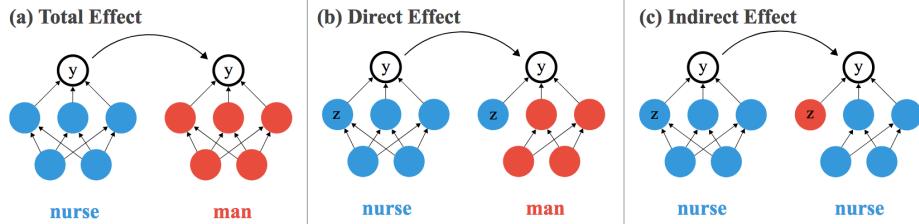


Figure 13: An illustration of causal mediation analysis (figure from Vig et al. (2020)). The input change x ($\text{nurse} \rightarrow \text{man}$) influences the output y , mediated by neuron z .

Intervening in model representations. Similar to input intervention, we also summarize model representation intervention methods according to the *target* and the *operation*. Here, the target can be broadly categorized into **neurons** and **feature representations**. The operation can still be **erasure** and **perturbation**.

Similar to the case of intervening in inputs, we will first classify existing work based on the target, and then on the operation:

(a) **Neuron-targeted intervention.** By intervening in individual neurons in the neural network, one can explain the importance of each neuron to the prediction. The intervention can still be either **erasure** or **perturbation**.

The simplest form of erasure is still **leave-one-out**. Using the same strategy as with input features, Li, Monroe, and Jurafsky (2017) study the effect of leaving out a single dimension in hidden units on the log-likelihood of the gold label. In text classification tasks, they find that compared to the input layer, the importance in higher layers is distributed more equally across dimensions. In other words, there are no particular dimensions that are strikingly more important than others, which might make the final prediction more robust against changes in any of them. Bau et al. (2019) adapt the method for Machine Translation models. Instead of erasing each hidden unit sequentially, they search for important neurons in a guided fashion. According to their ranking, it is further validated that more important neurons have a larger impact on translation quality than less important ones, as shown by masking out their activations during the inference.

Besides erasure, perturbation is another form of neuron-targeted intervention. One representative example is **causal mediation analysis** (Vig et al. 2020), which measures how a *control variable* influences a *response variable* through the mediation by an intermediate variable, or *mediator*. Using the example from Pearl (2001), consider a scenario where we want to study the effects of a drug (control variable) on a disease (response variable). However, the drug has certain side effects, causing the patient to take aspirin (mediator), which in turn has an effect on the disease. In machine learning, we can think of the input example as the control variable, the model output as the response variable, and an internal neuron as the mediator. Vig et al. (2020) use this framework to analyze gender bias in LMs. Given a prompt p such as *The nurse said that*, they compute the conditional probability of *he* versus *she* as the next generated token, and consider the ratio $y = \frac{P(\text{he}|p)}{P(\text{she}|p)}$ as a measurement of gender bias. Now, the goal is to study the effect of each individual neuron as the mediator. Specifically, they first perform a change on the input prompt (e.g., *The nurse said that* \rightarrow *The man said that*). Then, they measure three types of effect of the input change x on the output y , mediated by some neuron z . Figure 13 provides an illustration:

- (i) total effect (of x on y), i.e., the change in y resulting from the input change x ;
- (ii) direct effect (of x on y **without passing through** z), i.e., the change in y resulting from the input change x , but holding the mediator z constant;
- (iii) indirect effect (of x on y **only through** z), i.e., the change in y by only setting z to its value after the input change x , while holding all other neurons constant.

Intuitively, (iii) can represent the contribution of individual neurons to the prediction. Through their case study on GPT-2, the authors find that gender bias is concentrated in a relatively small proportion of neurons, especially in the middle layers. No empirical evaluation on faithful evaluation is reported though.

(b) **Feature-representation-targeted intervention.** Beyond intervening in neurons, directly targeting feature representations in the model allows us to answer more insightful questions like “*is some high-level feature, e.g., syntax tree, used in prediction?*”. This is particularly meaningful to the line of work on *what knowledge a model encodes* (Section 1.1.1), which oftentimes discovers linguistic features in the model, but it is unclear whether they are indeed used by the model.

As before, the most intuitive way to perform an intervention on feature representation is **erasure**. Two pieces of concurrent work, **Amnesic Probing** (Elazar et al. 2021) and **CausalLM** (Feder et al. 2021), are representative examples. They both aim to answer the following question: is a certain feature (e.g., POS, dependency tree, constituency boundary, gender, race, ...) used by the model on a task (e.g., language modeling, sentiment classification, ...)? To answer the question, they exploit different algorithms to *remove* the target feature from the model representation, via either linear projection (Ravfogel et al. 2020) or adversarial training. Then, with the new representation, they measure the change in the prediction. The larger the change, the more strongly it indicates that the feature has been used by the original model. In terms of Faithfulness, only CausalLM is validated with a white-box evaluation, whereas no explicit evaluation is provided for Amnesic Probing.

