Explanation from Specification

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Abstract

Explainable components in XAI algorithms often come from a familiar set of models, such as linear models or decision trees. We formulate an approach where the type of explanation produced is guided by a specification. Specifications are elicited from the user, possibly using interaction with the user and contributions from other areas. Areas where a specification could be obtained include forensic, medical and scientific applications. Providing a menu of possible types of specifications in an area is an exploratory knowledge representation and reasoning task for the algorithm designer, aiming at understanding the possibilities and limitations of efficiently computable modes of explanations. Two examples are discussed: explanations for Bayesian networks using the theory of argumentation, and explanations for graph neural networks. The latter case illustrates the possibility of having a representation formalism available to the user for specifying the type of explanation requested, for example, a chemical query language for classifying molecules. The approach is motivated by a theory of explanation in the philosophy of science, and it is related to current questions in the philosophy of science on the role of machine learning.

Introduction

Interpretability, explainability, transparency and other requirements for neural networks and other models built using machine learning pose an important challenge in many applications. The history of the problem in machine learning is illustrated by Sommer (1996): “This paper reopens the issue of understandability of induced theories, which, while prominent in the early days of ML, seems to have fallen out of favor in the sequel.” It is often noted that these notions are used with different meanings and precise definitions do not exist (see, e.g., Lipton 2018). Possibly the notions are inherently ambiguous, and therefore giving formal definitions is not necessary and perhaps not even possible. Precise definitions may not be of interest in themselves, but they can be useful, even in restricted cases, for understanding the possibilities and limitations of algorithmic approaches.

In view of the large variety of algorithms for interpretability, several papers provide taxonomies (e.g., Arrieta et al. 2020, Guidotti et al. 2019, Henin and Métayer 2019, Sokol and Flach 2020). These are not formal definitions, but describe various components of the algorithms, different types of those components and their interactions, objectives and evaluation methods. Doshi-Velez and Kim (2017) give a taxonomy of approaches for evaluating interpretability. The main criterion for evaluating interpretability of a result is its usefulness for humans.

Miller, Howe, and Sonenberg (2017), quoting Cooper (2004), refer to AI researchers designing interpretable learning algorithms without taking into account desiderata based on philosophy, cognitive science and other areas as “inmates running the asylum”. While this suggests that computer scientists have too large a role, it may also be the case that their task is narrow in the sense that interpretable models usually are of a familiar kind, such as linear models and decision trees. Are there other options? We formulate an approach to post hoc explainability which, while adhering to Miller’s warning, could help answer this question.

The proposed approach is that for an XAI application, instead of deciding on the explainable model to be used (say, a decision tree), one can try to obtain a specification of the kind of explanation required. The task then is to design an explainable learning model satisfying the requirements, or to argue that this is not possible, for informational or computational reasons. This view is related to the taxonomy of Doshi-Velez and Kim (2017). Another view is that the specification represents the type of question or query and the type of answer expected by the user, providing an abstraction of the user for the application.

It is to be emphasized that the approach is not expected to be feasible in every application, but it is hoped that in some cases it could lead to the development of new explainable representations. It could also provide an understanding of the relevant features of explainable models or, in the specification phase, provide a better understanding of the explainability requirements of the particular application. Such an approach is feasible in forensic, medical and scientific appli-
cations, where the user has an approximate idea of what is meant by an explanation. This approximate idea can then be refined in an interaction with the algorithm designer.

The algorithm designer can prepare for such an interaction by studying various types of explanations that are to be expected in a particular area. Thus the proposed framework includes exploring knowledge representation and reasoning aspects of explainability. For a given type of explanation, an alternative route is to learn a corresponding interpretable representation directly. The feasibility of this route can depend on the nature of data available for a particular application.

