

Explanation in the Era of Large Language Models

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Abstract

Explanation has long been a part of communications, where humans use language to elucidate each other and transmit information about the mechanisms of events. There have been numerous works that study the structures of the explanations and their utility to humans. At the same time, explanation relates to a collection of research directions in natural language processing (and more broadly, computer vision and machine learning) where researchers develop computational approaches to explain the (usually deep neural network) models. Explanation has received rising attention. In recent months, the advance of large language models (LLMs) provides unprecedented opportunities to leverage their reasoning abilities, both as tools to produce explanations and as the subjects of explanation analysis. On the other hand, the sheer sizes and the opaque nature of LLMs introduce challenges to the explanation methods. In this tutorial, we intend to review these opportunities and challenges of explanations in the era of LLMs, connect lines of research previously studied by different research groups, and hopefully spark thoughts of new research directions.

1 Outline of Tutorial

This tutorial will take about 3 hours:

- Introduction & Desiderata (30 minutes)
- Free-text, CoT, Structured Explanations (50 minutes)
- Importance Scores (40 minutes)
- Mechanistic, Causal, etc (40 minutes)
- Conclusion & Discussion (20 minutes)

The following subsections list some more detailed content for each section.

1.1 Introduction

Explanation has been an important component in languages and their use. Explanation can reveal

the underlying mechanism of the phenomena to be explained (Keil, 2006). Explanation is also a process (Achinstein, 1983). Explanation can be part of an argumentative tool that help humans exploit the uniqueness of societal environment (Mercier and Sperber, 2017), and have profound impacts on the cognition procedures of learning and inference (Lombrozo et al., 2019).

There are many types of explanations. In the literature of philosophy and psychology, one fruitful taxonomy is mechanistic explanations (citing the components and procedures), teleological explanations (citing the goals), and formal explanations (citing the categories) (Lombrozo, 2012). In the NLP and explainable AI literature, there have been many types of explanations as well. Taxonomizing by the nature of the explanandum, we have the explanations towards model predictions vs. the explanations towards other problems (for example, events). Taxonomizing by whether the explanations are produced with the predictions, we have pre-hoc explanations vs. post-hoc explanations. Taxonomizing by the methods to arrive at the explanations, there are many popular methods including free-text, attribution scores, and mechanistic explanations, many of which will be discussed in the next a few sections.

In recent years, the advance of LLM technologies has introduced unique opportunities for explanations. In some application scenarios of education (Khan, 2023; Duolingo, 2023) and commerce (Stanley, 2023), explanations can improve the AI systems. In this tutorial, we will focus on the recent opportunities and challenges introduced by LLMs, which have not been covered by prior tutorials.

1.2 Desiderata of Explanation

What is a good explanation? On a high level, good explanations are the ones that achieve the intended

communicative goals, which can help developers debug or improve human decisions. On a detailed level, the literature has also identified some desirable properties for measuring the quality of explanations, including but not limited to:

Faithfulness. An explanation should accurately reflect the reasoning process behind the model’s prediction (Jacovi and Goldberg, 2020; Lyu et al., 2023a).

Plausibility. An explanation should be understandable and convincing to the target audience (Herman, 2019; Jacovi and Goldberg, 2020).

Usefulness. An explanation should be helpful for the user to achieve a pre-defined goal (Zhou and Shah, 2022; Bansal et al., 2021; Chen et al., 2023).

Minimality. An explanation should only include the smallest number of necessary factors (Halpern and Pearl, 2005; Miller, 2018).

On an implementation level, the procedure to generate explanations has some desirable properties as well. The algorithms should require realistic data and computation resources. Depending on the accessibility of the models, the requirement to access the internal weights of the models can also be noteworthy.

Note that it may be difficult to satisfy all of the properties above at the same time (e.g., minimality and plausibility). One can also argue that these properties are not the “first-order principles” that determine the explanation qualities. We will describe the nuances in this tutorial.

When discussing each desideratum in the tutorial, we will impose a special focus on the challenges and opportunities brought by LLMs. For example, recent studies find that LLM can generate more *plausible* explanations (Marasović et al., 2022; Wiegrefe et al., 2022), which are, however, not necessarily faithful to their internal reasoning mechanism (Turpin et al., 2023; Lyu et al., 2023b).

1.3 Method: Free-Text/CoT

We then proceed with four sections describing the methods to generate explanations. For each category of method, we will also describe the corresponding evaluation criteria and illustrate how well the explanation methods work.

The advancement of LLMs introduces unique opportunities, including the chain-of-thought (CoT) (Wei et al., 2022). There have been various approaches to leverage LLMs’ reasoning abilities to explain the problems (Marasović et al., 2022).

Compared to prior, smaller models, larger LMs are able to generate free-text explanations on a zero-shot or few-shot setting. Specifically, the qualities of the generated explanations can be comparable to, and sometimes more preferable than those that were written by humans (Wiegrefe et al., 2022).