Similar to input erasure, a major problem with feature representation erasure lies in unrealistic representations. For instance, since syntax is such a fundamental component of language, what does it mean if an LM is *entirely ignorant of syntax*? Is it still an LM at all?

To address this issue, **perturbation**-based methods targeting feature representations are proposed. Ravfogel et al. (2021) introduce AlterRep, an algorithm to manipulate the target feature value in model representations. Specifically, they investigate the task of subject-verb agreement prediction. For example, given the sentence

The man that they see [MASK] here.

with an embedded relative clause (*that they see*), the correct verb to fill in the mask should be *is* as opposed to *are*, since it should agree with *man*. They now ask the question: does the model use syntactic information (e.g., the relative clause boundary) in making such predictions? To answer this, they first probe for syntactic knowledge in the model representation. If the model “thinks” that the [MASK] token is outside the relative clause (factual), AlterRep would flip this knowledge via linear projections, such that [MASK] is now inside the relative clause according to the model (counterfactual). Now, the probability ratio of *are* versus *is* increases significantly, as the model is potentially tempted to associate the verb with *they* in the relative clause. Such findings suggest that syntactic information is indeed used in predicting the verb. Tucker, Qian, and

Levy (2021) study the same task and feature, but improve the method by providing syntactically ambiguous contexts, e.g.,

I saw the boy and the girl [MASK] tall.

which can be interpreted as either

[I saw the boy] and [the girl [MASK] tall].

or

I saw [the boy and the girl [MASK] tall].

Therefore, [MASK] can be either singular or plural. Likewise, they first probe for the model’s syntactic representation, and then flip the structure of the syntax tree from one of the above interpretations to the other. The way they do the flipping is a gradient-based algorithm informed by trained probes. Similar findings are reported as in the AlterRep paper, suggesting BERT-based models are using syntax in agreement prediction. However, no extrinsic evaluation of Faithfulness is provided.

Tools. The following tools implement some type(s) of counterfactual intervention: Captum³¹, LIT³² (Tenney et al. 2020), LIME³³ (Ribeiro, Singh, and Guestrin 2016), SHAP³⁴ (Lundberg and Lee 2017), Anchors³⁵ (Ribeiro, Singh, and Guestrin 2018), Seq2Seq-Vis³⁶ (Strobelt et al. 2019), and the What-if Tool³⁷ (Wexler et al. 2020).

2.5.3 Advantages.

(a) Counterfactual intervention has its root in the causality literature, and is therefore designed to **capture causal instead of mere correlational effects** between inputs and outputs.

(b) Compared to other methods, counterfactual intervention methods are more often explicitly evaluated in terms of **Faithfulness** (e.g., Ribeiro, Singh, and Guestrin 2018; De Cao et al. 2020; Ribeiro, Singh, and Guestrin 2016; Lundberg and Lee 2017; Tsang, Rambhatla, and Liu 2020; Feder et al. 2021), mostly with predictive power or white-box tests.

2.5.4 Disadvantages.

(a) Compared to other methods, counterfactual intervention is relatively more expensive in **computational cost**, normally requiring multiple forward passes/modifications to the model representation. Searching for the right targets to intervene can also be costly.

31 <https://captum.ai>

32 <https://pair-code.github.io/lit>

33 <https://github.com/marcotcr/lime>

34 <https://github.com/slundberg/shap>

35 <https://github.com/marcotcr/anchor>

36 <https://seq2seq-vis.io>

37 <https://pair-code.github.io/what-if-tool>

(b) As mentioned before, erasure-based intervention can result in **nonsensical inputs**, which sometimes allow adversaries to manipulate the explanation (Slack et al. 2020).

(c) Intervening in a single feature relies on the assumption that features are **independent**. Consider the sentence *This movie is mediocre, maybe even bad* (Wallace, Gardner, and Singh 2020). If we mask out *mediocre* or *bad* individually, the predicted sentiment will probably not change much (still negative). Hence, an explanation method that relies on single feature erasure might report that neither token is important for the model prediction. However, it does capture feature interactions, like the OR relationship between *mediocre* or *bad* here – as long as one of them is present, the sentiment is likely negative. More examples are provided in Shrikumar, Greenside, and Kundaje (2017).

(d) Interventions are often overly **specific to the particular example** (Wallace, Gardner, and Singh 2020). This calls for more insights into the scale of such explanations (i.e., if we discover a problem, is it only about one example or a bigger issue?) and general takeaways (i.e., what do we know about the model from this explanation?).