In this paper we give several motivations for explanations from specifications, including functionally grounded evaluation of explainability methods, the pragmatic theory of explanations and the theoretical study of explainability. We describe several aspects of the realization of the approach, and we present two examples where there is initial work in the direction proposed: explaining Bayesian network classifiers using argumentation theory and explaining graph neural network. Future work is outlined in both cases. The philosophy of science gives a motivation for the approach, and we also mention a connection in the other direction as well, noting that the exploration of the approach could contribute to the discussion of current problems on the role of machine learning in scientific research.

Functionally grounded evaluation

In the taxonomy of (Doshi-Velez and Kim 2017) for interpretability evaluation methods, functionally grounded evaluation does not use human experiments. Instead, a “formal definition of interpretability [is used] as a proxy for explanation quality […][which is] most appropriate once we have a class of models or regularizers that have already been validated […] The challenge, of course, is to determine what proxies to use. For example, decision trees have been considered interpretable in many situations”.

A project in this direction, proposed in (Doshi-Velez and Kim 2017), is to create a matrix with rows corresponding to real-world tasks, columns corresponding to methods, and entries corresponding to the performance of methods on the task (like decision trees of a certain type for a medical interpretability task). An interesting hypothesis formulated in (Doshi-Velez and Kim 2017) is that such a matrix may be factored using latent interpretability requirements of tasks such as global versus local interpretability and the type of user expertise required, and latent properties of the methods, e.g., the structure of methods in terms of cognitive chunks. The approach proposed in this paper promotes these factors to a central role and makes their elicitation a separate task guiding algorithm design.

The pragmatic theory of explanation

Interpretability and explainability are much studied, distinct but related, notions in philosophy. Scientific explanation, in particular, is a central concept in the philosophy of science. Several approaches are formulated, starting with the deductive-nomological (DN) approach of (Hempel and Oppenheim 1948). The approaches are quite different and there is no generally accepted one. Whether this background is relevant for ML is debated (Krishnan 2019; P´aez 2019).

One possible answer is that approaches in the philosophy of science are of interest in AI as potentially useful views of what constitutes an explanation in ML. This position involves no commitment on the relationship between the corresponding notions in the philosophy of science and AI.

One difference to note is that the objective in the philosophy of science is to capture the notion of a scientific explanation precisely. Counterarguments against a particular approach may refer to capturing too much or too little. In AI, on one hand, the bar is lower, as useful approaches are sought for, without any claim of precise characterization. On the other hand, the bar in AI is higher, because the approaches are required to be algorithmically tractable. The distinction between explaining the learned model or explaining the phenomenon modeled is an important one. Robustness may provide a distinction between the two (Alvarez-Melis and Jaakkola 2018; Hancox-L-L 2020).

The approach proposed in this paper is inspired by the pragmatic theory of explanation of (van Fraassen 1980).

This theory is part of van Fraassen’s constructive empiricist approach to the philosophy of science. The main aspects that are explanations are viewed as answers to why-questions in a contrastive form in the context of a relevance relation.

As summarized in (Cross and Reuveni 2018), “to ask why is to ask for a reason, and [the relevance relation] R varies according to the kind of reason that is being requested in a given context. One can ask why in order to request causal factors, to request a justification, to request a purpose, to request a motive, to request a function, and so on”.

One objection to van Fraassen’s approach is that it is not specified what counts as a relevance relation. We describe briefly the definition in the version given by (Boniolo 2005).

A why-question is of the form “why P rather than the other elements of X”, where P is a proposition and X is a set of propositions containing P. The question also specifies

\[ a \text{ knowledge base } K, \text{ a scientist } s \text{ and the background knowledge } K_s \subseteq K \text{ of } s. \]

The relationship between scientific explanation and explanation in general is also open to debate.

Here “pragmatic” does not refer to claim of relevance for practice (which would apply to other approaches as well), but to aspects of the participation of the agents in the explanation process (the details of which are not needed for our discussion). See the distinction between pragmatic1 and pragmatic2 in (Woodward 2019).