The LLMs have the potential to build a special category of models, self-rationalizing models, which outputs both the prediction and the reasons toward that prediction at the same time. The self-rationalizing models can introduce unique advantages. For example, the models themselves may be less susceptible to spurious correlations, making more predictions “right for the right reasons” (Ross et al., 2022). The generated CoT could also be beneficial to “student models” (Wang et al., 2023; Pruthi et al., 2022).

LLMs are also known for “hallucination”: they tend to improvise and produce nonfactual content (Ji et al., 2023), so the LLM-produced explanations can be unreliable, even after few-shot demonstrations (Ye and Durrett, 2022). We will describe some recent works to improve this problem, e.g., the approaches of Lyu et al. (2023b). Relatedly, some recent works study prompt writing methods that aim at improving the reasoning qualities, including context faithfulness (Zhou et al., 2023) and help-me-think (Mishra and Nouri, 2023).

1.4 Method: Structured Explanations

Researchers have long wanted to figure out the underlying structures of the explanations. The study of the structures of explanations can be traced back to Hempel and Oppenheim (1948). Explanations can contain various structures. Inductive explanations present observed events that can improve the statistical likelihood that the explanandum event is true (Hempel, 1958). Deductive explanations provide logical arguments that can derive the explanandum event following a set of widely accepted rules (Hempel, 1962). Abductive explanations, on the other hand, aim at making the event more *plausible* while allowing more relaxed structures (Lombrozo, 2012; Zhao et al., 2023).

Wiegrefe and Marasović (2021) listed many structured explanation approaches. They can be presented in graphs (WorldTree (Jansen et al., 2018), OpenbookQA (Mihaylov et al., 2018)), symbolic rules (Lamm et al., 2020), semi-structured texts (Ye et al., 2020), etc.

More recently, many additional structures are

found to be useful, for example, Tree-of-thoughts (Yao et al., 2024), Graph-of-thoughts (Besta et al., 2024) and Everything-of-thoughts (Ding et al., 2023). The advance of LLMs allows unprecedented flexibility in controlling the structures and contents of explanations. We will describe some of the new approaches to make these controls possible. We will also describe some ways to evaluate the utility of these new approaches.

1.5 Method: Importance Scores

A category of methods to explain data-driven systems aim at attributing system behavior to the instances in the input data. This category of method is referred to as importance scores. We will discuss some popular importance score-based methods spanning two prominent paradigms (token-wise attribution and instance-wise attribution) in the context of NLP models, especially LLMs.

We will first set up some basics of importance score methods, covering the most commonly used token-level attribution methods (Ribeiro et al., 2016; Lundberg and Lee, 2017; Sundararajan et al., 2017) and instance-wise attribution methods (Koh and Liang, 2017). We plan to give a high-level introduction of these methods. We will omit the technical details, but emphasize on the cost of computation and the requirements on the access to model details for obtaining the interpretations using different methods, so as to better deliver the applicability of these methods on LLMs. We will also introduce the common evaluation protocols that are unique to the importance score methods, such as sufficiency and comprehensiveness (DeYoung et al., 2020).

Next, we will discuss the unique challenges and opportunities of applying the importance score methods on interpreting and developing LLMs. LLMs are associated with extreme scale in both model size and training data size, which can render many previously viable importance score methods prohibitively expensive. We will showcase how importance score methods such as influence function are adapted for interpreting LLMs (Grosse et al., 2023; Piktus et al., 2023), and how they are utilized for gaining deeper understanding of LLMs’ behavior (Wu et al., 2023; Madaan and Yazdanbakhsh, 2022) or for improving model performance (Krishtna et al., 2023).

1.6 Method: Mechanistic, Causal, Others

Explanations are not the only approaches that help us “open the black boxes”. There are many other

methods that aim at achieving similar goals. We will briefly mention some of these popular methods, and discuss how they relate to the explanation methods mentioned in our tutorial.

Mechanistic interpretability approaches try to describe the mechanisms of how the DNN-based AI systems work. A representative work in mechanistic interpretability is neural circuits (Conmy et al., 2023). Causal mediation analyses try to apply causal analysis tools to understand the models. Kiciman et al. (2023) provides an overview of the tools and frontiers related to causal analysis in DNN models.

Model editing provides explanations from a counterfactual aspect: “What would be the output, had this model been modified into the other way?” Some recent works include ROME (Meng et al., 2022) and MEND (Mitchell et al., 2022). Yao et al. (2023) provides a summary on this.

We recommend the readers to check out the EACL tutorial (Mohebbi et al., 2024) and the reviewing article by Ferrando et al. (2024) for more details, especially about Transformer-specific mechanistic interpretability. Our tutorial includes explanation topics that are beyond Transformers.