(e) Counterfactual intervention may suffer from **hindsight bias** (De Cao et al. 2020), which questions the foundation of counterfactual reasoning. Specifically, the fact that a feature can be dropped without influencing the prediction does not mean that the model “knows” that it can be dropped and has used it in the original prediction. For instance, consider a synthetic counting task where a model should decide if there are more 1’s than 8’s in the input digits. Now, suppose the input contains four 1’s, two 8’s, and three 5’s. Say we have a model with perfect accuracy, which correctly predicts TRUE. Through counterfactual intervention, we can either drop a 1, all of the 8’s, or all of the 5’s, without affecting the prediction. Does that mean that all these digits should be assigned zero importance? De Cao et al. (2020) argue that a more reasonable picture should be that all 1’s and 8’s have uniform importance, and all 5’s have zero. In the context of NLP, consider the Reading Comprehension task, where a model is given a context and a question, and should identify an answer span in the context. Now, using counterfactual intervention, if we mask out everything except the answer in the context, the model will for sure predict the gold span. Nonetheless, this does not imply that everything else is unimportant for the model’s original prediction. This again calls for our attention to the fundamental mechanism of counterfactual reasoning.

2.6 Self-Explanatory Models

2.6.1 Overview.

In contrast with all the above post-hoc methods, self-explanatory models provide built-in explanations. Typically, explanations can be in the form of feature importance scores, natural language, causal graphs, or the network architecture itself.

2.6.2 Past Work.

Prior work on self-explanatory models can be broadly categorized into two lines based on *how the explanation is formed*: **explainable architecture** and **generating explanations**. The former relies on the transparent model architecture, such that no extra explanation is necessary. The latter, though, may still involve opaque architectures, but generate explicit explanations as a byproduct of the inference process. The rest of the subsection will elaborate on each category.

Explainable architecture. While end-to-end NNs are a black-box, classic machine learning models like Decision Tree and linear regression have a highly interpretable

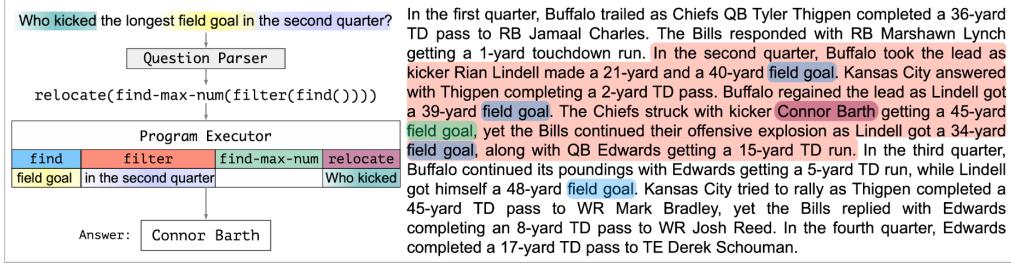


Figure 14: An illustration of Neural Module Network on the QA task (figure from Gupta et al. (2019)). Given a paragraph of context and a question, the model parses the question into a program of learnable modules, which is then executed on the context to derive the answer. Colors represent the correspondence between spans in the question, the modules, and the intermediate outputs in the context.

reasoning mechanism. Drawing inspiration from them, researchers attempt to design *neural* models with more structural transparency while maintaining their performance.

(a) **Neural Module Networks** (NMN) is one representative, specifically in the context of Question Answering (QA) tasks. Given a complex question (e.g., *Are there more donuts than bagels in the image?*), humans naturally decompose it into a sequence of steps (e.g., look for donuts and bagels, count them, and compare the counts). Motivated by the same idea, NMNs parse the input question into *a program of learnable modules* (e.g., `compare(count(donuts), count(bagels))`), which is then executed to derive the answer.

There are three potentially learnable components in NMNs: (i) the question parser (question \rightarrow dependency tree), (ii) the network layout predictor (dependency tree \rightarrow program), and (iii) the module parameters (program \rightarrow answer). Previous studies differ in whether and how each component is learned. Andreas et al. (2016b) introduce the earliest version of NMN, where only module parameters are learned and the other two components are pretrained or deterministic. In a follow-up study (Andreas et al. 2016a), they extend the framework to also jointly learn the network layout specific to each question, which is then named Dynamic Neural Module Network (DNMN). Hu et al. (2017) further propose to learn the question parser as well, resulting in their End-to-End Module Network (N2NMN).

The above methods prove effective on various visual QA tasks (including VQA (Antol et al. 2015), SHAPES (Andreas et al. 2016b), GeoQA (Krishnamurthy and Kollar 2013), and CLEVR (Johnson et al. 2017)), most of which are based on synthetic data, though. Recently, more studies investigate the application of NMNs on realistic data, especially in the language-only domain. Jiang et al. (2019) apply NMN to HotpotQA (Yang et al. 2018), a QA dataset involving reasoning across multiple documents. However, their model is incapable of symbolic reasoning, such as counting and sorting, so it can only solve questions with directly retrievable answers in the context. To address this issue, Gupta et al. (2019) introduce a set of modules for each symbolic operation, e.g., `count`, `find-max-num`, `compare-num`. Their model is capable of answering questions involving discrete reasoning in the DROP dataset (Dua et al. 2019), for example, *Who kicked the longest field goal in the second quarter?*, given a long description of the match. See Figure 14 for an illustration.