(Lipton 1990) cites van Fraassen as one of the sources of the contrastive approach. The critical review of (Worrall 1998) on van Fraassen’s book argues, among other things, that the contrastive approach is not applicable to scientific explanation, and context and relevance relations “lead to unnecessary complexity” by moving beyond classical logic. Lipton gives a counter-argument to Worrall’s first argument. Regarding the second argument, Worrall is actually right about complexity (whether the move is necessary or not is another question). Non-classical logics, like non-monotonic logic and argumentation theory, do have problems with intractability, and overcoming those is an important problem. See further discussion in the section on argumentation.
The proposed approach

The proposed view of explainability is summarized in Figure 1. The $N$ box represents a black box model ($N$ for network, neural or Bayesian), which on a given input $X$ produces output $f(X)$. The $R$ module ($R$ for relevance or reasoning) represents the user’s notion of an explanation. The missing component with the question mark is $E$ (the explainer), producing an explanation $\text{expl}(N, X)$ which explains $f(X)$ according to the user’s requirements. The task of the algorithm designer is to design an appropriate explainer. It is assumed that the designer knows $R$, and has to develop an explainer module which, given an $N$ and an $X$, produces a suitable explanation for $f(X)$.

The contrastive aspect is reduced here to “why $f(X)$ and not something else” for simplicity, but the general version could also be incorporated. The approach includes other scenarios as well, such as building an interpretable model directly or computing explanations from $N$ directly. The setup allows for the design of $N$ to take into consideration $R$, for the incorporation of explanation construction into the learning process (Park et al. 2018), for methods where the learning process of $N$ and the production of explanations are intertwined (Al-Shedivat, Dubey, and Xing 2018), and, depending on $R$, for interaction as well.

The diagram, mutatis mutandis, is also related to other tasks such as the verification (Katz et al. 2017) or testing (Zhang et al. 2019) of black boxes. (Dhurandhar et al. 2017) gave a formalization of the user in terms of a target model, the performance of which is to be improved using interpretability. (Overton 2011b, a) discusses the formalization of various kinds of explanations in science.

Being built around the relevance relation $R$, the approach implements van Fraassen’s theory of explanation. By moving part of the problem formulation to the user and leaving “only” algorithm design to the computer scientist, the “can is kicked down the road”. Furthermore, by building on the relevance relation and the context of the user, the approach is “as domain-specific as it gets”, thereby adhering to the domain-specificity of interpretability (Rudin 2019).

(Migliorati et al. 2019) consider an explanation to be an interface between the decision maker (the black box) and the user, which is an accurate proxy of the decision maker and is comprehensible to the user. The diagram suggests a way to achieve the simultaneous occurrence of the two conditions (accurate proxy and comprehensible) required for explanations to be useful. The user is supposed to provide $R$, which, by definition, is comprehensible to them. This could include statistical or logical aspects, background knowledge, etc. Then the designer has to come up with the explainer, which is an accurate local proxy in the form of the requested type of explanation, which can refer to either the model or the world.

The relevance relation should be formulated in cooperation with the user, building on psychology, cognitive science, HCI and other areas. This challenge seems to be somewhat different from tasks such as eliciting user preferences in terms of parameters of decision trees. It is interesting that the importance of contrastive explanations, emphasized by (Miller 2019) is already ‘built in’ into van Fraassen’s framework. It is noted by (Miller 2019) that eliciting a contrast case from a human observer may be a difficult problem. The present elicitation task may not be easy either, but it may be useful in other contexts as well. Elicitation and related aspects are described in (Cassens and Kofod-Petersen 2007; Lim, Dey, and Avrahami 2009; Kaur et al. 2020).