2 Reading List

In addition to the papers cited in this proposal, we also recommend [this reading list on Notion](#) and previous relevant tutorials: Belinkov et al. (2020) presented approaches to interpret the structures and behavior of neural network models; Wallace et al. (2020) described approaches to understanding the predictions of neural network models; Boyd-Graber et al. (2022) focused on the human aspect of explanation evaluation. Compared to the previous tutorials, our tutorial covers some new topics, including free-text / CoT explanations, and structured explanations, etc. We will present perspectives that connect the explanations as model interpretation tools and the explanations as communication procedures.

3 Type of the Tutorial

The tutorial is designed to be at the cutting edge, encompassing advanced technologies for explaining NLP models. In particular, the tutorial will emphasize on explanations in the context of LLMs, including generation and evaluation methods.

4 Target Audience and Prerequisites

Anyone interested in explainable NLP and LLMs is welcome. We anticipate an audience size of approximately 200.

Attendees are expected to have basic knowledge of NLP tasks (e.g., text classification, question answering) and neural language models (e.g., BERT, GPT). We plan to make tutorial materials (e.g., slides, media) public.

5 Breadth and Diversity

Our tutorial is ensured to cover a wide spectrum of explanation topics, ensuring that attendees are exposed to a comprehensive range of concepts, techniques, and advances. We will incorporate seminal works and recent advancements from a wide array of researchers in the field into the tutorial.

The instructors are diverse in terms of gender, nationality, affiliation, and seniority (from PhD students to postdocs to professors). We plan to organize open Q&A sessions to create a space for participants to directly engage with presenters, clarifying doubts and exploring different viewpoints. This format ensures that participants from various backgrounds can contribute to shaping the discussion. In particular, we encourage participants from underrepresented groups to share thoughts and insights and provide feedback.

6 Presenters

Zining Zhu is an incoming assistant professor at the Stevens Institute of Technology. He obtained his Ph.D. in 2024 at the University of Toronto. His research includes model control and interpretability. Zining co-instructed the Natural Language Computing course (CSC401) at UofT in 2023 and 2022, with class size around 200.

Hanjie Chen is an incoming assistant professor at Rice University, and is currently a postdoc at Johns Hopkins University. She obtained her Ph.D. in 2023 at the University of Virginia. Her research focuses on the interpretability/explainability of neural language models. As the primary instructor, she co-designed and instructed the course, CS 6501/4501 Interpretable Machine Learning, at UVA in Spring 2022. She received teaching awards at UVA.

Xi Ye is an incoming assistant professor at The University of Alberta. He obtained his Ph.D. in

2024 at the University of Texas at Austin. His research focuses on leveraging explanations to improve language models for complex textual reasoning tasks. He also works on program synthesis and semantic parsing.

Qing Lyu is a Ph.D. candidate at the University of Pennsylvania, advised by Chris Callison-Burch and Marianna Apidianaki. Her research interests lie in the intersection of linguistics and natural language processing, as well as the interpretability and robustness of language models.

Chenhao Tan is an assistant professor of computer science and data science at the University of Chicago, and is also affiliated with the Harris School of Public Policy. He obtained his PhD degree in the Department of Computer Science at Cornell University and bachelor's degrees in computer science and in economics from Tsinghua University. Prior to joining the University of Chicago, he was an assistant professor at the University of Colorado Boulder and a postdoc at the University of Washington. His research interests include natural language processing, human-centered AI, and computational social science. His work has been covered by many news media outlets, such as the New York Times and the Washington Post. He also won a Sloan research fellowship, an NSF CAREER award, an NSF CRII award, a Google research scholar award, research awards from Amazon, IBM, JP Morgan, and Salesforce, a Facebook fellowship, and a Yahoo! Key Scientific Challenges award.

Ana Marasović is an assistant professor in the Kahlert School of Computing at the University of Utah. Her primary research interests are at the confluence of NLP, explainable AI, and multimodality. Previously, she was a Young Investigator at the Allen Institute for AI and held a concurrent appointment in the Paul G. Allen School of Computer Science & Engineering at the University of Washington. She obtained her PhD in 2019 from Heidelberg University. She received Best Paper Award at ACL 2023, Best Paper Honorable Mention at ACL 2020, and Best Paper Award at SoCal 2022 NLP Symposium.

Sarah Wiegrefe is a Young Investigator (post-doc) at the Allen Institute for AI, where she is a member of the Aristo team. She also holds a courtesy appointment in the Allen School at the

University of Washington. Her research interests encompass interpretability + explainability of NLP models, with a focus on the faithfulness of generated text to internal LM prediction mechanisms and the utility of model-generated textual explanations to humans. She received her PhD in 2022 from Georgia Tech, advised by Mark Riedl.

7 Technical Equipment

No special requirements. We simply require fundamental technical equipment for our in-person tutorial, including essentials like projectors and screens, microphones, cables and adapters, etc.

8 Ethics Statement

This tutorial aims to provide a comprehensive overview of explanations for NLP, especially the challenges and opportunities in the era of LLMs. We hope the tutorial will provide the audience with a profound understanding of the pivotal role of explanations in enhancing human trust in LLMs, alleviating ethical concerns, and fulfilling societal responsibilities.

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