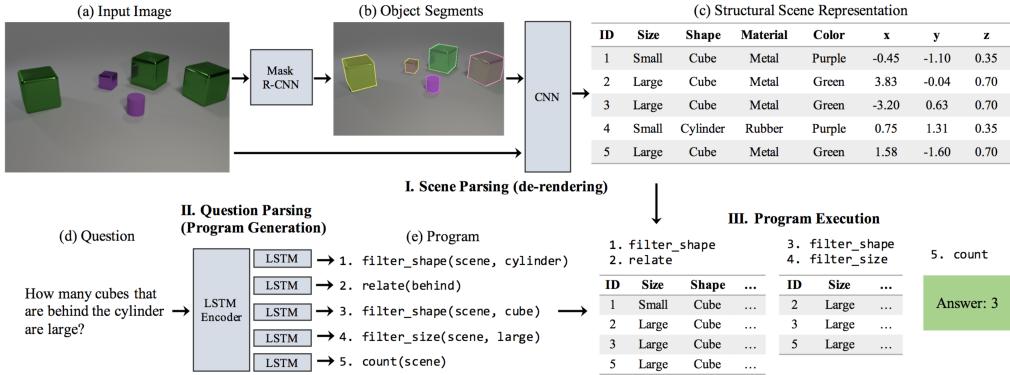


Figure 15: An illustration of the Neural-Symbolic VQA (NS-VQA) model (figure from Yi et al. (2018)). Given an image and a question, the scene parser converts the image to a structured representation; the question parser converts the image into a program; the program executor runs the program on the structured representation to obtain the answer.

Despite their presumably transparent structure, there are two main problems with NMNs: (i) The modules’ actual behavior may not be faithful to their intended function. Most NMNs pre-define modules only in terms of input/output interface. Their actual behavior – module parameters – are then typically learned from end-to-end supervision, i.e. only the question, context, and the final answer. Thus, there is no control over the intermediate output of individual modules. Consider our previous example `compare(count(donuts), count(bagels))`. Though we name the module `compare`, it may not perform the comparison function. Theoretically, it is possible that `compare` alone outputs the final answer, whereas `count` is ignored. Subramanian et al. (2020) empirically confirm such failure cases and experiment with several remedies, such as introducing intermediate supervision and limiting the module complexity. Curiously, the improved Faithfulness comes at the cost of end task accuracy. (ii) Symbolic modules may not be expressive enough for the flexible semantics of natural language. For example, Gupta et al. (2019) note that questions like *Which quarterback threw the most touchdown passes?* would necessitate modules with some key-value representation (`{quarterback: count}`), which are non-obvious to design. Other subtle semantic phenomena like context-conditional parsing and coreference pose similar challenges.

Nonetheless, the compositional nature of NMNs brings about promising research opportunities. In particular, it is possible to pretrain modules independently on other tasks. This allows us to ensure their Faithfulness as well as exploit transferable knowledge.

(b) **Neural-Symbolic Models (NSM)** are a more generic concept, loosely defined as neural models that integrate symbolic reasoning. This clearly includes NMNs, but here we will discuss the rest, i.e., methods that do not involve learnable neural modules.

Yi et al. (2018) introduce Neural-Symbolic VQA (NS-VQA) for answering questions based on synthetic images. As shown in Figure 15, it has three components: a scene parser, which derives a structured representation of the image, i.e., a database of object attributes; a question parser, which parses the question into a program; and a program executor, which runs the program on the database to obtain the answer. Note that, un-