The approach can be relevant for forensic, medical and scientific applications, as there are relevance relations in these areas which can serve as specifications. Although it is not indicated in the figure above, the use of background knowledge is especially important in these areas. Background knowledge can be incorporated explicitly and implicitly in different ways, including the design of neural networks (e.g., architecture, initialization and regularization) and the construction of explanations. Recent surveys of work relevant for these aspects are (von Kiden et al. 2019) on uses of background knowledge, (Karpatne et al. 2017) on theory-guided data science and (Roscher et al. 2020) on explainability aspects of current science research.

In biology there is a large variety of explanations, including non-causal forms of explanation as well, such as functional and evolutorial explanation (see (Braillard and Malaterre 2015)). Boniol, in his paper cited above, gave a
taxonomy of relevance relations for explanations in biology. Relevant types of explanation, besides those mentioned by (Boniol, 2005), are also given in (Trujillo, Anderson, and Pelaez, 2015). Their MACH (methods, analogies, context, how) model is obtained from interviews and data from experts in the context of biology education, and thus it gives an example of the elicitation process. (Overton, 2012, 2013) gives a theory of explanation in science, and relates it to an analysis of papers from Science. He uses the categories theory, model, kind, entity and data. For every pair there is a core relation for explanations involving that pair. These relations are further candidates to explore in the role of the R box.

**Explanations for Bayesian networks using argumentation**

Explanations for Bayesian networks have been studied for a long time (Lacave and Diez, 2002). The issue of interpretability of Bayesian networks requires some clarification. Bayesian networks are a clear and interpretable representation of dependencies in the joint distribution (although even that requires care to formulate exactly in terms of distribution-independence). On the other hand, inference given some evidence is computationally involved and hard to interpret for users not familiar with details of probabilistic reasoning.

Koller (Ford, 2018) noted that such models have an intermediate degree of interpretability. This intermediate position suggests that interpretability of probabilistic models may be more accessible than deep learning and may be of interest for exploring general issues.

**Argumentation** is a basic form of human reasoning (Mercier and Sperber, 2011), important in legal and medical contexts. Argumentation theory is a logic formalism for the mechanism of arriving at a decision making based on arguments for or against a decision, using relations like defeat, rebuttal and undercut between arguments (Pollock, 1995). The framework of (Dung, 1995) is a directed graph with the arguments as vertices and directed edges corresponding to the attack relation. This abstract framework is applied to a class of formulas by defining the attack relation over arguments for a decision, using relations like defeat, rebuttal and undercut between arguments (Pollock, 1995). The grounded extension semantics in (Timmer et al., 2017) is not a particularly good match. A relevant conclusion of (Cerutti, Tintarev, and Oren, 2014) is that domain specific knowledge needs to be considered. Taking more forms of background knowledge into account is also a consideration for further work on (Timmer et al., 2017).

Thus further work on argument-based Bayesian network inference explanations needs the cooperation of algorithm designers, cognitive scientists and users. It requires further work to identify desirable characteristics of the argument frameworks, followed by the design, if possible, of efficient algorithms producing arguments with those characteristics, making use of background knowledge.

**Explanations for graph neural networks**

The graph neural network (GNN) model is a neural network variant for problems on graphs (Hammond, 2020). Nodes in each layer correspond to vertices of the input graph. Computation and updating between layers are done along the edges of the graph, giving a deep learning version of message passing algorithms. GNN can be used, for example, for classifying nodes of a graph, or for classifying graphs.

GNN are an important tool for classifying molecules for problems in chemistry, biology and drug design. In these areas it is often noted that even though significant progress has been made by deep learning in terms of prediction, lack of interpretability of the results is a major problem to solve (see, e.g., (Ching et al., 2018)). Providing explanations for node and graph classification has been studied recently by (Preuer et al., 2019), Ying et al., 2019), Pope et al., 2019). Bal-dassarre and Azizpour (2019), Huang et al., 2020).

Properties of molecules are often studied by looking for relevant substructures. The GNNExplainer method of (Ying et al., 2019) finds explanations for the classification of a graph by a GNN in the form of a size-bounded subgraph and a subset of its node features that have large mutual information with the output. Thus in this case N is a neural network. X is a graph, an explanation is a subgraph, and the relevance relation is the subgraph relation.

Jiménez-Luna, Grisoni, and Schneider (2020) mention the development of new interpretable molecular representations as another major research problem. There are many different representations and explanation types for molecules, even for a single property (see, for example, the literature on aromaticity (Sanger, 2009), Sola, 2017). (Yang et al., 2019) investigate the predictive power of deep learning based representations when compared to fixed molecular input descriptions. A comparison with respect to explainability would also be interesting. In chemoinformatics there are several query languages describing properties of molecules, such as SMILES, SMARTS and CSRML. (Yang et al., 2015).

GNN learning algorithms and explainability methods are often evaluated on synthetic graph data as well. Synthetic
problems appear to be more realistic approximations of real-life properties for molecules than, for example, for image recognition. Therefore it seems to be of interest to explore synthetic problems in this context in more detail.

Our approach suggests that scientists can use classes of queries in the query languages to specify the type of explanation that is meaningful to them. As an exploratory research project, one can consider various classes of queries as candidate explanation types for synthetic problems, and study the possibilities and limitations of producing explanations of those types. Going beyond substructures, one could consider more general queries. Extensions could include, for example, properties involving the existence of multiple copies of substructures (perhaps in specified positions like being far away from each other), Boolean combinations or properties involving quantification and counting.

As noted in the introduction, for each such query class one could consider learning such a description directly. GNNs are known to have theoretical computational limitations [Xu et al. 2019; Morris et al. 2019; Garg, Jegelka, and Jaakkola 2020], Grohe 2020], and so their learning and explanatory aspects may differ from general neural networks. Direct learning is expected to be a hard problem in general.

An example of a class of properties going slightly beyond properties considered in [Ying et al. 2019] is having bounded radius. Here we assume that graphs are classified as positive if their radius is at most \( r \), for an unknown value of \( r \). In this case learning \( r \) directly is straightforward, but from the point of view of explainability it is of interest to see if a learned GNN provides meaningful explanations. For graphs classified positive a natural explanation is a spanning tree of bounded depth. Thus the relevant subgraphs do not have bounded size. Nevertheless, the GNNExplainer algorithm can be used with a minor change in the denoising part, which remains computationally efficient.

Figures 2 and 3 give an example of the explanation found in our ongoing experiments for the case \( r = 2 \). GNNExplainer assigns weights to the edges reflecting their importance for the classification. The denoising procedure (which differs from the one in [Ying et al. 2019]) then selects an explanatory subgraph. This procedure is designed knowing that the scientist is interested in the role of the radius. There are several options to extract a radius-related explanation from the weighted subgraph, and the preferred one could be chosen through interaction with the biologist. The syntactic data assume an idealized case, and it needs to be explored how robust the explanations are if the classification is not in terms of the radius alone.

**Prediction without explanation?**

ML providing prediction without explanation in the natural sciences raises fundamental questions in the philosophy of science. An upcoming special issue of *Minds and Machines* is devoted to these questions. Some questions are similar

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3The radius of a graph is the smallest number \( r \) such that for some vertex \( v \) every other vertex can be reached from \( v \) by a path of length at most \( r \).

4https://www.springer.com/journal/11023/updates/18180316
ML (at least to some extent) then ML fits van Fraassen’s constructive empiricist approach as a tool.

To put it another way, the gap would be bridged by incorporating ML into van Fraassen’s philosophy of science. (Hooker and Hooker 2013) mention ML interpretability as a form of intuitability. It is not a coincidence that explainability from specification is applicable for areas such as science, where a more rigorous form of explanation can be expected. Intuitability would apply to the types of explanation considered in most of XAI, describing explanations expected in societal contexts. In that sense the gap bridging we suggest is a meeting in the middle.