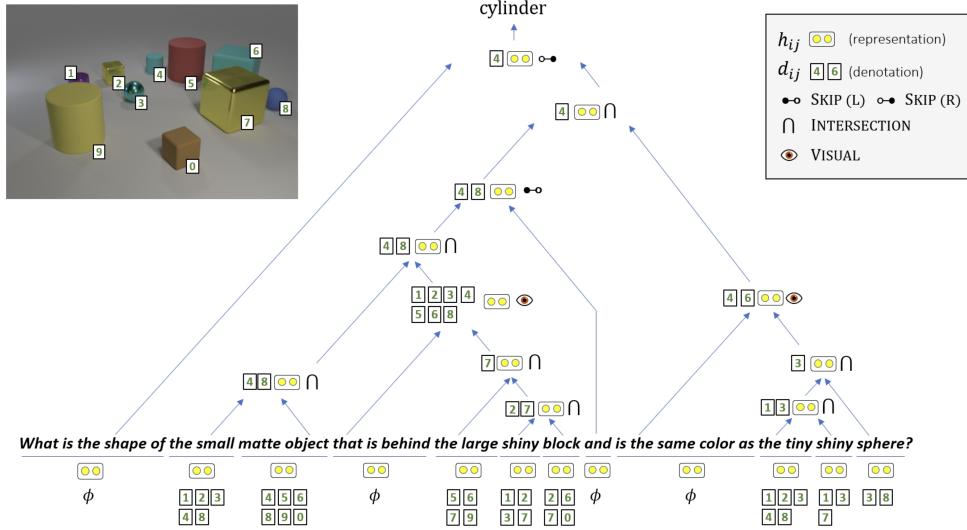


Figure 16: An illustration of the Grounded Latent Trees (GLT) model (figure from [Bogin et al. \(2021\)](#)). Starting from the leaves, the tree grows recursively upwards to reach answer.

like NMNs, here the program is composed of modules with fixed parameters, resulting in fully deterministic behavior. However, the model requires intermediate supervision on both the scene parser and the question parser, which limits its application to synthetic data only.

[Mao and Gan \(2019\)](#) extend NS-VQA by proposing Neuro-Symbolic Concept Learner (NS-CL), which requires no such intermediate supervision. It jointly learns visual scene representation of the question parse from (image, question, answer) triples directly. The scene is no longer converted to an explicit database, but has a probabilistic representation instead. This allows the model to be end-to-end differentiable and therefore applicable to real-world data as well.

[Bogin et al. \(2021\)](#) point out another weakness in existing NSMs concerning the question parser. To parse a question into a program, one needs to consider the enormous search space of possible programs. Most methods address this issue by techniques like reinforcement learning, which is not differentiable. In their model Grounded Latent Trees (GLT), the authors propose to parse the question into a latent tree, where each node corresponds to a span in the question. As shown in Figure 16, each span has a *denotation* (a symbolic set of objects it refers to in the image) and a *representation* (a continuous vector embedding of it). Starting from the leaves, the tree grows bottom-up, where each intermediate node is computed from its children. For example, the denotation of *the small matte object* is the intersection of *the small* and *matte object*. Finally, the denotation of the root node is the answer. During training, there is no supervision on the tree structure, but the model is capable of constructing valid trees only from end-to-end supervision.

(c) **Models with constraints** are the third family of explainable architectures. The idea is to incorporate constraints into neural networks from classic interpretable models, like generalized linear regression ([Alvarez Melis and Jaakkola 2018](#)) and

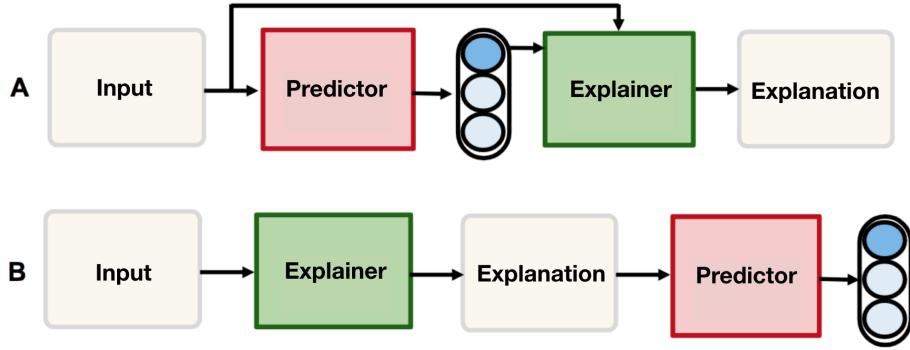


Figure 17: A comparison of the frameworks of generating explanations (figure adapted from Kumar and Talukdar (2020)): predict-then-explain (A), explain-then-predict (B), and jointly-predict-and-explain (no particular dependency between explainer and predictor, thus not visualized).

finite-state automata (Schwartz, Thomson, and Smith 2018; Deutsch, Upadhyay, and Roth 2019; Jiang et al. 2020). Still, a major challenge lies in the trade-off between interpretability and performance.

Generating explanations. Besides using architecture as an implicit explanation, another type of self-explanatory models generate explicit explanations as an additional task with the original prediction. For supervision, human-written explanations are often used as the training signal. According to the dependency of the *predictor* and the *explainer*, we can broadly classify existing work into three categories: **predict-then-explain**, **explain-then-predict**, and **jointly-predict-and-explain**. See Figure 17 for a comparison.

(a) **Predict-then-explain** models first make a prediction with a standard black-box predictor, and then justify the prediction with an explainer (Figure 17A). This is analogous to previous post-hoc explanation methods (from Section 2.2 to 2.5). This framework has been applied to many domains, including vision (Hendricks et al. 2016), language (Camburu et al. 2018), multimodal tasks (Park et al. 2018), self-driving cars (Kim et al. 2018), etc. However, it suffers from the same Faithfulness challenge as all other post-hoc methods: since the predictor does not depend on the explainer, there is no guarantee that the explanation accurately reflects the reasoning process behind the prediction. Moreover, as the supervision comes from human-provided explanations, the explainer is only explicitly optimized in terms of Plausibility, but not Faithfulness.

(b) **Explain-then-predict** methods are then introduced in response to this issue. In this framework, the explainer first generates an explanation, which is then provided as the *only* input to the predictor. In other words, the predictor can only access the explanation, but not the original input example. The intuition is that the prediction can only be made based on the explanation, which renders the predictor “faithful by construction”.

Methods within this framework differ in the *form* of explanation, which is typically either an **extract from the input** or **natural language**.

The former (an extract from the input as the explanation) is also known as rationale-based methods, where a *rationale* is defined as a part of the input that is short yet sufficient for the prediction (Zaidan, Eisner, and Piatko 2007).³⁸ For example, in sentiment classification, seeing the phrase *not good* is probably enough for predicting negative. The job of the explainer is to extract such a rationale, and thus it is also called *extractor* in this scenario. One major difficulty lies in how to effectively find the rationale span, given the formidably large search space. Lei, Barzilay, and Jaakkola (2016) proposes to guide the search with reinforcement learning. Bastings, Aziz, and Titov (2019) introduces a re-parameterization technique as an alternative, which makes the learning differentiable. Jain et al. (2020) discards searching and directly obtain candidate rationales from existing post-hoc explanation methods (e.g., backpropagation-based ones) instead. Although seemingly “faithful by construction”, there are some problems with rationale-based methods: (i) Clearly, only the rationale is used in the prediction, but this does not tell us anything about *how* it is used. For example, it is possible that the predictor only looks at the pattern of the rationale (e.g., the number of tokens that are retained) and makes a prediction based on this cue. Jacovi and Goldberg (2021) confirms the possibility of these so-called “trojan” explanations in practice. (ii) Similarly, the framework does not tell us *why* a rationale is selected. (iii) Finally, the validity of rationales is highly task-specific. For instance, it might make sense to classify the sentiment only based on a text fragment, but what about tasks that intrinsically require full sentence(s), such as Natural Language Inference (NLI)?

The latter (natural language as the explanation) generates explanations in natural language, more flexible than an extracted rationale from the input. Consider the NLI task as an example. Given a hypothesis (e.g., *An adult dressed in black holds a stick*) and a premise as input (e.g., *An adult is walking away, empty-handed*), the explainer should first generate an explanation (*Holds a stick implies using hands so it is not empty-handed*), and then the predictor should make a prediction (Contradiction) only based on the explanation. When experimenting with this model on the SNLI dataset (Bowman et al. 2015), Camburu et al. (2018) discover a trade-off between the task accuracy and the Plausibility of the explanation. It is also found that the model can generate inconsistent explanations (Camburu et al. 2020), e.g., *Dogs are animals* and *Dogs are not animals*. Moreover, the explanation might contain cues to the label, e.g., patterns like *X implies Y / X is a type of Y* oftentimes indicate Entailment, while *X is not the same as Y* is a strong signal of Contradiction. To overcome this issue, Kumar and Talukdar (2020) propose the Natural language Inference over Label-specific Explanations (NILE) model, where every class label has its own an explainer. Given an input, an explanation is generated for each label. Then, all three explanations are fed to the predictor, which makes a decision after comparing them. This precludes the possibility of the predictor exploiting cues in the explanation pattern. NILE is shown to have comparable accuracy with SOTA models on SNLI, as well as better transferability to OOD datasets. Through an extensive evaluation, the authors compare the Faithfulness of a few variants of NILE. Also, they argue that perturbation-based metrics (DeYoung et al. 2020) can sometimes be misleading, and task-specific metrics should be designed.

(c) **Jointly-predict-and-explain** methods have two possible structures: (i) there are still an explainer and a predictor, but the predictor can access both the explanation and

³⁸ This is analogous to the concept of “anchors” mentioned in Section 2.5.

the input example.³⁹ (ii) there are no separate explainer and predictor at all – everything is produced jointly.