A neural network predicting a property of molecules accurately contains empirically adequate knowledge and according to van Fraassen’s view that is the main objective. The scientist can also be interested in whether the network provides relevant explanations according to their relevance relation, and this is the form of explainability considered in this paper. As the scientist’s relevance relation is presumably adapted to the problem studied (like subgraphs for molecule classification), explainability may have a better chance to occur than a general purpose notion of explanation (for example, a DN explanation).

Thus the main question suggested by this argument is the following: to what extent can explainability from specification be achieved in ML scientific applications?

Positive results on explainability give information on the compatibility of scientific results using empirically adequate predictions from ML with the framework of a theory. Correspondence between concepts of a theory and concepts computed at a hidden node is a form of interpretability. Using the query languages mentioned above could be helpful in finding such correspondences. Negative results, i.e., the lack of interpretability could be a source for predicate invention (see, e.g., (Hocquette and Muggleton 2020)).

A relevant notion for these considerations is the Rashomon effect, i.e., the existence of multiple good models for data, introduced by (Breiman 2001). This phenomenon is explored further in ML, in particular for its relation to interpretability in (Semenova and Rudin 2019) [Dziugaite, Ben-David, and Roy 2020]. This effect also seems to match van Fraassen’s notion of theories through his semantic approach. (Hancox-Li 2020) notes that the Rashomon effect is argued as providing possibilities for interpretability in (Semenova and Rudin 2019), while he views it as relating to the lack of robustness, which is a limitation for relevance to reality.

Thus philosophy of science not only provided a motivation for the approach to XAI proposed in this paper but, in the other direction, it seems that an understanding of the possibilities and limitations of explainability by specification could contribute to answering some of the philosophy of science questions posed by ML.

Concluding remarks

We described an approach to explainability based on explicit specifications of the kind of explanations which the user deems relevant. Candidates for areas where this approach could be realized are natural sciences, medicine and forensic science, where there are basic forms of explanations, such as argumentation, causality and non-causal forms.

Besides the motivations and justifications mentioned earlier, the possibility to prove theoretical results on explanations in well-defined contexts is another reason to consider this approach. Proving such results is an interesting topic in itself for theoretical AI, but the considerations of the previous section give it additional significance.

(Colca 1996) initiated a study of the complexity of rule extraction, and (Barcelo et al. 2020) proved several hardness results. Obtaining knowledge representations with given tractability properties is related to knowledge compilation (Darwiche and Marquis 2002). Here knowledge representation formalisms, such as DNF and OBDD, are compared with respect to their expressivity, operations supported and efficiently decidable properties. Explainability aspects are discussed in (Darwiche and Hirth 2020). As learned models contain errors, it is of interest to consider approximate knowledge compilation. (Chubarian and Turán 2020) prove an approximate knowledge compilation result related to interpretability. (Macdonald et al. 2020) consider explanations with an approximate version of prime implicans.

Besides positive results, there are also results on limitations. (Wegener 1994) showed that, assuming prime factoring has no non-uniform polynomial time algorithms, there is no data structure for Boolean functions which can represent a version of multiplication in polynomial size and allows for efficient implementation of certain operations. Such negative results would be of interest for explainability as well.

Opening a black box and explaining a computational result in a form comprehensible to the user are two hard problems. The requirement to solve two interconnected hard problems at the same time contributes to the difficulties of XAI. The proposed approach to explainability separates the algorithm design task and the explainability aspect. This could help by disentangling the cognitive and algorithmic aspects of developing explainable learning algorithms.

(Rudin 2019) warns against using explanations provided by black boxes for high stakes decisions. Even though the scope of this warning is not quite clear, e.g., for self-driving cars, it seems that the areas suitable for the proposed approach are less of a concern from this point of view. The role of ML models in these applications is more of an assistant rather than a decision maker. Similarly, explainability has to address adversarial aspects, like “gaming” and privacy (see, e.g., (Milli et al. 2019)). Another common feature of the areas mentioned is that these issues seem less relevant there as well.

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