Among them, (ii) is more straightforward in structure. Given the input example as the prompt, a generation model outputs a continuation including both the explanation and the prediction in some designated order. This is analogous to any ordinary generation task. Existing studies along this line differ in the choice of the generation model and the end task. For example, Ling et al. (2017) use LSTMs to solve algebraic problems and provide intermediate steps, and Narang et al. (2020) rely on T5 to generate predictions with justifications for NLI, sentiment classification, and QA. Here, we will focus on a series of work on generating structured proofs for deductive reasoning. This is particularly interesting since most previous work only aims at generating single-step explanations (e.g., a single sentence), but complex tasks would require a structured reasoning chain as explanations (e.g., the classic syllogism – from *all humans are mortal* and *Aristotle is a human*, we can conclude that *Aristotle is mortal*). As one of the earliest studies of this kind, Tafjord, Dalvi, and Clark (2021) develop ProofWriter, which takes in a set of premises and a hypothesis, and then decides if the hypothesis is true as well as a structured proof. The method obtains SOTA performance on the synthetic RuleTaker dataset (Clark, Tafjord, and Richardson 2020). Specifically, there are two versions of ProofWriter, all-at-once (generating the entire proof in one shot) and iterative (generating one step at a time), with different strengths and weaknesses. The all-at-once ProofWriter cannot guarantee that the proof is faithful, since it may not “believe” in the proof that is generated. Consider the following example:⁴⁰

Premises:

- S1. Nails are made of iron.
- S2. If something is iron then it is metal.
- S3. If something is made of metal then it can conduct electricity.

Hypothesis:

- S4. Nails conduct electricity.

Suppose ProofWriter generates the correct answer and a reasoning chain as proof, all in one shot:

Answer: TRUE

Proof:

- S1 & S2
- “Nails are made of metal.”
- & S3
- S4

Now, if we isolate the first step in the proof ($S1 \& S2 \rightarrow \text{“Nails are made of metal.”}$), we can feed it back to the ProofWriter to *verify* it:

Premises:

- S1. Nails are made of iron.
- S2. If something is iron then it is metal.

Hypothesis:

- S5. Nails are made of metal.

³⁹ In contrast, the above-mentioned explain-then-predict methods do not allow the predictor to access the input example. This is why we categorize (i) as jointly-predict-and-explain methods.

⁴⁰ Example from Peter Clark’s talk at Penn’s NLP seminar in Feb 2022.

There is no guarantee that ProofWriter will still output TRUE, meaning that the step may not necessarily be verified. In other words, the proof might not faithfully reflect how the model arrives at the answer. In fact, in a similar verification experiment as exemplified above, the authors find that for proofs within the depths seen during training, almost all correct steps can be verified; however, when it comes to greater depths, the percentage drops rapidly. This confirms that the all-at-once ProofWriter is not always faithful.

The iterative ProofWriter does not have this issue, since it derives the proof one step at a time. All steps are already verified during generation. Therefore, it is faithful by construction. However, compared to the all-at-once version, it suffers from bottlenecks in efficiency and input lengths limit.

After ProofWriter, [Dalvi et al. \(2021\)](#) generalize the idea to real-world data as well, developing the EntailmentWriter. Nevertheless, only an all-at-once version is implemented, indicating that the same Faithfulness risk exists.

As opposed to generating everything jointly, work in (i) still has an explainer and a predictor separately, but there is no particular constraint on input access. For example, [Rajani et al. \(2019\)](#) introduce a QA model that takes in a question, generates an explanation first, and then produces an answer based on *both* the question and the explanation. Another example is a variant of NILE ([Kumar and Talukdar 2020](#)) previously mentioned in (b), which allows the predictor to look at both the premise-hypothesis pair and the explanations. These methods have the same Faithfulness issue, since the predictor can make its decision based on the input only using whatever reasoning mechanism, while totally ignoring the explanation.

2.6.3 Advantages.

- (a) By definition, self-explanatory methods provide built-in explanations, so there is **no need for post-hoc explanations**.
- (b) **The form of explanation is flexible**, e.g., model architecture, input features, natural language, or causal graphs.
- (c) It is possible to **supervise the explainer** with human-provided explanations. This is helpful for learning more plausible explanations, as well as encouraging the model to rely on desired human-like reasoning mechanisms instead of spurious cues.
- (d) Certain self-explanatory models, e.g., the iterative ProofWriter ([Tafjord, Dalvi, and Clark 2021](#)), are **faithful by construction** (we should be extra cautious about this claim, though).

2.6.4 Disadvantages.

- (a) Many self-explanatory models cannot guarantee **Faithfulness**, e.g., Neural Module Networks without intermediate supervision, predict-then-explain models, rationale-based explain-then-predict models, and certain jointly-predict-and-explain models.
- (b) There is often an observed **trade-off between performance and interpretability** in self-explanatory models ([Subramanian et al. 2020](#)). Faithfulness can come at the cost of task accuracy.
- (c) Large-scale human supervision on explanations can be **costly and noisy** ([Dalvi et al. 2021](#)). Also, it is **hard to automatically evaluate** the quality of model-generated explanations given the reference human explanations, since there can be multiple ways to explain a prediction.

3. Summary and Discussion

In this section, we summarize the five methods above by discussing their common virtues and challenges, as well as identify future work directions in model interpretability.

3.1 Virtues

Recent advances in model interpretability exhibit the following virtues:

(a) They are conducive to **bridging the gap between competence and performance** in language models. The two terms originate from linguistics: competence describes humans' (unconscious) knowledge of a language, whereas performance refers to their actual use of the knowledge (Chomsky 1965). For humans, there is a gap between competence and performance, e.g., we can theoretically utter a sentence with infinitely many embedded clauses, but in practice, we never do so. Similarly, for language models, *what they know* can be different from *what they use (in a task)*, as discussed in Section 1.1.1. Previous work on interpretability predominantly focuses on competence, whereas more recent studies (e.g., all five methods discussed in this survey) aim at answering the performance question. This allows us to better understand whether the same gap exists in models, and if so, how we can bridge it.

(b) There has been **increasing awareness of Faithfulness and other principles** of model explanation methods, especially since the seminal opinion piece by Jacovi and Goldberg (2020). A number of evaluation methods have been proposed; see Section 1.1.4 for details. Though each of them depends on assumptions and application scenarios, this is a good starting point for quantitatively assessing the quality of explanations.

(c) Explanations produced by most above-mentioned methods above are **intuitive to understand**, even for lay people. This is because the form of explanation is simple, mostly feature importance scores, visualization, natural language, or causal graphs. Though the model and the explanation method may be opaque, the explanation itself is easily understandable.

(d) There are a plethora of explanation methods that are **model-agnostic**, especially for classification tasks.

(e) Many studies **draw insights from work in vision** and develop adaptable methods in language. See Section 2.4 for more details.

(f) Numerous **toolkits** have been developed to help users apply explanation methods to their own models. See Section 2.3, 2.4, and 2.5 for more details.

3.2 Challenges and Future Work

Despite the remarkable advances, the area of model interpretability still faces several major challenges, which also provide exciting future work opportunities:

(a) A large number of explanation methods still lack **objective quality evaluation**, especially in terms of **Faithfulness**. There has not been any established standard on how to measure Faithfulness. \Rightarrow We need a universal evaluation framework, which is fundamental to measuring the progress of any research in this area.

(b) Most existing methods provide explanations in terms of **surface-level features**, e.g., pixels in vision and tokens in language. \Rightarrow Future work should explore how to capture the contribution of **higher-level features** in a task, including linguistic (case, gender, part-of-speech, semantic role, syntax dependency, coreference, discourse relations, ...), and extra-linguistic (demographic features, commonsense and world

knowledge, ...) ones. Several studies on counterfactual intervention provide inspiring examples (Ravfogel et al. 2020; Elazar et al. 2021; Tucker, Qian, and Levy 2021); see Section 2.5 for details.

(c) Most existing methods capture the **contribution of individual features to the prediction**, but not that of higher-order feature interactions. See Section 2.5.4 (c) for an example. \Rightarrow Future work can develop more **flexible forms of explanation** instead of flat importance scores, e.g., feature subsets as in certain counterfactual intervention methods (Ribeiro, Singh, and Guestrin 2018) and causal graphs as in several self-explanatory methods (Tafjord, Dalvi, and Clark 2021; Dalvi et al. 2021).

(d) Existing work mostly focuses on **limited task formats**, e.g., classification and span identification. This limits their downstream applicability to real-world scenarios. \Rightarrow Future work can study **alternative task formats** such as language generation and structured prediction, or even better, develop explanation methods that are generalizable across tasks.

(d) It is not always obvious whether insights from model explanations are **actionable**. For example, given the explanation of the model’s decision on one test example, the user finds that the model is not using the desired features. Then how should they go about fixing it – through the data, model architecture, training procedure, hyperparameters, or something else? How does the user **communicate** with the model? \Rightarrow **Interactive** explanations will be a fruitful area for future study. Several recent studies on knowledge editing have shown the plausibility of the idea (Madaan et al. 2021; Kassner et al. 2021).

(e) There has been a **tension between model performance and interpretability**. This issue is especially evident in self-explanatory models; see Section 2.6 for more details. \Rightarrow It will be greatly helpful to have a **theoretical understanding** of whether the tension is intrinsic or avoidable. In the meantime, we need to cautiously balance between performance and interpretability depending on application scenarios.

4. Conclusion

This survey provides an extensive tour of recent advances in NLP explainability, through the lens of Faithfulness. Despite being a fundamental principle of model explanation methods, Faithfulness does not have a well-established technical definition or evaluation framework. As a result, it is difficult to compare different methods in terms of Faithfulness, and many of them do not report it by any means at all.

We present a critical review of five categories of existing model explanation methods: similarity methods, analysis of model-internal structures, backpropagation-based methods, counterfactual intervention, and self-explanatory models. We introduce each category in terms of their representative work, advantages, and disadvantages, with a special focus on Faithfulness. Then, we summarize all methods by discussing their common virtues and challenges and outline a few directions for future research. We hope that this survey provides an overview of the area for researchers interested in interpretability, as well as users aiming at better understanding their own models.

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